Book of Abstracts

2008 E-MRS Fall Meeting & Exhibit

Book of Abstracts: 2008 E-MRS Fall Meeting & Exhibit

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Disclaimer

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Table of Contents

Welcome

The European Materials Research Society

Fall Meeting

* * *

Warsaw University of Technology

Warsaw (Poland)

15th - 19th September, 2008

We are pleased to welcome delegates and guests

to the 2008 Fall Meeting & Exhibit

of the European Materials Research Society (E-MRS)

Introduction

In 2002, EMRS decided to established a Fall Meeting as a twin conference to the annual Spring Meeting held in Strasbourg, France. Initially the Fall Meetings were intended to develop and enhance contacts between scientists from Central and Eastern European countries with those from Western Europe, Asia and America. The inaugural Fall Meeting consisted of three symposia and was held in three locations:

- Moscow - Software Development for Process and Materials Design;
- Warsaw - Interfacial Effects and Novel Properties of Nanomaterials;
- Zakopane - Solid Solutions of the II-VI Compounds, Growth, Characterization and Applications.

The success of the first meeting in Warsaw has led to the EMRS Fall Meeting being based entirely in Warsaw since 2003. In this period the conference has grown from 3 to the 10 symposia presented in 2007. The importance of the conference is such that the number of scientists attending the meetings has increased from 200 in 2002 to about 800 from over 60 different countries in 2007. The Conference is held in the Main Building of Warsaw University of Technology.

The Fall Meeting organizers follow the procedures developed over the years by the Society to host wide ranging multi-disciplinary conference to bring established scientists with a world reputation together to share their state-of-the-art knowledge and experience. The most important philosophy of E-MRS is to facilitate scientific and social contacts between established researchers, young scientists and Ph.D. students and to promote technology transfer from public institutions to industry.

The Czochralski Award

One of the most important and prestigious events which take place during the Fall Meetings is the Presentation Ceremony of the annual "Jan Czochralski" Award. The Award in the name of Professor Jan Czochralski was instituted by the E-MRS, to commemorate his lifelong contribution to materials science, technology transfer to industry and international collaboration. The Society has formally legalised the Czochralski Award for Achievements in Materials Science.

In 2006 – the European Materials Research Society, the Polish Academy of Sciences, the Polish Materials Science Society, and the Polish Society for Crystal Growth jointly established the International Chapter of the Jan Czochralski Award which together select the Award Laureate.

To dare, four distinguished scientists have been presented with the Czochralski Award:

- 2004 – Professor Walter Heywang (former Director of Research of Siemens),
- 2005 – Professor Boris Paton (the long term President of the National Academy of Sciences of the Ukraine),
- 2006 – Professor Thaddeus B. Massalski (Carnegie-Mellon University in Pittsburgh),
- 2007 – Professor Shuji Nakamura (ERATO, JST, UCSB group, Santa Barbara), the inventor of the Blue Laser Diode.
- 2008 laureate will be Professor Kurt Heinz Juergen Buschow (University of Amsterdam)

Organisers

Conference Organisers:

- Polish Materials Science Society
- Warsaw University of Technology (*)
- Institute of Physics, Polish Academy of Sciences (**)
- European Materials Research Society (***)

Organising Committee:

- J. Franc (Prague, Czech Republic)
- K. Kurzydłowski (*)
- M. Lewandowska (*)
- A. Mycielski (**)
- P. Siffert (***)
- F. Tuomisto (Helsinki, Finland)

Conference Chairpersons:

- Gabriel Crean
- Jozsef Gyulai
- Andrzej Mycielski
- Urszula Narkiewicz

Conference Secretariat:

Agnieszka Rytel

Warsaw University of Technology

Woloska 141, 02-507 Warsaw, Poland

Phone/Fax: +48 22 234 87 94

e-mail: emrs@inmat.pw.edu.pl

E-MRS European Co-ordination Group:

A. Slaoui *E-MRS President*

P. Siffert *E-MRS General Secretary*

F. Priolo *Vice-President*

E-MRS Headquarter

BP 20 67037 Strasbourg, Cedex 2, France

Phone: +33 3 88 10 63 72; Fax. + 33 3 88 10 63 43

E-mail: emrs@emrs.c-strasbourg.fr

Sponsors

The 2008 E-MRS Fall Meeting is supported by:

E·MRS	**European Materials Research Society**
	Polish Ministry of Science and Higher Education
PMS SOCIETY	**The Polish Materials Science Society**
	Faculty of Materials Science and Engineering, Warsaw University of Technology
	Institute of Physics, Polish Academy of Sciences

The 2008 E-MRS Fall Meeting & Exhibition is sponsored by:

NT-MDT
Molecular Devices and Tools for Nano Technology

TheEuropean Materials Research Society

(E-MRS) a non profit scientific association founded in 1983 focuses on creating the synergy between interdisciplinary, innovative technologies, spreading and exchanging information and promoting technology transfer from public institutions to industry. The primary objective of E-MRS is to promote and enhance the efficiency of research in Europe in the field of Advanced Materials. E-MRS seeks to quickly inform researchers of the scientific and technological developments in their field of interest from the rest of the world through the society's links with other MRS societies belonging to the International Union (IUMRS). In 2002 E-MRS decided to launch in parallel to the well established spring meetings in Strasburg also the fall meetings in Warsaw.

The Polish Materials Science Society

The Polish Materials Science Society (PMSS) was founded in December 2004. PMSS promotes interdisciplinary cooperation between scientists working in different scientific areas - materials science and engineering, chemistry, physics, biology, medicine etc. PMSS works in close collaboration with E-MRS.

The main aims of the PMSS are:

- provide a platform facilitating interdisciplinary cooperation between materials scientists from different fields,
- strengthening the interdisciplinary meetings, conferences, workshops and schools important for the PMSS members,
- distribution of information among scientists working in the field of materials research

Faculty of Materials Science and Engineering; WUT

The former of Materials Science and Engineering, with almost a century of experience in the teaching of materials science at Warsaw University of Technology, became a fully independent Faculty in 1991. The main lecture theatres and research laboratories are located in a new building on the southern campus. The Faculty offers a BSc-equivalent and MSc degree education as well as doctoral studies, with places for about 350 undergraduates and 40 places in its doctoral program. There are over 40 scientific and academic staff members, including: 16 professors and associate professors and 20 assistant professors. These are supported by 30 technical and administrative staff.

The Faculty's scientific projects are carried out by the research groups of each of the four Divisions. The nature of the work is both fundamental and technological and in 1998 included over 20 grants awarded by the State Committee for Scientific Research, the Faculty statutory activities, commissions from industry and cooperation with similar institutions abroad. Cooperation with Polish industries includes: Polish Petroleum Concern, The Nitrogen Chemical Plant in Pulawy, The "Boleslaw" Mining and Foundry Plant.

In addition, the Faculty is the coordinator of the Warsaw University of Technology's priority research program entitled "New Materials", which includes such issues as new generation highly resistant materials, anti-wear materials and corrosion resistant materials.

The main areas of scientific research include:

- the theory of mechanical properties in poly-crystalline materials,
- microstructure degradation problems and properties of materials,
- grain boundary properties,
- applied image analysis in material micro-structures,
- modern methods of surface engineering, corrosion problems, amorphous and nanocrystalline materials, magnetic materials, advanced ceramic materials, polymers and composite materials, biomaterials, recycling of metals and polymers.

Institute of Physics PAS

The Institute of Physics was established on 24th September 1953 by a special Government decision. It was rooted in the physics faculties of seven universities: Warsaw University and Warsaw Technical University, Jagiellonian University in Kraków, Adam Mickiewicz University in Poznań, Nicolaus Copernicus University in Toruń, as well as the University and Technical University of Wrocław. The Institute was relying on their research staff, premises and laboratory facilities. The Institute was established as a country-wide scientific institution conducting research in all areas of experimental and theoretical physics, including educational obligations. The first director of the Institute, Prof. Stefan Pieńkowski, and the first chairman of its Scientific Council, Prof. Leopold Infeld, were the most prominent physicists of that time in Poland. Since the establishment of the National Agency for Nuclear Energy in 1955, the nuclear physics has ceased to constitute a part of the research program of the Institute. Those units of the Institute which were specifically active in this field (the Departments of Radioactive Isotopes, Elementary Particles, and Nuclear Physics in Krakow) formed the kernel of Nuclear Research Institutes. The fast rate of development of the Institute has led, in the course of years, to the formation of independent research units grown on its basis. In 1975 the Department of Ferromagnetics, Department of Dielectrics, together with the Radiospectroscopy Laboratory created in 1966 in Poznań, became incorporated into the Institute of Molecular Physics of the Polish Academy of Sciences. The Wrocław branch of the Institute became a part of the Institute of Low Temperature and Structural Research, of the Polish Academy of Sciences. The Institute of Physics was also the founder of the Department of Solid State Physics in Zabrze. The industrial, high-tech centers of the Academy of Sciences, such as "UNIPAN" (specializing in scientific electronic instruments) and "WILMER" (humidity meters), as well as the High Pressure Research Center "UNIPRESS", are also rooted in the Institute.

In September 2003 the Institute celebrated its 50th anniversary. On this occasion the achievements of the Institute were recognized by the

Academy and State authorities: 28 of our scientific and technical staff were decorated by various state medals.

NT-MDT Europe BV

NT-MDT enjoys a 15-year history in instrumentation created specifically for nanotechnology research, leading the field in originality, quality, and high tech development.Our mission is to enable researchers, engineers and developers to conduct nanoscale research by creating ever more perfect nanotechnology instrumentation. Along the way, we maintain a global perspective, always taking into consideration the needs of student in the classroom, the researcher at the cutting edge in the laboratory, and the practicalities of industrial R&D. We strive for next-generation SPM technology, whether it be in pure modularity that allows a university or industrial lab to start with a cost-effective core product and build to a grand, multi-user research center or the ultimate amalgamation of SPM with related technologies that has resulted in ultramicrotomy for nanotomography and spectroscopy-based instruments that meld the world of imaging with the world of chemical analysis. We believe passionately in pushing the envelope for rapid innovation while still delivering superb customer service.

Whether you are engaged every day in nano research or just contemplating
it, coupling your specific scientific knowledge and expertise with our competence in instrument creation will produce the highest quality research results currently available.

NT-MDT offers expert service and applications development through more than 20 representative offices and distributor centers around the globe including two key branch offices in Holland and America. In the past five years, our installed base has grown to over 700 instruments, promoting growth of both lab and research programs worldwide.

Our role as leaders in the field of innovation in nanotechnology is illustrated by the recent award of the "R&D 100" for the NTEGRA Spectra.

Frame programme

Plenary Sessions:

1. Monday, September 15th , 10:00 - 12:30 (including Czochralski Award Ceremony)
2. Friday, September 17th, 09:00 - 10:30 (E-MRS & EPDIC Joint Plenary Session)

Poster Sessions (both obligatory for all authors):

1. Monday, September 15th, 16:00 - 17:30
2. Wednesday, September 17th, 16:00 - 17:30
3. Wednesday, September 17th, 17:00 Best Poster Award Ceremony

Symposia:

- SYMPOSIUM A, Room 315:

Raman scattering in materials science

- SYMPOSIUM B, Room 226:

Transparent Electronics: from materials to devices

- SYMPOSIUM C, Room 231:

Smart Materials for Smart Devices and Structures

- SYMPOSIUM D, Room 134:

Novel synthesis processes and design of nanomaterials for catalytic applications

- SYMPOSIUM E, Room 206:

Plasmonic nanostructures for application in the life sceinces

- SYMPOSIUM F, Room 219:

Nanocomposite materials

- SYMPOSIUM G, Room 144:

Morphology and dynamics of nanostructures and disordered materials via atomic-scale modelling

- SYMPOSIUM H (as a part of SYMPOSIUM L), Room 213:

Crossing frontiers in designing of bio-inspired materials - a novel breakthrough in material science

- SYMPOSIUM I, Room 208:

Functional and Structural Ceramic and Ceramic Matrix Composites (CCMC)

- SYMPOSIUM J, Room 309:

New Opportunities and Challenges in Material Research using Phonon and Vibrational Spectra

- SYMPOSIUM K, Room 215:

Mechanics of nanomaterials

- SYMPOSIUM L, Room 213:

New Scaffolds for Tissue Engineering: Materials and Processing Methods

Satellite event:

- WORKSHOP, 16th and 17th September, Room 123:

Current trends in nanostructured polymer and sol-gel thin films

- COMPLEXEIT WORKSHOP, 16th September, Room 124:

ComplexEIT on Entrepreneurship in Education

Reception

Please note the Main Reception will be open according to the hours given below:

Day	Date	From	To
Sunday	September 14 th	12:00	19:00
Monday	September 15 th	08:00	18:00
Tuesday	September 16 th	08:00	18:00
Wednesday	September 17 th	08:00	18:00
Thursday	September 18 th	08:00	18:00
Friday	September 19 th	08:00	16:00

Fall Exhibit

Welcome

The 2008 E-MRS Fall Exhibit is scheduled to coincide with the Conference programme and will provide exhibitors with ample opportunity for in depth discussion with participants.

Participation in the exhibition will enable companies to make further contact with existing customers or clients and make new fruitful contacts with those engaged in interdisciplinary 'state of the art' research on behalf of industry at universities throughout the world.

The goal of the exhibition is to drive participants to develop their skills and to give them a deeper insight into technology coupled with market demand. The preparation and presentation of projects will challenge them to mix and match their theoretical and practical skills. Past exhibitions have been an invaluable networking opportunity for local and international participants. In addition the exhibition drives research and development in the materials since and engineering sector.

Following companies will welcome you at their booth:

No.	Company name	booth
1	ELSEVIER LTD	B9
2	HiNanoAnalytics CeNTech	B10
3	Goodfellow Cambridge Ltd	B11
4	L.O.T. - Oriel GmbH & Co.	B18
5	Atomic Force GmbH	B16
6	WITec GmbH	B17
7	Schaefer Technologie GmbH	A4
8	NT-MDT Europe B.V.	A5
9	RENISHAW PLC	B15
10	SCANCO Medical AG	B1
11	PREVAC	B12/13
12	COMEF	A2/3
13	PRECOPTIC	B6

The booths are located in the Main Hall of Conference Venue.

Exhibition Coordinator

The 2008 E-MRS Fall Exhibit is organised and coordinated by:

Mr. Grzegorz Wojas

Warsaw University of Technology
Faculty of Materials Science and Engineering
141 Wołoska Street
02-507 Warsaw, Poland
Phone / Fax: (+48 22) 234 81 08
e-mail: emrs.exhibit@gmail.com

Please visit the reception desk in case of any requests or questions concerning the Exhibition.

Sponsors

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Molecular Devices and Tools for Nano Technology

http://www.ntmdt.com

The main Sponsor of the 2008 E-MRS Fall Meeting & Exhibit

Exhibitors profiles

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We strive for next-generation SPM technology, whether it be in pure modularity that allows a university or industrial lab to start with a cost-effective core product and build to a grand, multi-user research center or the ultimate amalgamation of SPM with related technologies that has resulted in ultramicrotomy for nanotomography and spectroscopy-based instruments that meld the world of imaging with the world of chemical analysis. We believe passionately in pushing the envelope for rapid innovation while still delivering superb customer service.

NT-MDT offers expert service and applications development through more than 20 representative offices and distributor centers around the globe. There are two key branch offices opened in Holland and Ireland. In the past five years, our installed base has grown to over 800 instruments, promoting growth of both lab and research programs worldwide. Whether you are engaged every day in nano research or just contemplating it, coupling your specific scientific knowledge and expertise with our competence in instrument creation will produce the highest quality research results currently available.

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Precoptic Co, Arkuszowa 60, Warsaw 01-934, Poland

Programme

Exhibitions

Alphabetical order

Exhibition

Atomic Force GmbH

Ludger Weisser, Roland Goschke, Roger Proksch

ATOMIC FORCE GmbH, Hauptstrasse 161, Mannheim 68-259, Germany

e-mail: weisser@atomicforce.de

http://www.atomicforce.de

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Exhibition

Comef Aparatura Naukowo-Badawcza

Maria Tymieniecka[1], Bogusław Burak[2], Andrzej Czuma[2], Andrzej Wiśniewski[2], Renata Lewandowska[3], Melanie Gaillet[3], Reiner Brings[3]

1. *COMEF Aparatura Naukowo-Badawcza, Rakowiecka 36/317A, Warsaw 02-532, Poland* **2.** *COMEF, Kalinowa 41, Katowice, Katowice 40-750, Poland* **3.** *Horiba Jobin Yvon, Rue de Lille, Villeneuve d'Ascq 59650, France*

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Product Specialty:

Hitachi: Electron microscopes: SEM, TEM, STEM; **Thermo Fisher Scientific** : AUGER and ESCA Spectrometers , EDS and WDS Spectrometers for Electron Microscopy ; **Cameca :** Magnetic sector SIMS and electron microprobe (EPMA), OTAP; **Horiba Jobin Yvon**: Raman Spectrometers, Emission Spectrometers: ICP, GD-OES, Monochromators, Diffraction Gratings, Spectroscopic Ellispometer; **JANIS:** Cryosystems; **Riber**: MBE; **Newport:** Photonics, Vibration and Motion Control, Optics and Opto-Mechanics, Oriel Light Sources, Spectroscopy Instruments, Detectors and Detection Systems, Optical Filters, Hilger Crystals, Diffraction Gratings; **Spectra-Physics**: lasers; **SETARAM:** Calorimeters (CALVET, DSC), high temperatures dilatometers; thermal analyzers (TG, TG-DTA, TG-DSC, TGA-MS, TG-FTIR)

The effort put into continuous improvement of quality and customer service motivated us to apply for ISO 9001:2000 certificate. We received it according to TÜV CERT procedure in December 2005.

Exhibition

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Jonathan Agbenyega, Jonathan Simpson

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Exhibition

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Paul Everitt

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Exhibition

HiNanoAnalytics Network

Monika Lelonek, Heinrich Lothar, Nina Baumjohann, Holger Winter

HiNanoAnalytics Network, Heisenbergstasse 11, Münster 48149, Germany

e-mail: monika.lelonek@marcotech.de

www.hinanoanalytics.org

The network "High Performance Nano-Analytics for Medicine and Biomedical Materials" (= **HiNanoAnalytics**) represents a broad platform of nanoanalytic expertise and nanotechnological competence based on an excellent scientific infrastructure, as well as experienced experts and synergies of nano-science and specialized enterpreneurial practice. The network partners provide an forward integrated structure for research projects to clients and services for industry, scientific institutions and clinically contracting partners.
All members of **HiNanoAnalytics** are involved successfully in several public funded projects, and are experienced in international cooperation. A large number of national and international conferences were already organized and executed.
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- Development of nano-based analytical methods
- Production of analytical devices and instruments
- Analytical service
- Nanomaterials for biological and medical applications
- Technology transfer
- Training and education

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Ignacy Mościcki[1,2], Grzegorz Kaszyński[1,2], Dimitry Kozodaev[1]

1. *NT-MDT Europe BV (NT-MDT), De Pinckart 54, Nuenen 5674CC, Netherlands* **2.** *IGHT s.c., Marszałkowska 80, Warszawa 00-517, Poland*

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1. *Renishaw Plc, Old Town Wotton under Bridge, Gloucestershire GL127DW, United Kingdom* **2.** *Renishaw Plc, Szyszkowa 34, Warsaw 02-285, Poland*

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Wim Koelewijn

Scanco Medical AG, Fabrikweg 2, Bruettisellen 8306, Switzerland

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Martin Schaefer

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Symposia

Plenary session

Programme

Monday, 15 September

Opening & Plenary Session

Czochralski Award Ceremony
Monday morning, 15 September, 10:00
Small Hall (237)

10:30 Invited oral

Magnetic Refrigeration: A New Challenge for Materials Scientists

Kurt H. Buschow

Van der Waals-Zeeman Institute Univ. of Amsterdam, Valckenierstraat 65, Amsterdam NL-1018XE, Netherlands

e-mail: k.h.j.buschow@uva.nl

Magnetic refrigeration can be viewed as an alternative to the conventional vapor-compression technology. Magnetic refrigeration owes its renewed interest not only to its comparatively high efficiency but also to the fact that it is an environmentally friendly techniques, avoiding ozone-depleting or global-warming gases. This opens new research opportunities that have culminated in a worldwide search for novel magnetocaloric materials. In practice, magnetic refrigeration requires the combination of a magnetic field source of high strength and a material with a sufficiently high magnetocaloric effect (MCE). When looking at domestic applications, the best choice of the field source would be a permanent magnet. However, the field generated by permanent magnets falls typically into the 1-2 Tesla range and the MCE of most magnetic materials is too small for such a low field change to result in sufficient cooling power. Recent research activities have therefore been focused on materials with higher than average MCE value, and the prerequisites for attaining high MCEs will be briefly addressed in this talk. A commercially important aspect is the materials cost. Magnetocaloric materials based on magnetic 3d elements are much less expensive than those based on rare earth elements. In the present talk we will concentrate mainly on the results obtained with the former type of materials.

11:30 Invited oral

C.V. Raman and the Impact of Raman Effect in Quantum Physics, Condensed Matter, and Materials Science

Anant K. Ramdas

Purue University, Department of Physics, 525 Northwestern Avenue, West Lafayette 47907-2036, United States

e-mail: akr@physics.purdue.edu

Raman's momentous discovery in 1928 that the spectral analysis of the light scattered by matter, illuminated with monochromatic light of frequency ω_{L}, reveals new signatures at $(\omega_{L \pm} \omega_{i})$, ω_{i}'s being the internal frequencies of the matter [Nature **121**, 501 (1928); Indian Journal of Physics **2**, 387 (1928)]. In a cable to Nature [**122**, 349 (1928)], R.W. Wood, the renowned American Physicist, hailed it as a "very beautiful discovery, which resulted from Ramans's long and patient study of the phenomenon of light scattering" and underscored its significance as "one of the most convincing proofs of the quantum theory of light we have at present time".
After a brief account of Raman's extraordinary scientific career, I will recount the profound impact made by Raman effect, which launched a new branch of spectroscopy, with two illustrative examples: (1) Rotational Raman Spectra of homonuclear diatonic gases and Bose-Einstein & Fermi-Dirac Statistics and (2) The parity related rule of mutual exclusion in the Raman *vs* infrared activity of vibrational modes of centro-symmetric matter.
The dramatic change and the vastly expanded scope of Raman spectroscopy brought about by the invention of the Laser in 1960 will be illustrated with select examples from Condensed Matter Physics and Materials Science. In particular, the focus will be on the collective and localized vibrational, electronic, and magnetic excitations in semiconductors and their nanostructures.

Lunch break

Inner Courtyards
Monday afternoon, 15 September, 12:30

Friday, 19 September

E-MRS & EPDIC Joint Plenary Session
Friday morning, 19 September, 9:00
Small Hall (237)
Chair: Prof. A. Mycielski & Prof. B. Pałosz

9:00 Invited oral

Synthesis and applications for catalysis of carbon and carbides nanostructures

Marc J. Ledoux

European Laboratory for Catalysis and Surface Sciences, ELCASS (CNRS-ULP), 25 rue Becquerel, Strasbourg 67087, France

e-mail: ledoux@ecpm.u-strasbg.fr

Development of new supports for catalytic active phases is one of the most important research fields in heterogeneous catalysis, for use in many gas-phase and liquid-phase reactions.

Since the discovery of carbon nanotube, an increasing interest has been devoted to the preparation of new one-dimensional (1D) nanostructured materials such as nanowires or nanotubes – initiated from sp2 carbon and rapidly extended to oxides – for fundamental studies as well as for a wide range of applications. The field of catalysis also benefits from this (nano)material approach, and carbon nanotubes and nanofibers as well as high surface area silicon carbide (b-SiC) nanotubes obtained by a Shape Memory Synthesis process, used as catalytic active phase supports led to significant breakthroughs with interesting catalytic behaviors, due to their peculiar 1D morphology.

However, severe drawbacks are inherent to the use of fluffy 1D nanostructures, including an almost impossible recovery of the catalysts in liquid-phase medium, huge pressure drops and moving bed phenomena in fixed-bed reactors, and a health impact during handling. Therefore the macronisation of 1D catalysts is of great interest.

This talk details the synthesis, characterization and catalytic use of 1D carbon and b-SiC nanostructures, and focuses on the approach for designing safe and efficient macronized 1D carbon and b-SiC nanostuctures. A wide panel of environmental and energy impact target reactions is taken as key-reactions for highlighting the interest of using 1D carbon and b-SiC nanostructures as catalyst supports, in order to target new conversion and selectivity patterns. Supported by the development of a new electron tomography tool (3D microscopy) for getting more insight on the active phase location inside/outside of a nano-tube shaped support, the nanoreactor concept is pointed out, in which each carbon or b-SiC nanotube, either as fluffy or macronized material can be considered as a single nanoscale reactor.

9:45 Invited oral

Negative thermal expansion materials

John S. Evans

Department of Chemistry, University of Durham, Science Labs, South Road, Durham DH1-3LE, United Kingdom

e-mail: emrs@inmat.pw.edu.pl

We've an on-going interest in materials that show the unusual property of "Negative Thermal Expansion" and contract in volume on heating. Much of this was stimulated by ZrW2O8, which contracts isotropically and continually over a temperature range of 2 to 1050 K with a coefficient of thermal expansion of alpha = -9 x 10-6 K-1. In addition to this behaviour this and related materials show oxide ion mobility at remarkably low temperatures. Other materials such as Ag3Co(CN)6 show a remarkable "colossal" negative thermal expansion, with alpha = -130 x 10-6 K-1 in one direction. The observation of NTE behaviour is often intimately related to phase transitions in materials and in many cases these can lead to structures with a remarkable degree of complexity which present a considerable challenge for powder diffraction methods. A full understanding the synthesis and properties of such materials requires application of a range of complementary techniques such as diffraction, total scattering and multi-nuclear solid state NMR. In this presentation

I'll discuss recent advances in our understanding of these materials and highlight in particular the information available from powder methods. I'll also use the presentation to highlight methods for analysis of diffraction data such as "parametric" Rietveld refinement which can allow the extraction of "unusual" information from powder diffraction data such as temperatures or activation energies for processes in the solid state.

Raman scattering in Materials Science

Symposium A

Welcome

Raman spectroscopy is one of the fastest growing analytical techniques in use today. The conference is focused on the recent progress in the various fields of Raman scattering spectroscopy investigation of properties of different kind of materials. It covers the wide range of frequencies (from IR through visible to X-rays) and has now become a highly sophisticated research field as it is versatile and is a promising tool for advanced studies in areas of new materials, molecular dynamics, space exploration and several other areas. This conference seeks to gather both leading experts and young researchers to discuss the recent developments in this field, to stimulate exchanges among active researchers and to provide a global platform for the research community in Raman spectroscopy. The scientific programme will include a wide variety of topics on Raman Spectroscopy like:

- Theory
- Time-Resolved Raman Spectroscopy and Ultrafast Phenomena
- Non-Linear Raman Spectroscopy
- Surface-Enhanced Raman Spectroscopy
- Vibrational Analysis and Molecular Structure
- Solids, Crystals, Glasses, and Gels
- Thin Layers, Surfaces, and Interfaces
- Application to Material Science and Technology
- New Functional Materials, Fullerenes, Carbon Nanotubes, Conducting Polymers
- Application to Solid-State Physics; Conductivity, Magnetic Properties, and Phase Transition
- Raman Imaging; Confocal/Near-Field/Tip-Enhanced Raman Microspectroscopy, Bioimaging, and Stress Analysis
- Raman Spectroscopy under Extreme Conditions: High Temperature, High Pressure, and High Magnetic FieldsNew Raman Spectroscopy: Near-Infrared and X-Ray

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Programme

Monday, 15 September

Opening & Plenary Session

Czochralski Award Ceremony
Monday morning, 15 September, 10:00
Small Hall (237)

Lunch break

Inner Courtyards
Monday afternoon, 15 September, 12:30

Parallel Session

Monday afternoon, 15 September, 14:00
Room 315

14:00	Invited oral

Raman Scattering by Electrons in Semiconductor Quantum Structures*

Aron Pinczuk

Columbia University, New York, NY 10027, United States

e-mail: aron@phys.columbia.eu

Electron fluids in semiconductor quantum structures support low-energy excitation modes that manifest the remarkable quantum phases that emerge from fundamental interactions in two-dimensions. The benchmark semiconductor system is that of the ultra-high mobility 2D electron gas in GaAs-AlGaAs heterostructures. Atomic layers of graphene with density tunable by electric field doping are of enormous current interest.

Inelastic light scattering (or electronic Raman scattering) at very low temperatures (reaching below 50 milliKelvin degrees) are experimental venues to study excitations of electron fluids hosted by semiconductor heterostructures.

This talk presents a brief introduction to applications of inelastic light scattering methods to studies of 2D electron systems. Recent results in quantum Hall regimes are the examples that demonstrate the power of light scattering experiments to study the low-lying excitations. These are the excitations that express distinct quantum phases of the electron liquids.

Recent inelastic light scattering studies explore excitations of the quantum Hall fluids that reside in the second Landau level at filling factors such as nu=5/2 and nu=7/3. The quantum Hall fluids in higher Landau levels are of great current interest for applications in topologically protected quantum computations. The recent light scattering results will be evaluated to show how these experiments directly reveal spin properties and seek to elucidate the interplay among competing quantum phases of electrons that occur in higher Landau levels.[1]

(*) Work supported by the U.S National Science Foundation, by the U.S. Department of Energy, and by the U.S. Office of Naval Research.

[1] T.D. Rhone, X. Yang, J. Yan, Y. Gallais, A. Pinczuk, L.N. Pfeiffer, K.W. West, work in progress.

14:30 Invited oral

Phonon properties and structural phase transitions in ferroelectrics - high pressure Raman scattering studies

Mirosław Mączka[1], Waldeci Paraguassu[2], Antonio G. Souza Filho[3], Paulo T. Freire[3], Andrzej Majchrowski[5], Josue Mendes Filho[3], Jerzy Hanuza[4]

1. *Institute of Low Temperature and Structure Research, Polish Academy of Sciences, P.Ne 1410, Wrocław 50-950, Poland* **2.** *Departamento de Fisica, Universidade Federal do Maranhão, São Luis 65085-580, Brazil* **3.** *Departamento de Fisica, Universidade Federal do Ceara, Fortaleza 60455-970, Brazil* **4.** *Department of Bioorganic Chemistry, University of Economics, Wrocław 53345, Poland* **5.** *Institute of Applied Physics, Military University of Technology, Warsaw 00-908, Poland*

e-mail: m.maczka@int.pan.wroc.pl

Raman spectroscopy is a very powerful tool in studies of ferroelectric materials since it gives information about the symmetry changes and the mechanisms by which phase changes proceed. In particular, there has been great interest in studies of soft modes since such studies give direct information on the nature of lattice instabilities. High pressure is a clean probe for investigating the delicate balance between long and short range forces which in turn should shed light on the lattice instabilities and ferroelectric order.

In this contribution, we present and discuss high pressure Raman scattering results for two ferroelectric materials, Bi_2WO_6 and $K_2MgWO_2(PO_4)_2$.

Bi_2WO_6 is a member of bismuth layered compounds (Aurivillius family). Its room temperature structure (space group symmetry $Pca2_1$) can be regarded as derived from a high symmetry body centered tetragonal structure (space group symmetry I4/mmm) [1]. We will show that Bi_2WO_6 exhibits two reversible second order phase transitions at 3.4 and 6.2 GPa. It will also be shown that the phase transition at 6.2 GPa is triggered by instability of the low frequency mode, which behaves as soft mode. The observed soft mode is weak and it may be easily overlooked in the temperature dependent studies. Our results demonstrate therefore that the Raman studies under high pressure are an alternative way to study soft mode dynamics in ferroelectrics with high Curie temperature.

$K_2MgWO_2(PO_4)_2$ is derived from $KTiOPO_4$ (KTP) by replacement of two Ti^{4+} ions with Mg^{2+} and W^{6+} cations. This material exhibits five temperature-induced structural transitions from the $P4_12_12$ to P1 structure [2]. We will show that this material exhibits a reversible first order phase transition near 2.0 GPa, which is driven by the soft mode corresponding to motions of the K^+ ions.

References

[1] N. A. McDowell, K. S. Knight, and P. Lightfoot, Chem. Eur. J. 12, 1493 (2006).

[2] U. Peuchert, L. Bohaty, and J. Schreuer, J. Appl. Cryst. 31, 10 (1998).

15:00 Invited oral

Raman spectroscopy involving individual single and multicomponent nanowires

Jonathan E. Spanier

Drexel University, 3141 Chestnut St, Philadelphia 19104, United States

e-mail: spanier@drexel.edu

The Raman scattering by phonons from individual single- and multicomponent semiconducting nanowires and nanocones exhibits a number of noteworthy features owing to the finite size and shape of the nanowire[1,2]. In this presentation I will present and discuss our recent experimental and theoretical work involving remarkably strong enhancements of the spontaneous Raman scattering from these nanostructures, as compared with bulk Si, including the diameter, excitation wavelength and optical polarization dependence. Application of these findings to surface enhanced Raman scattering by molecules chemisorbed on hybrid metal-semiconductor nanostructures and its implications for chemical sensing will also be presented and discussed. Work supported by the US Army Research Office.

[1] L. Cao, B. Nabet and J. E. Spanier, Phys. Rev. Lett. 29, 157402 (2006).

[2] L. Cao, B. Garipcan, E. Piskin, B. Nabet and J. E. Spanier, Nano Lett. 8, 601 (2008).

Coffee break

Main Hall
Monday afternoon, 15 September, 15:30

Joint Poster Session 1

Monday & Wednesday
Monday afternoon, 15 September, 16:00
Main Hall

Tuesday, 16 September

Joint session with Symposium J

Tuesday morning, 16 September, 9:00
Room 315

9:00 Invited oral

Vibrational modes in suspended carbon nanotubes probed by transport measurements

Herre S. Van der Zant

DIMES, Mekelweg 4, Delft 2628 CD, Netherlands

e-mail: h.s.j.vanderzant@tudelft.nl

Single-walled carbon nanotubes (SWNTs) are promising building blocks for nano-electromechanical systems because they have a low mass, are easily scalable through their length and have a high Young's modulus of 1.25 TPa, which is almost an order of magnitude higher than that of silicon. At room temperature, we have used a suspended, semiconducting carbon nanotube as a frequency mixer to detect its own mechanical motion. In the range of 200 MHz, a single gate-dependent resonance is observed, which we attribute to the bending mode vibration of suspended carbon nanotubes [1]. A continuum model [2] describes the gate-dependence of the resonance frequency very well and the analysis shows that the nanotube can be tuned from a regime without strain to a regime where it behaves as a vibrating string under tension. At low temperatures, the suspended nanotubes act as quantum dots. Vibrational modes then become visible as harmonic excitation spectra in single-electron tunneling. Phonon-assisted tunneling mediated by (long-wavelength) longitudinal vibration modes has been observed [3] and comparison with a Franck-Condon model indicates a rather strong electron-phonon coupling factor of order unity. Issues that are currently investigated include mechanisms for electron-vibron coupling, mechanical relaxation, mechanical modes in higher-order tunneling and "distortion blockade of current" in ultra-short (< 100 nm) nanotube segments.

[1] B. Witkamp, M. Poot and H.S.J. van der Zant, Nano Lett. **6** (2006) 2904.

[2] S. Sapmaz, Ya. M. Blanter, L. Gurevich, and H.S.J. van der Zant, Phys. Rev. B. **67** (2003) 235414.

[3] S. Sapmaz, P. Jarillo-Herrero, Ya. M. Blanter, C. Dekker and H.S.J. van der Zant, Phys. Rev. Lett. **96** (2006) 026801.

EMAIL: h.s.j.vanderzant@tudelft.nl

9:45 Invited oral

Quantum tunneling through moving nanoobjects

Konstantin Kikoin

Tel Aviv University (TAU), Ramat Aviv, Tel Aviv 69787, Israel

e-mail: konstk@post.tau.ac.il

Among many possibilities provided by nanotechnologies one of the most challenging is the possibility of study quantum tunneling through nanoobject moving in space by means of nanomechanical or electrostatic forces or due to excitation of vibration eigenmodes. We discuss various aspects of quantum tunneling through molecules and/or quantum dots in Kondo resonance regime. Kondo anomalies in tunnel conductance of molecular complexes may be induced by phonon absorption and emission assisting single-electron tunneling [1]. Kondo shuttling through double quantum dots arises due to specific dynamical symmetry of spin multiplets characterizing magnetic state of these nanoobjects [2]. This dynamical symmetry allows also conversion of time-dependent charge input signal applied to the gate into Kondo response in tunnel conductance [3]. All these effects may be described by means of the Anderson model applied to molecular complexes or double quantum dots in a contact with metallic electrodes with time-dependent tunneling between various components of nanodevice.

[1] K. Kikoin, M.N. Kiselev, M.R. Wegewijs, Phys. Rev. Lett. **96**, 176801 (2006)

[2] M.N. Kiselev, K. Kikoin, R.I. Shekhter, and V.M. Vinokur, Phys. Rev. B **74**, 233403 (4) (2006)

[3] M.N. Kiselev, K. Kikoin, J. Richert, arXiv:0803.2676

Coffee break

Main Hall
Tuesday morning, 16 September, 10:30

Joint session with Symposium J

Tuesday morning, 16 September, 11:00
Room 315

11:00 Invited oral

The widths of phonons

Manuel Cardona

Max-Planck-Institut FKF, Heisenbergstr. 1, Stuttgart D70569, Germany

e-mail: M.Cardona@fkf.mpg.de

Most information on the width of phonons in crystals has been obtained by laser Raman spectroscopy: The resolution usually available in INS, and more recently in Inelastic X-ray Scattering, is too poor to yield precise results on phonon widths. Recently, phonon width data have also been obtained by coherent phonon techniques (in the time domain) and by neutron echo experiments, but these methods apply only to phonons of relatively low frequency. Theoretically, the phonon widths are described as the imaginary part of a self-energy, its real part representing a phonon shift beyond the harmonic approximation. The self energy is temperature dependent, a fact that accounts for an increase in width with increasing temperature. The shift usually corresponds to a softening with increasing temperature, although the opposite is sometimes found. The mechanisms involved in this self- energy are either anharmonic interactions (e.g. decay into two phonons) and electron-phonon interactions (in the case of metals and semiconductors).

Several typical and also unusual experimental results involving semiconductors and high Tc superconductors will be discussed together with their theoretical interpretation on the bases mantioned above.

11:45 Invited oral

Raman-Mie scattering from spherical microparticles

Wolfgang Kiefer

Institut für Physikalische Chemie, Am Hubland, Würzburg 97074, Germany

e-mail: wolfgang.kiefer@mail.uni-wuerzburg.de

Spherical particles in the size range of micrometers are excellent resonators for visible light. The elastically (Mie) as well as inelastically (Raman) scattered light is significantly dominated by this property, which leads to so-called morphology dependent resonances (MDRs) in both types of light scattering mechanisms.

The lecture first describes the various ways of trapping single microparticles free in space. Then, applications of combined Raman/Mie scattering from single microdroplets are discussed. This includes evaporation studies, phase transitions, acid/base reactions and polymerization in a single microdroplet. Finally, stimulated Raman scattering from and femtosecond pulse excitation experiments on single microdroplets are described. To interpret the observed femtosecond-Mie spectra, a time-dependent Mie-theory had to be developed.

The work presented had been performed in the author's former laboratories by my former co-workers M. Lankers, J. Musick, J. Popp, V.E. Roman, O. Sbanski, K. Schaschek, S. Schlücker, T. Siebert, and M. Trunk to whom I am most thankful.

Lunch break

Tuesday afternoon, 16 September, 12:30
Inner Courtyards

Parallel Session

Tuesday afternoon, 16 September, 14:00
Room 315

14:00 Invited oral

Lattice dynamics studies by inelastic x-ray scattering

Michael Krisch

European Synchrotron Radiation Facility, Grenoble, France

e-mail: krisch@esrf.fr

Starting from pioneering work in the 1980's [1], and profiting from the development of dedicated synchrotron radiation sources and performing x-ray optics, inelastic x-ray scattering (IXS) with meV energy resolution has become a powerful tool in the study of phonon dispersion in condensed matter. The most important aspects distinguishing IXS from inelastic neutron scattering (INS) techniques, are the absence of kinematic limitations and the possibility to study very small samples (down to 10^{-5} mm^3). This has opened up new possibilities in a range of research fields. The talk will illustrate the present capabilites of the technique by discussing a few representative examples of recent reseach conducted on beamline ID28 at the ESRF. These shall comprise studies at high pressure using diamond anvil cell techniques [2], work on BN [3], and experiments probing phonons in the near-surface region [4,5]. The presentation shall conclude with the discussion of some novel applications and perspectives.

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14:45 Oral

Strain imaging in SiGe waveguides

Emiliano Bonera[1], Fabio Pezzoli[1], Mario Guzzi[1], Emanuele Grilli[1], Riccardo Gatti[1], Leo Miglio[1], Daniel Chrastina[2], Giovanni Isella[2], Hans Von Känel[2], Fabian Gramm[3], E. Müller[3], Andrea Trita[4], Ilaria Cristiani[4]

1. *LNESS and Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, via Cozzi 53, Milano 20125, Italy* **2.** *LNESS and Dipartimento di Fisica del Politecnico di Milano, via Anzani 42, Como 22100, Italy* **3.** *Solid State Physics Laboratory ETH, Schafmatstr. 16, Zürich CH-8093, Switzerland* **4.** *Dipartimento di Elettronica, Università di Pavia, Via Ferrata 1, Pavia 27100, Italy*

e-mail: emiliano.bonera@unimib.it

The quest for the extension of silicon from the base material for electronics towards the base material for photonics spans the development of a small number of key building-block components. One such component is a waveguide which can transmit near-infrared radiation among the different devices of a photonic circuit. A practical implementation can be realized by Si/SiGe/Si heteroepitaxial structures. For these guides, uniformity of the refractive index is an extremely important parameter, since even small local variations can result in large differences in transmission properties.

We present a work where images of small local variations of strain in planar waveguides are acquired by Raman spectroscopy, the only characterization technique which combines strain sensitivity with submicron spatial resolution. The strain modulation is of the order of 0.02% with a length scale of the order of several microns and explains a modulation of the refractive index observed in infrared transmission images. The correlation of Raman results with finite-element models show that the physical origin of the modulation is consistent with bunching of dislocations.

Coffee break

Main Hall
Tuesday afternoon, 16 September, 15:30

Parallel Session

Tuesday afternoon, 16 September, 16:00
Room 315

16:00 Invited oral

Low frequency Raman scattering in characterization of nanostructured materials

Mile Ivanda[1], Davor Ristic[1], Kresimir Furic[1], Svetozar Music[1], Mira Ristić[1], Marijan Gotić[1], Goran Štefanić[1], Uros V. Desnica[1], Maja Buljan[1], Maurizio Montagna[2], Maurizio Ferrari[3], Alesandro Chisaera[3], Yoann Jestin[3]

1. *Ruđer Bošković Institute, Bijenička 54, Zagreb 10000, Croatia* **2.** *Dipartimento di Fisica, Universita' di Trento, via Sommarive, 14, Trento 38050, Italy* **3.** *CNR-IFN, CSMFO group (CSMFO), via Sommarive 14, Trento 38050, Italy*

e-mail: ivanda@irb.hr

A short theoretical introduction of the Lamb theory on the vibrations of elastic spheres will be described for the free nanoparticles as well as for the nanoparticles embedded in matrix. The spherical case is well understood – the normal modes of the sphere are divided into torsional and spheroidal and, experimentally, have been measured in various situations. Here, the application of the Lamb theory will be illustrated by the low frequency Raman scattering (LFRS) measurements on different powder samples: TiO_2, SnO_2, and CdS. The effects of sintering of nanoparticles will be described with the ZrO_2 nanoparticles doped with Sn, Ge and Cu. For the nanoparticles embedded in matrix a theoretical treatment of polarization-dependent low-frequency off-resonant Raman scattering which establishes a relation between the particle size, the frequencies, and the widths of various phonons. The selection rules for the Raman scattering of the spherical particles and of the particles of irregular shape will be discussed. Polarized and depolarized scattering from confined acoustic phonons were distinctly resolved near the laser line. A good agreement between the experimental and the theoretical results will be illustrated by TiO_2, CdS_xSe_{1-x}, and HfO_2 nanoparticles in glass matrix. The nanoparticle sizes and even sizes distribution obtained from Raman scattering agree well with those obtained from transmission electron microscope proving the LFRS to be a simple, fast and reliable method for the size distribution measurements. By inverse procedure, starting from the Raman spectra and known particles size distribution, the mean sound velocities of longitudinal and transverse phonons of nanoparticles could be deduced, providing LFRS to be unique technique for determination of the sound velocities in nanoparticles. The possibility of coherent Raman scattering will be illustrated by the LFRS on the self-organized Ge superlattice.

16:30 Invited oral

Acoustic vibrations for nanoscale metrology

Adnen Mlayah[1], Nicolas Large[1,2], Javier Aizpurua[2]

1. *CEMES-CNRS (CEMES-CNRS), 29, rue Jeanne Marvig, Toulouse F31055, France* **2.** *Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal, 4., San Sebastián 20018, Spain*

e-mail: Adnen.Mlayah@cemes.fr

Acoustic vibrations with frequencies ranging from few hundreds of GHz to few THz have wavelengths varying from few tens of nanometers to few nanometers depending on the material sound velocities. Hence, these sound waves are well adapted probes of nano-objects (Quantum wells, semiconductor quantum dots, metal nanoparticles) and can be excited and detected using optical techniques (e.g. Raman/Brillouin, time resolved pump-probe experiments). In this talk, I will review recent advances in the use of acoustic phonons Raman/Brillouin scattering as a tool for nanoscale metrology. I will first introduce the basic concepts of interaction between extended acoustic vibrations and electronic states in semiconductor quantum wells and in self-organized quantum dots. When the coherence lengths of light and sound is much larger than typical correlation lengths of excited electronic states, the inelastic light scattering process is spatially coherent, thus leading to interference effects in the scattered intensities. This property is here used to extract the size and the spatial distributions of nano-objects from the spectral feature of the low-frequency Raman/Brillouin scattering.

Acoustic vibrations can also be confined to nano-objects. Their density of states is then discretized and size effects are very important. The confinement of acoustic vibrations in two-dimensions is clearly observed by inelastic light scattering in silicon/silicon oxide layers and in silicon membranes. These structures are widely used in the silicon based micro-electronic industry, thus providing a good example of the use of fundamental concepts for applications in nanotechnoloy. The discussion will be extended to one dimensional (Carbon nanotubes and metal nanowires) and zero-dimensional (semiconductor quantum dots and metal nanoparticles) systems.

17:00 Oral

Raman intensity : an important tool in the study of nanomaterials and nanostructures

Aneta Slodczyk, Philippe Colomban

LADIR-CNRS (LADIR), 2 rue Henry Dunant, Thiais 94320, France

e-mail: slodczyk@glvt-cnrs.fr

The measurements of the relative Raman intensity are used mainly to map quantitatively the amount, distribution and degree of crystallisation of different phases in a material [1,2]. Our studies reveal that the analysis of the relative or absolute Raman intensity is much more powerful tool which allows to understand and characterize the modifications of the crystal/amorphous structure due to:

- changes of the long range order correlations as the function of the nanoregion organization in the case of PMN-PT [3] relaxor ferroelectric materials. The significant decrease of Raman intensity with the temperature increasing reveals the continuous evolution of the local symmetry towards the long range cubic one.
- changes of the Si-O network caused by the depolymerisation resulting from the substitution of the Si4+ ions (covalent bonds) by the M+ cations (ionic bonds) [4,5] or by the incorporation of the metallic nanoprecipitates [5,6]. SiO4 tetrahedron is a strong chemical and vibrational entity and the Raman signature reveals the different conformations. The transition from a highly connected tetrahedral structure to a weakly connected tetrahedral units as caused by the addition of fluxing agents is reflected in the Raman spectrum by modifications of the Si-O intensity. If the laser excitation interact with the Plasmon absorption of Ag° or Cu° nanoparticles dispersed in the glass (ancient or modern) the Raman scattering probes only the Si-O bonds interacting with the M° nanoparticles and strong intensity changes are measured [6].

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Wednesday, 17 September

Parallel Session

Wednesday morning, 17 September, 9:00
Room 315

9:00 Invited oral

Raman studies of corrosion layers formed on archaeological iron. From characterisation to imaging and quantification

Ludovic Bellot-Gurlet[1], Delphine Neff[2], Solenn Reguer[3], Judith Monnier[2], Phillippe Dillmann[4]

1. *Lab Dynamique Interaction et Reactivite, CNRS and Univ Paris VI (LADIR), 2 rue Henry Dunant, Thiais 94320, France* **2.** *Laboratoire Pierre Süe, CEA and CNRS, CEA Saclay, Gif-sur-Yvette 91191, France* **3.** *Beamline DIFFABS, Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, BP 48, Gif-sur-Yvette 91192, France* **4.** *UMR IRAMAT LMC CNRS and Laboratoire Pierre Sue, CEA Saclay, Gif-sur-Yvette 91191, France*

e-mail: bellot-gurlet@glvt-cnrs.fr

Prediction of corrosion behaviour of metallic materials over several 100 years could be assessed through the study of ancient archaeological artefacts [1]. The observation and characterisation of corrosion layers at a microscopic scale provides information helping formulating hypothesis for long term mechanisms. Raman micro-spectroscopy is a versatile tool for structural identification of iron corrosion products, thanks to its easy implementation, spatial resolution and ability to detect even low crystallised phases.

Various environment of iron corrosion were considered [2-6]: soil, atmosphere and concrete. For each case, Raman spectroscopy imaging had allowed to propose a schematic organisation of the corrosion layer, with phase identification and organisation. Some unexpected facts were encountered. For instance for buried artefacts, in the specific situation of the identification of chlorinated iron phases which are especially involved in active corrosion processes, we underlined the importance of a newly identified ferrous hydroxychloride (β-FeOOH). About atmospheric corrosion Raman spectroscopy emphasised the large presence of poorly crystallised phases as Maghemite, Ferrihydrites and Ferroxyhite.

Because each phase does not present the same activity in these corrosion mechanisms, it is not only needed to recognise and localise, but furthermore to quantify their proportions. But even at a microscopic scale Raman spectra display phase mixes, so that spectral decomposition is required to quantify the different phases. For that linear combination of reference spectra is used to extract "quantitative" structural composition. Thus normalised compositional images are deduced and by scanning a representative part of each sample "global" phase proportions are obtained. The final aim is one hand to provide data for alteration diagnosis and on the other hand to confront the results to existing predictive corrosion models.

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9:30 Invited oral

Micro-Raman scattering of semiconductor nanostructures

Andres Cantarero

Universidad de Valencia-ICMUV (ICMUV), Polígono La Coma s/n, Valencia 46980, Spain

e-mail: cantarer@uv.es

Micro-Raman scattering is a non destructive characterization tool which allows us to extract local and valuable information of semiconductor nanostructures. The technique can be applied to analyze first and second order phase transitions, anharmonicities, strain states of the nanostructures, etc. Playing with the wavelength, resonance Raman scattering can provide information of single quantum objects. We will describe here the main techniques based on Raman scattering applied to nanostructures, some experimental examples and some models of the vibrational properties of nanostructures.

10:00 Invited oral

Light scattering from photo-tunable carbon nanosponge suspensions.

Ratnasingham Sooryakumar[1], Wei Zhou[1], Ranjit Annamalai[2], Rakesh P. Tiwari[1], David Stroud[1], Vish Subramaniam[2]

1. *The Ohio State University, Department of Physics, 191 W. Woodruff Avenue,, Columbus 43210, United States* **2.** *The Ohio State University, Department of Mechanical Eningeering, 201 W. 19th Avenue, Columbus 43210, United States*

e-mail: soory@mps.ohio-state.edu

Propagation of acoustic and electromagnetic waves in inhomogeneous media is a phenomenon of fundamental importance and increasing technological relevance. In contrast to the case of electromagnetic waves, to date only a few experiments on sound propagation in the strongly scattering regime have been performed. In this talk we report on the creation of nanosponges made by dispersing networks carbon nanotube bundles in a fluid and exposing the suspension to low levels of laser radiation. Remarkably, exposure to laser light leads to agglomeration of the dispersed bundles into a nanoporous structure whose average pore dimensions are tunable with light. The acoustic properties of the suspension are measured by inelastic light scattering and reveal dramatic softening of the sound velocity with increasing weight fraction of the stiff nanotube bundles. The resulting reduction in sound speed as calculated using an effective medium approximation is comparable to that seen in the experimentally studied suspension. We interpret the observed acoustic mode as the analog of the slow compressional mode in porous solids having a length scale of order 100 nm.

Coffee break

Main Hall
Wednesday morning, 17 September, 10:30

Parallel Session

Wednesday morning, 17 September, 11:00
Room 315

11:00 Invited oral

Raman scattering in strongly correlated electron systems

Milan J. Konstantinovic

Belgian Nuclear Research Centre-Centre d'Etude de l'Energie nucléaire (SCKCEN), Boeretang 200, Mol 2400, Belgium

e-mail: mkonstan@sckcen.be

Strongly correlated electron systems exhibit a wealth of effects such as magnetic ordering, mixed valence, charge ordering phase transition, metal-insulation transition etc. The discovery of high-temperature superconductivity in lightly-doped transition-metal oxide antiferromagnets teaches us that these materials can do other remarkable things as well, which still need to be explored. In this talk I will review few results obtained along one particular research direction, motivated by the question: Is there something specific in the magnetism of transition metal oxides which is a prerequisite for the appearance of high-Tc superconductivity? Interestingly, some of these materials show low-dimensional magnetic properties due to strongly reduced electron interaction along one or two crystallographic directions. For example, as a consequence of quasi one-dimensionality, the spin-dimerization may occur in the spin-chains (spin-Peierls transition) or spin-ladders leading to the non-magnetic ground states at low temperatures. These structures exhibit complex excitation spectra which can be studied by Raman spectroscopy.

Firstly, I will discuss what kind of quantum effects are observed in the magnetic systems with restricted geometry, in particular the antiferromagnetic, S=1/2, two-leg-ladder, CaV_2O_5. Then, I will analyze the electronic order-disorder effects in the Raman spectra of NaV_2O_5, and discuss the charge ordering phase transition in this compound. Finally, I will present the orbital dimerization in $NaTiSi_2O_6$. I will argue that the novel type of the phase transition at T=210 K can be regarded as an orbital analogue of the spin-Peierls phase transition.

11:30 Invited oral

Correlated electrons and competing interactions in Raman scattering

Peter Lemmens

Inst. Condensed Matter Physics (IPKM), Mendelssohnstr. 3, Braunschweig 38108, Germany

e-mail: p.lemmens@tu-bs.de

Raman scattering is a valuable tool to investigate the magnetic excitation spectrum of quantum spin systems based on insulating transition metal oxides. Information on characteristic energy scales, dimensionality and competing interactions can be gained [1-5]. We will demonstrate experimentally that coupling a larger number of spins leads to more complex excitation spectra including magnetic bound states of singlet and triplet character up to a continuum of excitation if the ground state degeneracy is as large as in a Kagome system. In correlated electron systems also the lattice symmetry may be locally or globally be modified. We will discuss here the example of CdCr2S4, a ferromagnetic system with magneto-capacitive effects, where local distortions are proposed to lead to a very large coupling of magnetic to lattice degrees of freedom.

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Acknowledgement: This work was supported by DFG and the ESF program “Highly Frustrated Magnetism” (ESF-HFM).

12:00 Invited oral

Raman imaging approach to the study of ferroelectric domains and Raman spectra of multiferroic boracites

Milko N. Iliev, Victor G. Hadjiev, Jordi Pascual

University of Houston, Texas Center for Superconductivity and Advanced Materials, Houston, TX 77204, United States

e-mail: miliev@uh.edu

The boracites with general formula $M_3B_7O_{13}X$ (M=divalent metal, X=Cl,Br,I), shortly denoted as M-X, are among the first known multiferroic materials. They exhibit a sequence of transitions from the high temperature paraelectric cubic phase to ferroelectric orthorhombic, monoclinic, trigonal phases, and finally to a monoclinic phase at low temperatures, where both ferroelectric and magnetic orders coexist. The reports on the lattice dynamics of boracites have been restricted so far to the paraelectric cubic phase, the main problem with other phases being the coexistence of twin variants with different crystallographic and polarization orientation. It will be demonstrated on the example of $Co_3B_7O_{13}Cl$ (Co-Cl), $Co_3B_7O_{13}Br$ (Co-Br) and $Ni_3B_7O_{13}Br$ (Ni-Br) that using Raman microscopy imaging one can visualize the twin variants, obtain Raman spectra from untwined domains in exact scattering configurations, determine the Raman mode symmetries, and assign the Raman lines to definite atomic motions. The variations of the ferroelectric domains and Raman spectra through crystallographic transitions will also be discussed.

Lunch break

Inner Courtyards
Wednesday afternoon, 17 September, 12:30

Parallel session

Wednesday afternoon, 17 September, 14:00
Room 315

14:00 Invited oral

High-pressure induced phase transitions and amorphisation in $Gd_2(MoO_4)_3$ polarized Raman spectra and ab-initio analysis

Guy Lucazeau, Pierre Bouvier, Alain Pasturel, Olivier Le Bacq, Thierry Pagnier

Grenoble Institute of Technology, Laboratoire d'électrochimie et de physicochimie des matériaux (LEPMI-CNRS), 1130 rue de la piscine BP75, Grenoble 38402, France

e-mail: guy.lucazeau@lepmi.inpg.fr

Polarized Raman spectra of single crystal gadolinium molybdate, $Gd_2(MoO_4)_3$ were obtained between 1atm and 7 GPa. Ab initio calculations were performed on the isostructural europium compound for reproducing pressure induced structural changes. Using a mixture of alcohol and water as a pressure transmitting medium, YY, ZZ, XY components of scattering matrices were measured. The ZZ spectra were also obtained in argon. Five phase transitions and amorphization were identified. In alcohol, amorphisation is observed above 6.5 GPa. In argon the amorphisation is progressive and begins above 3 GPa and thus the chemical decomposition is not considered to drive the amorphization. The spectral changes with pressure concern as well high-frequency bands attributed to symmetric and antisymmetric MoO4 stretching modes as the very low frequency modes such as librations of tetrahedra. This means that both tetrahedra short range and long-range organisation are involved in these phase transitions. The disordering mechanism is strongly dependent on the pressure-transmitting medium. The TO and LO low frequency modes of A_1 symmetry, observed in the Y(ZZ)Y and c(bb)c geometries respectively below 50 cm^{-1}, soften continuously through the first three phases when increasing pressure. The strong A_2 mode observed in the Z(XY)Z spectra exhibits the same anomalous behaviour by decreasing from 53 down to 46 cm^{-1} at 2 GPa. The softening of these modes, probably due to librations of tetrahedra, is related to the orientation change of tetrahedra observed by ab initio calculations when the volume cell is decreased. Symmetry coordinates for these modes are identical to cooperative orientation changes observed in ab initio results. These orientation changes can explain the frequency decrease of Mo-O stretching modes above 2 GPa, which indicates an increase of Mo coordination. Among the different amorphization mechanisms, the steric hindrance between polyhedra is believed to be the most relevant.

14:30 Invited oral

High pressure Raman spectroscopy in carbon nanotubes

Gerasimos A. Kourouklis[1], John Arvanitidis[1,2], Dimitris Christofilos[1], Sotirios Ves[3]

1. *Aristotle University, Physics Division, School of Technology, University Campus, Thessaloniki 54124, Greece* **2.** *Technological Educational Institute of Thessaloniki, Department of Applied Sciences, Sindos, Thessaloniki 57400, Greece* **3.** *Dept. of Physics, Aristotle University of Thessaloniki, 54 124 Thessaloniki, Greece, Thessaloniki 54 124, Greece*

e-mail: gak@gen.auth.gr

This work focuses on the high pressure Raman study of carbon nanotube structures comprising of single or multiwall tubes. The detailed examination of the Raman peaks as a function of pressure, especially those attributed to the radial breathing modes (RBM) of the inner and outer tubes of the structure, provides a wealth of information concerning the pressure response of individual nanotubes as well as the inner-outer tube (intratube) interactions. The pressure response of the inner tubes, expressed by the normalized pressure slopes $\gamma_i = (1/\omega_i)\ (\delta\omega_i/\delta P)$ *vs.* frequency of their RBMs, shows a remarkable grouping in quasi-linear distributions wherein G_i increases with w. This behaviour is explained by assuming that the pressure response of an internal tube is strongly dependent on the intratube spacings and thus the structural characteristics of the encapsulating tube. This information is of particular interest for the characterization of carbon nanotubes as well as in evaluating the encapsulation effects on systems incorporated in these structures.

15:00 Invited oral

New imaging techniques in Raman spectroscopy - Defining new standards for high speed image data acquisition.

Ken Williams

e-mail: ken.williams@renishaw.com

Raman spectroscopy continues to provide analytical solutions in a variety of applications offering chemical specificity on a micrometer scale.

The ability to create chemical and compositional images by acquiring Raman spectra from an array of positions and then processing them to reveal the parameters of interest is a powerful technique. Traditionally, these spatially-related data have been collected by raster scanning the sample beneath the incident laser spot, typically in micrometer intervals. New approaches to Raman imaging have been developed that enhance the capabilities of modern Raman instruments.

A new method of acquiring confocal Raman images has been developed – ‘Streamline’. Spectra are collected in parallel, rather than in series using the traditional methods. Shorter total acquisition times result, with high quality individual spectra recorded in the order of fifty milliseconds. The method also benefits from ‘on the fly’ data analysis resulting in real time image creation. This innovative approach allows the technique to succeed where others have failed: producing uncompromised data and images for small or large areas at speeds much greater than possible with competing methods. Geological, polymer and materials examples will be shown to illustrate the benefits of this method. For example large area mineral samples yield Raman chemical images that can be produced in less than thirty minutes which offers real advantages for surveying and identifying the real areas of interest.

Coffee break

Main Hall
Wednesday afternoon, 17 September, 15:30

Joint Poster Session 2

Poster Award Ceremony
Wednesday afternoon, 17 September, 16:00
Main Hall

Thursday, 18 September

Parallel symposia

Thursday morning, 18 September, 9:00
Room 315

9:00 Invited oral

Materials Engineering inside Carbon Nanotubes

Rudolf Pfeiffer

University of Vienna, Faculty of Physics, Boltzmanngasse 5, Wien 1090, Austria

e-mail: rudolf.pfeiffer@univie.ac.at

Research on carbon nanotubes (CNTs) is now in its second decade and Raman spectrsocopy was a main tool for unravelling many of their unique optical properties. From a materials engineering standpoint, one of the most interesting properties of CNTs is that they have an interior which can be filled with various molecules and in which chemical reactions inside a 1D nano cleanroom can be studied. The most prominent examples are C_{60} peapods, i.e. C_{60} fullerenes filled into single-wall CNTs, and their reaction to double-wall CNTs (DWCNTs) at temperatures around 1200 °C. We used Raman spectrsocopy and x-ray diffraction to study this growth process in detail [1]. Several other carbon-rich precursor molecules were subsequently filled into the tubes and further transformed into DWCNTs. A very interesting molecule in this regard is ferrocene, which gives rise to a completely different growth process (already at 600 °C) for the inner tubes than C_{60} (catalytic vs. non-catalytic growth). [2] Another important point is the engineering of the distance between the encaged molecules inside the tubes. Especially for 1D spin chains having control over the spin separation is crucial. In this presentation we will show how Raman spectroscopy together with other techniques can be used to characterize and analyze all these various materials.

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9:30 Oral

Raman scattering study of CdSe nanorods

Holger Lange[1], Christian Thomsen[1], Ulrike Woggon[2]

1. *Institut für Festkörperphysik, TU Berlin, Hardenbergstr. 36, Berlin 10623, Germany* **2.** *Fachbereich Physik, Otto-Hahn-Str. 4, Dortmund 44227, Germany*

e-mail: holger.lange@physik.tu-berlin.de

Raman scattering experiments are a versatile method to characterize different aspects of nanostructures.

We present Raman spectra from CdSe nanorods of various sizes and discuss features that can be extracted from them.

In particular the nanorod diameter can be estimated from the frequency of the radial breathing mode, similar to carbon nanotubes. ab-initio calculations of CdSe nanowires indicate the presence of this fully symmetric vibrational mode which's frequency is highly diameter dependent. This mode can be characterized by Raman spectroscopy and is especially interesting for very small structures. The RBM frequency rises for decreasing diameter, which makes it experimentally easier to detect, while other suitable techniques like high resolution transmission electron microscopy become more sophisticated. Another discussed feature is the exciton-phonon coupling strength. The coupling strength in nanorods can be deduced from the integrated intensities of the Raman bands and their overtones. Simultaneous measurement of the fundamental and overtone allows the study of e.g. the size dependence of the coupling strength. We find an increasing coupling strength for decreasing nanorod diameter in the diameter regime from 2-10 nm, while still being lower than the coupling strength in bulk material. This is explained within a model for spherical nanocrystals. Couplings to higher frequency phonons increase for smaller structures while the coupling strength compared to bulk material is reduced due to the decreased Coulomb interaction and confinement effects.

9:45 Oral

Low-frequency Raman Spectroscopy of Pure and La-doped TiO_2 Nanopowders Synthesized by Sol-gel Method

Maja J. Šćepanović[1], Sonja Aškrabić[1], Vesna I. Berec[1], Aleksandar V. Golubović[1], Zorana D. Dohcevic-Mitrovic[1], Aleksandar Kremenovic[2], Zoran V. Popovic[1]

1. *Institute of Physics (IF), Pregrevica 118, Belgrade 11080, Serbia* **2.** *Faculty of Mining and Geology, Laboratory for Crystallography, University of Belgrade,, Djusina 7, Belgrade, Belgrade 11000, Serbia*

e-mail: maja@phy.bg.ac.yu

Pure and La-doped titania (TiO_2) nanopowders are synthesized by sol-gel technology. The crystallite sizes determined by XRD measurements range from 10 and 15 nm. Dependence of structural and morphological characteristics of nanopowders on synthesis conditions and La^{3+} content is investigated by Raman spectroscopy. Very intensive modes observed in Raman spectra of all nanopowder samples are assigned to anatase phase of TiO_2. Additional Raman modes of extremely low intensity can be related to the presence of small amount of brookite amorphous phase in nanopowders, which is in accordance with the results of XRD structural analyses. The particle size distribution in TiO_2 nanopowders was estimated from the low frequency Raman spectra, using the fact that the phonon modes in nanosized TiO_2 observed in the low frequency region ($\omega < 40$ cm^{-1}) can be well described by the elastic continuum model, assuming that nanoparticles are of perfect spherical shape and isotropic. The nanosized particle distribution obtained by this method is used for the calculation of the frequency and shape of the most intensive E_g Raman mode in anatase TiO_2 by the phonon confinement model. The calculated broadening of this mode, associated with the particle size distribution, coincides well with the characteristics of E_g mode observed in measured Raman spectra of TiO_2 nanopowders. This confirms the Raman spectroscopy method as a powerful tool for determination of particle size distribution in nanosized materials.

10:00 Oral

Optical Control of Molecular Magnets

Tom Lummen, Esther Vertelman, Petra Van koningsbruggen, Ria Broer, Regis Gengler, Petra Rudolf, Paul Van Loosdrecht

Zernike Institute for Advanced Materials, Nijenborgh 4, Groningen 9747AG, Netherlands

e-mail: p.h.m.van.loosdrecht@rug.nl

A variety of applications require control of the physical state of matter using, for instance, optical techniques. In order to achieve this, one would like to design novel, functional materials capable of changing for instance their magnetic state or their optical properties upon application of external optical stimuli. One of the most promising materials in this field are the transition metal polycyanides (Prussian Blue Analogues) which posses an electronic and magnetic bistability over a broad range of temperatures, even close to room temperature, which allows for optical switching of both the magnetic as well as the optical properties. Raman spectroscopy of the CN vibrations is a very sensitive probe for the physical state of the materials, since this bistability involves a charge transfer between the CN bridged 3d elements. Optically induced switching of one such system ($RbMn[Fe(CN)_6]\cdot H_2O$) has been observed using Raman spectroscopy, XPS, and direct imaging techniques. In addition, Magnetic, Mössbauer and Raman measurements on single crystals [1] reveal that only ~ 50 % of the magnetic entities change their properties, which is suggested to be due to an intrinsic presence of two distinct crystal sites.

[1] Esther J. M. Vertelman *et al.* Chem. Mater. **20**, 1136 (2008)

10:15 Oral

Investigation of structural and interfacial defects in oriented $LiNbO_3$ thin films

Swati Shandilya, Monika Tomar, Kondepudy Sreenivas, Vinay Gupta

Department of Physics and Astrophysics, University of Delhi, Delhi 110007, India

e-mail: swatishandilya@rediffmail.com

Lithium Niobate ($LiNbO_3$) is one of the most ideal candidate for electro-optic, optical waveguide and SAW devices because of its good electro-optic, piezoelectric, pyroelectric, photo-elastic and non-linear optical properties. $LiNbO_3$ in thin film offers great advantages over the bulk because of producing high electric field with low applied voltage, the possibility to produce step-index profiles and ease introduction of dopant. It is desirable to grow $LiNbO_3$ films with c-axis orientation to couple the large eleectro optical and non- linear optical coefficients along this direction

In this work highly *c*-axis oriented $LiNbO_3$ films have been deposited by pulsed laser deposition technique on the silicon substrate using a transparent conducting Al doped ZnO inter-layer. X-ray diffraction and Raman spectroscopic analysis show the fabrication of single phased $LiNbO_3$ films with minimal intrinsic defect structure under the optimized deposition conditions. The presence of possible intrinsic defects in the films deposited under varying processing conditions has been investigated and correlated with the presence of superfluous peaks in Raman spectra. Dielectric properties of the $LiNbO_3$ films deposited under the static and rotating substrate mode have been studied in the metal-insulator-metal configuration. Films deposited under the rotating substrate mode are found to result in dielectric properties close to the single crystals and attributed to the further reduction in the intrinsic and interfacial defects. The origin of the possible defects and its influence on the optical and structural properties of the films has been discussed.

Coffee break

Main Hall
Thursday morning, 18 September, 10:30

Parallel Session

Thursday morning, 18 September, 11:00
Room 315

11:00 Invited oral

Micro-Raman and XAS study of V_2O_5 and WO_3 nanostructured thin films for electrochromic applications

Danilo Bersani[1], Alessandro Cremonesi[2], Gianluca Calestani[2], Pier Paolo Lottici[1]

1. *Dipartimento di Fisica, Università, Viale G.P. Usberti 7/a, Parma 43100, Italy* **2.** *Dip. Chimica Generale ed Inorganica, Chimica analitica, Chimica fisica (GIAF), V.le G. Usberti, Parma 43100, Italy*

e-mail: danilo.bersani@fis.unipr.it

Tungsten oxide is the most widely studied electrochromic (EC) oxide due to his mixed oxidation states; V_2O_5 is a good candidate to form counter electrodes in EC devices, having high ion storage capacity and providing a coloration complementary to the tungsten oxide. Nanocrystalline oxides are expected to show improved EC performances during the optical switching process. In order to develop low-cost and low-environmental impact synthesis routes, macro-porous vanadium and tungsten oxides films were produced by sol–gel method with the addition of different structure-directing agents.Micro-Raman spectroscopy was employed for the determination of the phases and XAS measurements were performed to study the local order. SEM was used to study the films morphology.A first series of samples was deposited directly on soda-lime glass substrates using polyethylenglycol (PEG) as templating agent. At low temperatures spherical shaped mesostructure (in tungsten oxide) and ribbons (in vanadium oxide) are observed. After heating, many different phases arise, due to the interaction with the soda lime substrate: together with minor stoichometric V_2O_5 and WO_3, hydrous phases and bronzes are obtained, not suitable for EC applications. The structure of the sodium vanadate $Na_2V_2O_6$ is refined from the EXAFS data. A second series of films was deposited on glass substrates covered with ITO (indium tin oxide) in order to avoid the diffusion of alkali ions, using four different surfactants. In the new series the heating treatments from 250 to 500 °C give pure orthorhombic V_2O_5 or monoclinic WO_3, with very good homogeneity of the films.In vanadium oxide the strong anisotropy of the crystalline network leads to unidirectional growth: nanorods and nanobelts are observed. In tungsten oxide the effect of the surfactant gives mesostructures composed by micro-sphere aggregated to give a network of filaments. All the obtained structures are well suitable for EC applications.

11:30 Invited oral

Optically induced phase transition on Bi and Sb single crystal

Daniele Fausti[1], Oleg Misochko[2], Paul Van Loosdrecht[1]

1. *Zernike Institute for Advanced Materials, Nijenborgh 4, Groningen 9747AG, Netherlands* **2.** *Institute of Solid State Physics, Russian Academy of Sciences (ISSP RAS), Institutskaja,2, Chernogolovka 142432, Russian Federation*

e-mail: d.fausti@rug.nl

When writing data to a dvd, your dvd-drive does something really interesting: it optically induces a phase transition in the active material of your dvd. This is an example of the much broader, rapidly developing field of optically induced changes in condensed matter. The present contribution focuses on optically induced phenomena in the semimetals bismuth and antimony. The structure of these semi-metals is not the usual cubic one, as found in other simple metals, but rather a distorted one called the arsenic-A7 structure. The origin of this distortion lies in the electron-phonon interaction, and in particular depends on the charge density in the conduction band of these materials. At a high enough density this distortion should vanish, leading to a cubic phase, and one would expect that it is possible to induce a phase transition to this state by photo-doping. Recent experiments, using direct probing of the phonon excitation spectrum via time resolved optical pump/Raman probe spectroscopy, have shown that one can indeed reduce the distortion by photo-doping. Moreover, they yield strong indications for an optically induced phase transition in the semimetals, albeit that it does not appear to be a transition to the cubic phase. Apart from introducing the novel experimental technique, the observed transient phonon spectra of Bi and Sb will be discussed in terms of thermal and non-thermal effects, and screening of the crystal potential by the photo induced charge density in the conduction band.

Finally, the experimental evidence for, and the nature of the observed phase transition will be discussed.

12:00 Oral

Ab initio calculation of the Raman spectrum of $Li_2SrTa_2O_7$ using generalized forces and symmetry coordinates

Thierry Pagnier

LEPMI, 1130 rue de la Piscine, Saint Martin d'Hères 38402, France

e-mail: thierry.pagnier@lepmi.inpg.fr

In spite of an increasing efficiency of the ab initio DFT codes, the calculation of Raman spectra of crystals is still uncommon. Whatever the method, e.g. frozen phonons for the VASP/Phonon couple, second derivatives calculation for Abinit, the calculation starts with the determination of the whole dynamical matrix and its diagonalization. If the dynamical matrix elements are expressed in the basis of the displacements of all atoms in the x, y, and z directions of a fixed coordinate system, it has no special symmetry and the dynamical matrix diagonalization can be very difficult. Moreover, if one in only interested in the Raman bands, the calculation of the whole dynamical matrix is not necessary.

A new method has been developed, using atom displacements along the symmetry coordinates bases of the Raman active irreducible representations. If S_i and S_j are two symmetry coordinates bases of the same irreducible representation, the dynamical matrix element $D_{ij}=\partial^2E/(\partial S_i\partial S_j)$ can be calculated from the forces observed in the S_j direction when atoms are moved according to S_i. If S_i and S_j are bases of different irreducible representations, the corresponding D_{ij} is zero by definition. The method described here allows therefore the calculation of a block-diagonalized matrix. Band frequencies and normal mode displacements can then be calculated independently for each symmetry.

This technique has been applied to $Li_2SrTa_2O_7$, a Ruddlesden-Popper-type oxide which structure and Raman spectrum have been recently obtained (1). The DFT code was Abinit (2), in the Local Density Approximation (LDA) framework. Despite the known limitations of this technique, a good fit with the experimental data has been obtained.

(1) T. Pagnier, C. Galven, F. Le Berre, M.P. Crosnier-Lopez, ICORS 2008, Uxbridge, West London, UK 17-22 august 2008

(2) www.Abinit.org

Dr F. Le Berre and M.P. Crosnier Lopez are kindly acknowledged for having provided the $Li_2SrTa_2O_7$ samples.

12:15 Oral

Raman spectroscopy for the analysis of temperature-dependent plastic relaxation of SiGe layers

Fabio Pezzoli[1], Emiliano Bonera[1], Monica Bollani[1], Stefano Sanguinetti[1], Emanuele Grilli[1], Mario Guzzi[1], Giovanni Isella[2], Daniel Chrastina[2], Hans Von Känel[2]

1. *University of Milano-Bicocca, Department of Materials Science, via Cozzi 53, Milano 20125, Italy* **2.** *LNESS and Dipartimento di Fisica del Politecnico di Milano, via Anzani 42, Como 22100, Italy*

e-mail: fabio.pezzoli@mater.unimib.it

Novel architectures for electronics and photonics are expected to be developed using the forthcoming SiGe technology. However, in SiGe-based heterostuctures, material and design issues rely on accurate control of strain and composition of the alloy. Raman spectroscopy has rapidly emerged as a reliable technique to the quantitative determination of such parameters on a sub-micrometric scale. In particular, we demonstrated that Raman spectroscopy enables measurements of concentration and strain with a sensitivity comparable to that of x-ray diffraction.

In this work we present an investigation of the effects of the growth conditions of SiGe graded layers on dislocation nucleation and interaction. In particular, we focus on the crucial role the deposition temperature plays in the dislocation kinetics. The analysis of threading dislocation densities is accompanied with a quantitative measurement of the residual strain in SiGe/Si heterostructures, which is carried out by means of Raman scattering. Our approach is effective to study the physical mechanism governing dislocation multiplication and the sharp transition from a state of brittleness to a state of ductility within a narrow temperature window.

Lunch break

Inner Courtyards
Thursday afternoon, 18 September, 12:30

Parallel Session

Thursday afternoon, 18 September, 14:00
Room 315

14:00 Invited oral

Non-linear Raman spectroscopy of molecular hydrogen

Michele Marrocco

ENEA, via Anguillarese 301, Roma 00123, Italy

e-mail: michele.marrocco@casaccia.enea.it

The non-linear optical response of a medium can be used to explore the fundamental physical properties of molecules. In the present work, coherent anti-Stokes Raman spectroscopy is employed to investigate the intra-molecular interaction caused by the vibration-rotation coupling, whose effect is of great importance in the precise determination of spectroscopic strengths of very light molecules. More precisely, the coupling is defined by the so-called Herman-Wallis (HW) factor $F = |\langle v,J|O|v',J'\rangle|^2 / |\langle v,J|O|v',J'\rangle|^2$ where O is the operator responsible for the rovibrational molecular transition [1]. Although the Herman-Wallis factor is well known, its calculation is not easy and, in the literature, either the correction is not considered at all, or different authors suggest different Q-branch HW factors in manifest disagreement with each other.

To gain more insight into the problem, an experiment based on vibrational CARS applied to H_2 molecules is illustrated [2]. Here, the measured spectroscopic strength for the line Q(7) is compared with the calculated line strengths obtained from different HW factors found in the literature. The idea behind this experimental proof is very simple. The spectra have been acquired from a flat flame produced in a Hencken burner fed with H_2 and air. Since the flame is very stable and works under adiabatic conditions, the flame temperature is well known and its maximum value is at stoichiometric condition. On the other hand, the acquired CARS spectra are temperature dependent and they can be fitted with theoretical spectra that incorporate the given temperature and, alternatively, the expressions of different HW factors. The conclusion of this analysis clearly shows that the experimental results help in the determination of the most reliable factor needed to define the non-linear Raman spectra of hydrogen.

[1] R. Herman and R. F. Wallis, J. Chem. Phys. **23**, 637 (1955).

[2] M. Marrocco, Chem. Phys. Lett. **442**, 224 (2007).

14:30 Oral

High Resolution, High Speed Confocal Raman AFM Imaging of Heterogeneous Materials

Ute Schmidt, Jan Toporski

WITec GmbH, Hoervelsingerweg 6, Ulm 89081, Germany

e-mail: ute.schmidt@witec.de

Raman imaging is a rapidly evolving technology for noninvasive chemical imaging of microscopic composites and biological materials. The power of Raman imaging stems from the high chemical information content of molecular vibrational spectra. However, Raman spectroscopy is an inelastic light scattering process and therefore the acquisition of Raman spectra is the time limiting factor in Raman imaging. By combining an ultrahigh throughput confocal microscope with an extremely sensitive spectroscopy system the integration time for the acquisition of Raman spectra can be reduced below 100 milliseconds. This short integration time enables the acquisition of arrays of thousands of complete Raman spectra within minutes. The confocal setup reduces in addition unwanted background signals, enhances contrast and provides depth information. The images are evaluated from the two dimensional array of the collected Raman spectra by isolating spectral characteristics such as peak intensity, width, position, etc. Differences in chemical composition, although completely invisible in optical images, will be apparent in the Raman image and can be analyzed with a resolution down to 200 nm. If higher resolution is required, by simply turning the microscope turret, the confocal Raman microscope can be transformed in to an AFM. Using this imaging technique, structures below the diffraction limit can be visualized from the same sample area.

Aim of this contribution is to present the key features required for high speed confocal Raman microscopy and to prove its capabilities with Raman and AFM images obtained on composite materials and polymeric films.

14:45 Oral

Raman spectroscopic evidence of a coherent room temperature hybrid structure of $BaTiO_3$ single crystal

Efthymios P. Liarokapis[1], Anastasios Antonakos[1], Akira Kojima[2], Yukio Yoshimura[3]

1. *National Technical University of Athens (NTUA), Heroon Polytechneiou 9, Athens 157 80, Greece* **2.** *Department of Material Science, The University of Shiga Prefecture, Hikone 522-8533, Japan* **3.** *Faculty of Science and Engineering, Ritsumeikan University, Nojihigashi Kusatsu-shi 525-8577, Japan*

e-mail: eliaro@central.ntua.gr

Recently, a precession X-ray study has discovered that ferroelectric $BaTiO_3$ single crystals have a coherent hybrid structure (CHS) that consists of tetragonal and monoclinic lattices that share the (101) face of the tetragonal [1,2]. Microscopic observations attest that the single crystal has two kinds of stripes (grey and yellow regions). Raman spectra were measured at room temperature in a backscattering geometry on a 4x4x4 mm^3 single crystal, with the sample placed under the microscope with ×10, ×40 and ×100 magnifications. The difference of the relative intensities between the different magnifications at the 90° domain indicates that the stripes consist of several elongated domains, which are consistent with the CHS. Two kinds of domains have been observed by the Raman measurements, which are identified as light and dark spots under the optical microscope. Raman spectra of all sides of the cubic crystal have been collected at several scattering configurations. The spectra structures and line-widths are strongly affected when the laser direction is parallel to the b-axes and the polarization parallel to the a- or c-axes of the 90^o domain (ac-side). It appears that there is a symmetry reduction, which affects the polarization selection rules of the Raman active phonons. The results are in agreement with the coexistence of the two (tetragonal and monoclinic) lattices.

References

[1] Y. Yoshimura, A. Kojima, N. Tokunaga, K. Tozaki, T. Koganezawa, Phys. Lett. A **353**, 250 (2006).

[2] Y. Yoshimura, M. Morioka, A. Kojima, N. Tokunaga, T. Koganezawa, K. Tozaki, Phsy. Lett. A 367, 394 (2007).

15:00 Oral

Raman spectroscopy and magnetic properties of bulk $Zn_{0984}Co_{0.016}O$ crystal

Wojciech Szuszkiewicz[1], Jean-Francois Morhange[2], Andrzej Lusakowski[1], Zbigniew Golacki[1], Monika Arciszewska[1], Beata B. Brodowska[1], Marcin Klepka[1], Witold Dobrowolski[1]

1. *Polish Academy of Sciences, Institute of Physics, al. Lotników 32/46, Warszawa 02-668, Poland* **2.** *Institut des nanosciences de Paris (INSP), 140 rue de Lourmel, Paris 75015, France*

e-mail: szusz@ifpan.edu.pl

An analysis of the structural and magnetic properties of bulk $Zn_{0984}Co_{0.016}O$ mixed crystal have been performed using Raman scattering and magnetization measurements. The exact Co content in crystals grown by chemical vapour transport was determined using an electron microprobe. The optical measurements were performed at several temperatures between 15 K and 295 K, the magnetic properties were investigated in a wide temperature range from 5 K to 295 K.

Beside the phonons characteristic for the ZnO host lattice, in the Raman spectra we observed a disorder-induced lattice vibration modes and a structure which was assigned to a local vibration mode of the Co impurity. Moreover, in the Raman spectra we also observed lines resulting from light scattering on phonons in hcp-Co and on magnons in CoO. This may be considered as an experimental confirmation of the presence of such precipitates in the investigated sample. The temperature dependence of the Raman spectra confirms this interpretation.

Apart from the high frequency structures mentioned above, we observed also two lines in the low frequency region (at 5 cm^{-1} and at 13 cm^{-1}). The first line may be ascribed to the splitting of the ground state of Co^{2+} ion in the crystal field of wurtzite symmetry. The second line may be due to the ground state splitting of Co^{2+} ion in CoO. Some other explanations, like possible presence of other precipitates ($ZnCo_2O_4$) or local deformation of Co^{2+} ion neighborhood are also analyzed and discussed.

Finally, we discuss an influence of precipitates on the magnetization of the sample.

15:15 Oral

Distorted forms of metalloporphyrins probed by Raman and high resolution luminescent spectroscopy

Aleksandr S. Starukhin[1,2], Mikalai M. Kruk[1], Jacek Waluk[2]

1. *B.I. Stepanov Institute of Physiscs National Academy of Sci. of Belarus (IF), Independence Av., 68, Minsk 220072, Belarus* **2.** *Polish Academy of Sciences, Institute of Physical Chemistry, Kasprzaka 52/56, Warszawa 01-224, Poland*

e-mail: astar@imaphbas-net.by

In our report the spectral manifestation of different spectral forms obtained for Mg-, Zn-, Pd- and Pt-porphins in different solid matrices at cryogenic temperatures have been discussed. The planar and two kinds of distorted conformations of Mg-, Zn-porphins in highly-resolved fluorescence spectra were detected. Distorted forms of “saddle” and “dome” types have been detected in the luminescence and absorption spectra. For Zn-porphin distorted forms have been detected in the fluorescence and phosphorescence spectra simultaneously. In the phosphorescence spectra of the Pd- and Pt-porphins the manifestation of the two forms in the ground state has been proved also. Energy splitting in the phosphorescence spectrum of the Pd-porphin in n-octane at 4,2 K comes to 78 cm^{-1} for two forms. Under selective excitation in singlet-singlet channel the large set of sharp lines was detected for each of two forms and vibrational frequencies have been determined. In highly-resolved phosphorescence spectra of Pt-porphin in n-octane at 4,2 K we have detected similar manifestation of the two spectral forms in the phosphorescence spectrum. The set of temperature activated bands in phosphorescence spectra were found. Analysis of phosphorescence spectra at elevated temperatures and excitation of phosphorescence spectra under direct excitation in the singlet-triplet channel make possible the value of zero-field splitting of quasi-degenerate triplet states for two forms to be determined. The splitting values in n-octane matrix amount to 40 and 57 cm^{-1} for planar and nonplanar conformations of PdP, respectively. To estimate the type of molecule distortion the information about the frequencies of vibronic modes from well-resolved spectra of metalloporphins have been used. For distorted forms of metalloporphyrins the greatest shifts are observed for the lines in the range 1500-1650 cm^{-1} that well correlate with data of resonance Raman spectra of metalloporphyrins with Ni, Pd, Fe, Zn etc..

Coffee break

Main Hall
Thursday afternoon, 18 September, 15:30

Parallel Session

Thursday afternoon, 18 September, 16:00
Room 315

16:00 Invited oral

Development of a new ultrahigh vacuum tip-enhanced Raman scattering (UHV-TERS) experimental setup

Niculina Peica[1], Serge Roehrig[2], Andreas Ruediger[2]

1. *Central Division of Analytical Chemistry, Research Center Juelich (ZCH), Leo-Brandt Strasse., Jülich 52425, Germany* **2.** *Research Centre Jülich, Institute of Solid State Research (IFF), Jülich, Germany*

e-mail: n.peica@fz-juelich.de

Tip-Enhanced Raman Spectroscopy (TERS) is a high-sensitivity and high spatial-resolution analytical technique based on the strong field enhancement provided by a sharp metallic tip. TERS holds the promise for a structural and chemical analysis of insulators on the nanoscale, where established techniques like AES are blurred due to surface charge accumulation. In order to conduct spectroscopy sensitive to ambient conditions on a variety of specimens, the use of an UHV environment is mandatory. Using a commercial non-contact Atomic Force Microscope (AFM) combined with a confocal optical setup in reflection geometry, we are targeting samples on non-transparent electrodes. The resulting design challenges with respect to quantum efficiency, optical accessibility of the tip and the optics themselves, e.g. numerical aperture and stability, were balanced and taken into consideration for the presented UHV-TERS setup. The entrance window to the UHV environment has been found to only influence the measured Raman spectra due to reflection losses. No influence due to birefringence or tension in the window was observed. Combining various laser wavelengths with different tip coatings provides a powerful analysis tool for a large variety of samples.

16:30 Invited oral

Pushing the Limits of Raman Microscopy towards Nanomaterials Analysis and Fast Imaging

Renata Lewandowska

Horiba Jobin Yvon, Rue de Lille, Villeneuve d'Ascq 59650, France

e-mail: renata.lewandowska@jobinyvon.fr

Raman microscopy has become an important tool for materials analysis, providing crucial information to experimentalists working in the fields of semiconductor, ceramics or composite materials. The unique confocal and spatial resolution of micro-Raman systems enables optical far field resolution to be pushed to its limits with often sub-micron resolution achievable for chemical imaging of small structures.

The next step to material analysis on a smaller scale is the combination of Raman spectroscopic analysis with near field optics and Atomic Force Microscopy (AFM). This combination enables nanometric topographical information to be coupled to chemical information. Unique designs enable Raman measurements to be made upon different AFM units for the exploration of new and evolving techniques such as nanoRaman spectroscopy based on the TERS (tip enhanced Raman spectroscopy).

Raman Imaging is sometimes seen as rather slow in comparison to other techniques such as NIR or Fluorescence. Now, things have evolved much further, pushing the limits of systems to obtain high quality Raman images with unprecedented acquisition speeds. Recent advances in detection and hardware communication enable us to reach measurement times as low as a few ms/point, opening the door to quasi-instantaneous chemical imaging.

In addition, HORIBA Jobin Yvon has launched a new imaging mode, the revolutionary DuoScan^{TM} (patent pending), which offers the best of both the micro and the macro world, as it generates Raman maps across both µm-scale and cm-scale areas with FULL coverage of your sample. When looking at large sample surfaces to measure component distribution or to search for contaminants, it often comes down to finding a needle in a haystack. The DuoScan allows you to vary the spot size from 1 µm to 300 µm to match your image pixel size, ensuring that you don't miss a spot.

Examples emphasizing Raman capabilities in the field of semiconductor or carbon materials will be discussed.

17:00 Invited oral

Numerical simulations of Raman spectra as a tool in nanomaterial science

Malgorzata Makowska-Janusik

Institute of Physics, Jan Dlugosz University, Al. Armii Krajowej 13/15, Częstochowa 42200, Poland

e-mail: m.makowska@ajd.czest.pl

Nanocrystalline semiconductors are promising materials due to their versatile electronic and optical size-dependent properties significantly different from those of the corresponding bulk-like lattice. Their investigation has recently caused considerable experimental and theoretical interest. Powerful optical methods for study the electronic property of nanograins contains technique as: fluorescence, Raman scattering or electroluminescence. The Raman spectra are closely dependent upon the microstructure of the material, size and surface reconstruction of crystalline arrangement. The vibrational properties of nanosized heteroatom particles XY also change as the results of X/Y ratio. An analysis of experimentally obtained Raman spectra is difficult because of different stoichiometry of nanocrystallites and their amorphisation at the surface. Because of mentioned reason, the theoretical calculations may be helpful in analysis and explanation of experimentally obtained results. The theoretical frequencies allow a quantitative assignment of the experimental spectrum details. However, the calculation of Raman spectra of crystals and especially nanocrystallites are still uncommon. In the presented speech the simulations of the Raman spectra of nanocrystalline silicon carbide will be discussed. Performed calculations implement cluster approach for the computations of electronic property of SiC nanocrystals possessing different diameter, stoichiometry and Si/C ratio. Presented technique of computational methods includes *ab initio*, DFT and semi-empirical methods and compares their results. The implemented approach presents the solution of the boundary space restriction problem and the surface reconstruction effect. All theoretically obtained results are compared to the experimental data published earlier and presented in connection with other results receiving for organic materials, especially macromolecules.

Friday, 19 September

E-MRS & EPDIC Joint Plenary Session

Friday morning, 19 September, 9:00
Small Hall (237)

Coffee break

Main Hall
Friday morning, 19 September, 10:30

Parallel Symposia

Friday morning, 19 September, 11:00
Room 315

11:00 Invited oral

Magnetoplasma and impurity excitations in GaAs studied by resonant Raman scattering in high magnetic fields

Andrzej Wysmolek

University of Warsaw, Institute of Experimental Physics (IFDUW), Hoża 69, Warsaw 00-681, Poland Grenoble High Magnetic Field Laboratory, CNRS (GHMFL), 25 Avenue Des Martyrs BP166, Grenoble 38042, France

e-mail: Andrzej.Wysmolek@fuw.edu.pl

Plasmonic and shallow donor excitations in *n*-type GaAs are studied in extreme magnetic-fields (up to 28T) using the method of inelastic light scattering (Raman scattering). [1] The strength of magnetic field was sufficient to made cyclotron frequency comparable to all important frequencies in the system, namely the plasma frequency, and the frequencies of longitudinal (LO) and transverse (TO) optical phonons. The physics of mixed plasma and phonon excitations under these particular and interesting conditions has never been fully explored in Raman scattering experiments.

Experimental data are analyzed using a standard, dielectric function theory. Results obtained for samples with high electron concentration are well understood in terms of observation of longitudinal, plasmon-phonon excitations. A strong interaction of coupled LO-phonon-plasmon modes with the collective cyclotron resonance excitations (Bernstein modes) is observed.
In samples with lower electron concentration, the unexpected feature in the vicinity of the undressed optical phonon is observed at high magnetic fields. This effect is explained in terms of transverse excitations, which can appear in the Raman spectrum due to disorder-activated selection-rule breaking. A field induced metal-insulator transition GaAs is shown to be traced with Raman scattering experiments in samples with the lowest electron concentration. In the insulating state, the repulsion (magnetopolaron effect) is observed between the intra-donor 1s-2p excitation and the LO-phonon mode. This is explained in terms of Fröhlich interaction. Interestingly, the analogous effect involving the cyclotron resonance excitation is not observed in the metallic phase. Our observation may give some additional insight into the physics of the resonant magnetopolaron effect, which has been recently reviewed in two-dimensional systems.

11:30 Oral

Raman and IR study of chalcohalide Ge-S-AgI glasses

Ofeliya Kostadinova[2], Tamara Petkova[1], Boris Monchev[1], Plamen Petkov[3], Soghomon Boghosian[2], Spyros Yannopoulos[2]

1. *Institute of Electrochemistry and Energy Systems (IEES), Acad.G.Bonchev str.Bl.10, Sofia 1113, Bulgaria* **2.** *Foundation for Research and technology-ICEHT, Patras, Greece* **3.** *Uniersity of Chemical Technology and Metallurgy (UCTM), 8, Kl.Ohridsky Blvd, Sofia 1756, Bulgaria*

e-mail: tpetkova@bas.bg

Glasses that contain both chalcogen and halogen atoms, known as chalcohalide glasses, have attracted considerable attention in view of their IR transparency and other photonic properties. Novel glasses from the chalcohalide system $(AgI)_x\ (GeS_{1.5})_{100-x}$ with atomic ratio S/Ge=1.2 and 1.5 and AgI content $5 \leq x_{AgI} \leq 20$ have been synthesized. Structural information for these glasses has been obtained by studying their vibrational properties by Raman and FTIR spectroscopy. The combination of these complementary techniques enabled us to identify the structural units building up the glassy network and elucidate the role of AgI as component of the $(AgI)_x\ (GeS_{1.5})_{100-x}$ quasi binary system.

The structure of Ge–rich glassy matrix is composed of mixed GeS_nGe_{4-n} tetrahedra, being appreciably different than that of the stoichiometric GeS_2 glass. The addition of AgI causes considerable structural changes due to the distinctive roles of silver and iodine. The network terminating role of iodine atoms, as well as the presence of silver cations and their impact on vibrational modes are discussed and compared with literature data on similar chalcohalide glasses.

11:45 Oral

Atomic Force Microscope Combined With Confocal Raman Microscopy – a Tool for Subwavelength Optical Resolution

Pavel Dorozhkin, Alexey Schekin, Artem Shelaev, Evgenii Kuznetsov, Victor Bykov

NT-MDT Co., Build. 100, Zelenograd Moscow 124482, Russian Federation

e-mail: dorozhkin@ntmdt.ru

We demonstrate various applications of confocal Raman/fluorescence microscope integrated with Atomic Force Microscope (AFM). Firstly, we report on “classical” applications of such combination, where 2D AFM and confocal Raman maps are acquired simultaneously from the *same* part of the sample, but “independently” one from another. Physical characterization and modification capabilities of AFM merge with chemical resolution of confocal Raman microscope and general capabilities of optical microscope to provide complete information about sample investigated. We demonstrate results on various promising nanoelectronics materials: carbon nanotubes, semiconductor nanowires etc. Graphene flakes (a few monolayers of graphite) are studied. AFM topography and phase pictures combined with Raman spectroscopy of the *same* sample area allow one to distinguish flakes of different thickness (down to single layer flake) and analyze flake’s structural uniformity. Advanced AFM techniques such as Kelvin probe microscopy and Electrostatic force microscopy applied to the same flake give further insight into its physical properties.

The ultimate goal of integrating AFM with Raman/fluorescence spectroscopy is to break diffraction limit and to bring spatial resolution of optical methods down to resolution of AFM (a few nm). We will focus on the results of Tip Enhanced Raman Scattering (TERS) experiments – where Raman signal from narrow sample area below the metallized AFM tip is resonantly enhanced due to interaction with plasmons localized at the tip apex. The resulting resolution of 2D Raman mapping is about 60 nm that goes far beyond the optical diffraction limit. Different materials are studied: carbon nanotubes, dielectric films, C60 layers etc. Both etched gold wires and silver coated cantilevers are used for localized enhancement of electromagnetic field. Special emphasis is put on the difference between transmission (transparent samples) and reflection (opaque samples) TERS geometries.

Lunch break

Inner Courtyards
Friday afternoon, 19 September, 12:30

Posters

Monday, 15 September

Joint Poster Session 1

Monday & Wednesday
Monday afternoon, 15 September, 16:00
Main Hall

16:00 Poster A01

Confinement and morphological effects on the Raman response of porous silicon: theory and experiment

Adriana Cazares[1], Monserrat Bizarro[1], Miguel Cruz-Irisson[2], Chumin Wang[1]

1. *Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico (UNAM), A.P. 70-360, México 04510, Mexico*
2. *ESIME-Culhuacan, Instituto Politécnico Nacional (IPN), Av. Santa Ana 1000, México 04430, Mexico*

e-mail: monserrat@iim.unam.mx

The Raman scattering in porous silicon (PSi) is modeled by means of a local bond-polarization model based on the displacement-displacement Green’s function within the linear response theory, where the Born potential is used, including central and non-central interatomic forces [1,2]. Using the supercell method, the ordered pores are produced by removing columns of Si atoms from a crystalline silicon (c-Si) structure [3]. On the other hand, the samples of PSi are obtained by anodizing p^--type (001)-oriented c-Si wafers in a hydrofluoric acid bath [4]. The morphology of PSi samples at nanometric scale is characterized by the atomic force microscopy (AFM). Both theoretical and experimental results show a notable shift of the main Raman peak towards lower energies, in comparison to the bulk c-Si signal. This shift is quantitatively analyzed within the quantum confinement framework and the morphological effects are also discussed.

[1] R.J. Elliott, J.A. Krumhansl, and P.L. Leath, *Rev. Mod. Phys.***46**, 465 (1974).

[2] C. Wang and R.A. Barrio, *Phys. Rev. Lett.***61**, 191 (1988).

[3] P. Alfaro, M. Cruz and C. Wang, *Nanoscale Res. Lett.***3**, 55(2008).

[4] R. Cisneros. C. Ramirez, and C.Wang, *J. Phys.:Condens.Matter.***19**, 395010 (2007).

16:00 Poster A02

Use of Phonon Confinement Model in Simulation of Raman Spectra of Nanostructured Materials

Mirjana Grujić-Brojčin, Maja J. Šćepanović, Zorana D. Dohcevic-Mitrovic, Zoran V. Popovic

Institute of Physics (IF), Pregrevica 118, Belgrade 11080, Serbia

e-mail: myramyra@phy.bg.ac.yu

The simulation of Raman spectra is an important technique in systematic characterization of nanostructured materials. The effects of frequency shift and asymmetric broadening play an important role in modeling the spectra. Several approaches for calculating Raman spectra by using phonon confinement model are discussed in this work. The phonon confinement model is considered both from the viewpoint of different confinement function and the confinement strength, as well as the dimensionality of the confinement model. The influence of particle size distribution on the shape of the spectra is discussed and some possible distributions such as Gaussian, asymmetric Gaussian and log-normal distribution are compared. The phonon dispersion relations and the choice of the approximation of its shape are also studied. The results of the phonon confinement model are compared to experimental spectra of CeO_2 and anatase TiO_2 nanopowders, with particle size about 7 and 13 nm, respectively. This work points out the possibility of qualitative modeling of Raman spectra of nanostructured materials as a function of confinement effect, particle size distribution and the dispersion relation.

16:00 Poster A03

Raman scattering from acoustic phonons confined in small spherical nanoparticles

Radmila Kostic

Institute of Physics (IF), Pregrevica 118, Belgrade 11080, Serbia

e-mail: radmila.kostic@phy.bg.ac.yu

Low-frequency Raman scattering from small spherical particles is analyzed. Frequencies of vibrational modes are calculated in elastic continuum approximation, which considers one nanoparticle as homogeneous elastic sphere and no force acting on the surface (so called stress-free boundary conditions). Procedure, similar to one presented in this paper, but for different boundary conditions, can also be done.

Vibrational modes are classified according to the symmetry group of the sphere by the sphere angular momentum quantum number *l*. Index *n* (*n*=0,1,...) labels the sequence of eigen modes, in increasing order of frequency. On the basis of symmetry consideration, the only Raman-active modes of a sphere are the symmetric *l*=0 and quadropolar *l*=2 spheroidal modes.

Parameters of this model are transverse (v_t) and longitudinal (v_l) sound velocities of material i.e. elastic properties of bulk material. Calculated vibrational frequencies for nanospheres of dimension *d*, on the basis of bulk material parameters, are usually used to verify w~1/*d* relationship and to compare nanoparticles dimension determined by this method (experimental low-frequency Raman spectra combined with calculations within this model) and other (XRD, optical phonon region Raman, etc) experimental and calculation methods.

In this paper, vibrational modes frequencies are scaled as function of mentioned bulk parameters for *l*=0 and *l*=2 spheroidal modes up to n_{max}=4, to establish relations between vibrational modes frequencies in the case of stress-free boundary conditions. Calculated relations are compared with low-frequency Raman experimental results from literature (Ge, Si, CdS, CdSe,...) and also with our results for CeO_2 nanoparticles.

These calculated relations can be practically used to examine nanoparticles of unknown bulk parameters material. One procedure, how to establish v_l and v_t of material from low-frequency Raman spectra of dimension *d* particles, is presented.

16:00 Poster A04

Low frequency Raman scattering in free-standing single, double and triple layer silicon-based membranes

Nelson Lou[1], Jesse Groenen[1], Gérard BenAssayag[1], Antoine Zwick[1], Monique Dilhan[2], Eléna Bedel-Pereira[2], Emmanuelle Daran-Schmidt[2]

1. *CEMES-CNRS (CEMES-CNRS), 29, rue Jeanne Marvig, Toulouse F31055, France* **2.** *LAAS-CNRS, Toulouse 31077, France*

e-mail: nelson@cemes.fr

Inelastic light scattering was shown to be a valuable tool for probing elastic properties of thin free-standing membranes (See for instance Ref. [1]). We report on a low frequency Raman scattering study of silicon-based membranes. Thin silicon membrane spectra display a series of peaks assigned to standing acoustic modes. It was shown that both acoustical and optical cavity effects have to be considered in order to account for their scattering efficiencies. [2] Here we focus on the optical cavity effects by modifying the environment of the thin silicon layer. We present low frequency Raman spectra from three different free-standing membrane structures : a silicon single layer membrane (32 nm), a Si/SiO_2 double layer membrane (32 nm/200 nm) and a $Si_3N_4/Si/SiO_2$ triple layer membrane (100 nm/32 nm/200 nm). These membranes were fabricated using a silicon nitride coated silicon on insulator wafer.

The three different membranes present specific spectral signatures (peak positions and intensities) which point out the specific role of the optical cavity effects. The membrane spectra are systematically compared to those recorded on the equivalent (multi)layer supported on a thick silicon substrate. Experimental data are compared to spectra calculated within the frame of the photoelastic model. It is shown that such comparisons are required in order to perform a quantitative analysis of the experimental data.

[1] R. S. Bandhu, X. Zhang, R. Sooryakumar, and K. Bussmann, Phys. Rev. B 70, 075409 (2004).

[2] J. Groenen, F. Poinsotte, A. Zwick, C.M. Sotomayor Torres, M. Prunnila and J. Ahopelto. Phys. Rev. B 77, 045420 (2008).

16:00 Poster A05

Low-frequency Raman scattering from transition-metal-doped ZnO nanoparticles

Radmila Kostic[1], Nebojsa Romcevic[1], Maja Romcevic[1], Branka Hadzic[1], Zorica Lazarevic[1], Izabela Kuryliszyn-Kudelska[2], Witold Dobrowolski[2], Daniel Sibera[3], Urszula Narkiewicz[3]

1. *Institute of Physics (IF), Pregrevica 118, Belgrade 11080, Serbia* **2.** *Polish Academy of Sciences, Institute of Physics, al. Lotników 32/46, Warszawa 02-668, Poland* **3.** *Szczecin University of Technology, Institute of Chemical and Environment Engineering, Szczecin 70-322, Poland*

e-mail: romcevi@phy.bg.ac.yu

Nanocrystaline samples of transition-metals (Fe, Mn) doped ZnO are synthesized by wet chemical method. Samples are characterized by X-ray diffraction in order to determine composition of the samples and the mean crystallite size (8-52 nm). Raman spectroscopy and the magnetic measurements were performed too.

In this paper we report experimental spectra of low-frequency Raman scattering (below 100 cm^{-1}) at low temperatures, from these doped ZnO nanoparticles. In order to make low-frequency Raman modes visible we subtracted the intensity of the elastic scattering background by A/ω^n approximation. Observed modes are deconvoluted using the Lorentzian line profile technique. In almost all samples, two low-frequency Raman modes are identified. For example: in a case of $(ZnO)_{0.95}(Fe_2O_3)_{0.05}$ with mean crystallite size ~10 nm , modes are at about 19 cm^{-1} and 39 cm^{-1}; in a case of $(ZnO)_{0.05}(MnO)_{0.95}$ with mean crystallite size ~43 nm modes are at about 22 cm^{-1} and 46 cm^{-1}. Position of these modes is connected to the dimension of particles and dopant concentration. Low-frequency modes are analyzed as confined acoustic vibrations of nanoparticles.

As the dimension of the particles is already determined and having in mind specific frequency to diameter dependence, we established material parameters and analyzed behavior of these nanocrystaline doped ZnO samples.

16:00 Poster A06

Dopping Effects on Multiwalled Carbon Nanotubes: Influence of Different Acid Treatments

Sara Costa, Ewa Borowiak - Paleń

Szczecin University of Technology, Institute of Chemical and Environment Engineering, Szczecin 70-322, Poland

e-mail: scosta@ps.pl

In the present study we report the surface modification of multiwalled carbon nanotubes (MWCNT) using HCl, HNO_3 and H_2SO_4. Acids are commonly used in purification procedures to remove catalyst particles from the raw material. However, it is known that MWCNT upon acid treatment have many surface functionalized groups or intercalate within the walls, modifying their electronic properties [1]. Several studies on doping of different CNT have been previously developed, however none of them provide a comparison between different acids.

Here, we present a comparative study between samples of MWCNT modified with the most common acids used in the purification of carbon materials and the influence of the treatment time on their properties. The samples were analyzed via Raman and Infrared (IR) spectroscopies. While the first method is a very helpful tool to understand the electronic modifications of the carbon nanotubes (CNT), the second one supports to identify the functional groups attached on the MWCNT surface (such as carboxylic and nitrile groups).

Data show in this contribution proved that different acids treatments result in different changes in the bands of the Raman spectra. HNO_3 influence the most in the disorder band (D band), while H_2SO_4 and HCl are responsible for affecting more the graphite band (G band) as well as the two-phonon second order raman band (G' band). The treatment time showed to be directly correlated with the shift of the different Raman bands.

[1] EB Barros *et al.*, Physical Review B 76 (2007) 045425

16:00 Poster A07

Raman evidences for the interface interactions in poly(bithiophene)/single-walled carbon nanotubes composites

Mihaela Baibarac[1], Ioan Baltog[1], Serge Lefrant[2], Cristina Bucur[1]

1. *National Institute for Materials Physics, Bucharest- Magurele 010555, Romania* **2.** *LPCM, Institut des Matériaux Jean Rouxel, 2 rue de la Houssinière, Nantes 44322, France*

e-mail: barac@infim.ro

Electrochemical polymerization of 2,2'-bithiophene (BTh) in a tetrabutylammonium tetrafluoroborate ($TBABF_4$)/acetonitrile solution on a single-walled carbon nanotubes (SWNTs) film has been studied by cyclic voltammetry and Raman scattering. Two composites result from the electrochemical synthesis: i) poly(bithiophene) (PBTh) doped with carbon nanotubes and ii) PBTh functionalized SWNTs. In the case of PBTh doped SWNTs, a charge transfer process is argued by change of the position of Raman lines associated with the radial breathing modes (RBM) of SWNTs and the C=C stretching vibration of PBTh. For the latter composite, an analysis of the Raman band with the maximum situated to 1595 cm^{-1} associated with the tangential mode of SWNTs reveals a functionalization of side-walls of nanotubes with polymer. A post chemical treatment of the PBTh functionalized SWNTs composite with a basic solution induces the increase in the intensity of the Raman band at 178 cm^{-1} associated with radial breathing modes of SWNTs bundles, which suggests an additional nanotubes roping with PBTh as a binding agent. For a better understanding of the above results, Raman studies concerning the oxidation-reduction process at the interface SWNTs films/the $TBABF_4$ solution in the absence of BTh are shown, too.

16:00 Poster A08

Resonance Raman study on carbon nanotubes formation and characterisation

Anna Stęplewska, Ewa Borowiak - Paleń

Szczecin University of Technology, Institute of Chemical and Environment Engineering, Szczecin 70-322, Poland

e-mail: asteplewska@ps.pl

Carbon nanotubes can be obtained from verity of the molecular precursors in chemical vapor deposition (CVD) processes. The growth mechanism of carbon nanotubes (CNTs) still remains unsolved puzzle for the researchers. Therefore, this contribution presents *in situ* study on the formation of CNTs in CVD process in TGA analyzer. In addition, TGA analysis was applied to estimate the quality of the produced sample. Resonance Raman spectroscopy was used to determine the quality of the final sample and characterize it, e.g. to estimate the diameter of the tubes. High resolution transmission electron microscope with Energy dispersive X-ray spectroscopy was a tool to determine the morphology and elemental composition of the samples, respectively.

16:00 Poster A09

Raman spectroscopy of single and multilayer graphene on SiC substrates

Kacper Grodecki[1,2], Andrzej Wysmolek[1], Rafał Bożek[1], Roman Stępniewski[1], Jacek Baranowski[1], Jolanta Borysiuk[2], Wlodek Strupinski[2]

1. *University of Warsaw, Institute of Experimental Physics (IFDUW), Hoża 69, Warsaw 00-681, Poland* **2.** *Institute of Electronic Materials Technology (ITME), Wólczyńska 133, Warszawa 01-919, Poland*

e-mail: Andrzej.Wysmolek@fuw.edu.pl

Graphene obtained by annealing of silicon carbide (SiC) substrates has recently attracted a lot of interest as a promising material for future carbon-based electronics. On the contrary to graphene made by micromechanical cleavage [1], epitaxial graphene [2] is compatible with industrial processing techniques. However, the electronic and optical properties of the epitaxial graphene can be substantially modified by interaction with the SiC substrate.

Raman spectroscopy has been proved to be very efficient and useful method to study single- and multi-layer graphene structures. In this communication Raman spectroscopy of epitaxial graphene are presented. Investigated samples were prepared in Epigress VP508 SiC hot wall CVD reactor on 4H-SiC(0001) substrates with Si and C polarity as well as with exact and 4° off orientation. The appearance of single and/or multiple graphene layers on the SiC surface was verified by Scanning Tunneling Microscopy and Transmission Electron Microscopy. Micro-Raman experiments where performed at room temperature, using 532 nm line from Nd-YAG as a source of continuous wave excitation. Highly oriented pyrolitic Graphite (HOPG) was used as a reference sample.

It is observed that the Raman shifts of characteristic 2D bands observed for layers deposited on Si-face of the SiC substrates are blue shifted with respect to the 2D peak observed for the graphene made by micromechanical cleavage [4] as well as the G' band of reference HOPG sample. Interestingly the blue shift as well as the FWHM of the 2D transition observed for the 4^0 off-axis substrate is larger than measured for on-axis sample. The observed effects could be explained in terms of strain induced by 4H-SiC substrates. Other mechanisms including unintentional doping are also discussed.

[1] K.S. Novoselov et al. Science **306**, 666 (2004)

[2] C. Berger et al. J. Phys. Chem. B **108**, 19912 (2004)

[4] A. C. Ferrari, Solid State Commun. **143**, 47 (2007)

16:00 Poster A11

Synthesis and characterization of Mn-doped $BiFeO_3$ nanoparticles

Hideo Fukumura[1], Satoshi Matsui[1], Nobuhiko Tonari[1], Takaaki Nakamura[1], Kenji Kisoda[2], Noriyuki Hasuike[1], Kohji Nishio[1], Toshiyuki Isshiki[1], Hiroshi Harima[1]

1. *Department of Electronics, Kyoto Institute of Technology, Kyoto 606-8585, Japan* **2.** *Department of Physics, Wakayama University, Wakayama 640-8510, Japan*

e-mail: d6821004@edu.kit.ac.jp

$BiFeO_3$ is a unique material that exhibits ferroelectric and weak ferromagnetic (or canted anti-ferromagnetic) orderings simultaneously far above room temperature (Curie temperature T_C ~1100K and Néel temperature T_N ~640K). This property, called multiferroics, results in a coupling between electric field and magnetization; the so-called electromagnetic effect. Because of this attractive nature, $BiFeO_3$ now gathers great attention as a prominent candidate for future innovative electronc devices such as energy-saving memories and transisters. For device applications, however, further investigations for its basic physics both in electric and magnetic properties are strongly expected. For example, as a recent hot topic, $BiFeO_3$ thin films greatly increased their remanent electric polarization by doping with Mn, though the mechanism has been left an open question.[1]

To solve this problem, we synthesized here Mn-doped $BiFeO_3$ samples by a sol-gel process with molar compositions of [Mn]=0-10%, and investigated their lattice properties by Raman scattering, x-ray diffraction and transmission electron microscopy. Our results showed that the samples included no seconadary phases and the Mn ions substituted Fe sites of host lattice. Small lattice distortion from the rhombohedral structure of $BiFeO_3$ was observed with increasing [Mn]. Moreover, phonon Raman spectra observed at 300-800K showed anomalous behavior near T_N. This was interpreted by a coupling between the phonon and spin systems.

[1] S. K. Singh, H. Ishiwara and K. Maruyama , Appl. Phys. Lett. **88** 26908 (2006)

16:00 Poster A12

Micro-Raman study of $BiFeO_3$ thin films fabricated by chemical solution deposition using different Bi/Fe ratio precursors

Takaaki Nakamura[1], Hideo Fukumura[1], Noriyuki Hasuike[1], Hiroshi Harima[1], Yoshitaka Nakamura[2], Kenji Kisoda[3], Seiji Nakashima[4], Masanori Okuyama[4]

1. *Department of Electronics, Kyoto Institute of Technology, Kyoto 606-8585, Japan* **2.** *Institute for Chemical Research, Kyoto University, Kyoto 611-0011, Japan* **3.** *Department of Physics, Wakayama University, Wakayama 640-8510, Japan* **4.** *Graduate School of Engineering Science, Osaka University, Osaka 560-8531, Japan*

e-mail: m7621022@edu.kit.ac.jp

Recently, there has been increasing interest in so-called multiferroic materials, where two or more ferroic orderings (ferroelectricity, ferromagnetism and ferroelasticity) coexist simultaneously. In a multiferroic material with ferroelectricity and ferromagnetism, magnetization can be controlled by applied electric field and polarization can be controlled by external magnetic field (magnetoelectric effect). Such materials lead us to future innovative electronic devices. $BiFeO_3$ (BFO) is a promising candidate for such applications because it shows ferroelectric and weak ferromagnetic orderings above room temperature (Curie temperature T_C~1100K and Néel temperature T_N~640K).

Recently, the influences of surface texture and Bi/Fe ratios on electric properties of BFO thin films have been investigated.[1] According to [1], two regions with μm-order size were observed on the film surface by atomic force microscopy (AFM). The sample containing lots of one region shows good electric properties. Therefore, in order to improve electric properties of BFO thin films, it is important to investigate their properties in these regions.

Here, we prepared BFO thin films grown by chemical solution deposition using precursor solutions with different Bi/Fe ratios and were characterized by micro-Raman scattering. Micro-Raman scattering is a very useful tool to study their crystallinity with μm-order spatial resolution. Our Raman results demonstrated that the surface of samples consisted of two regions ; one region crystallized in perovskite units and the other not. These are consistent with AFM observation.[1] We found that the electric properties on BFO thin films are dependent on their crystallinity.

[1] Y.Nakamura, S.Nakashima and M.Okuyama, Jpn. J. Appl. Phys. (submitted)

16:00 Poster A13

Raman scattering study of polycrystalline $BiFeO_3$ obtained by mechanochemical synthesis

Zorica Marinkovic-Stanojevic[2], Nebojsa Romcevic[1], Branka Hadzic[1], Biljana Stojanovic[2]

1. *Institute of Physics (IF), Pregrevica 118, Belgrade 11080, Serbia* **2.** *Center for Multidisciplinary Studies, University of Belgrade, Kneza Viseslava 1, Belgrade 11000, Serbia*

e-mail: romcevi@phy.bg.ac.yu

A powder mixture of Bi_2O_3 and Fe_2O_3 was mechanically tretaed in a planetary ball mill in air atmosphere for 120, 240, 360 and 720 minutes.

Samples were denoted according to the time of milling as BFO120, BFO240, BFO360 and BFO720. Mechanochemical reaction leads to the gradual formation of polycrystalline $BiFeO_3$ (BFO) at room temperature. After 240 min of synthesis, all of the reflection peaks can be indexed as BFO rhomohedral R3c crystallographic structure. Highly dense and single-phase BFO ceramics were prepared by conventional solid-state reaction at the temperature of 810^oC for 1^h followed immediately by quenching process.

Raman scattering study of polycrystalline BFO ceramics were carried out at room temperature. Most of the 13 Raman modes predicted by group theory ($\Gamma_{Raman,\ R3c} = 4A_1 + 9E$) for R3c structure of BFO are observed in the present work. There are nine normal modes, including A_1-1, A_1-2, and A_1-3 modes with strong scattering intensity, and six E modes with medium scattering intensity. The results of Raman spectra matches well with the recently reported single crystal and epitaxialy grown thin film of BFO. The observed three A_1 modes should be governed by the Bi-O covalent bonds, which are the origin of the ferroelectric distortion. The Raman spectra suggest that the ferroelectric distortion of BFO360 sample is more stable than that of BFO120, BFO240 and BFO720 due to the weakening of the scattering intensities of the A_1 modes in these samples.

The slight difference in some of the peak positions observed in investigated samples can be attributed to the sample preparation details. It is known that mechanochemical synthesis influences the oxygen stoichiometry. This is expected to show changes in oxygen bonding and disorder that is reflected in the vibrational frequencies of mode involving oxygen.

16:00 Poster A14

Raman spectroscopy of $Pb_{0.85}Sn_{0.15}Te$ (In) single crystal

Dusanka Stojanovic[1], Nebojsa Romcevic[1], Maja Romcevic[1], Dmitry R. Khokhlov[2]

1. *Institute of Physics (IF), Pregrevica 118, Belgrade 11080, Serbia*
2. *M.V. Lomonosov Moscow State University, Vorobyevy gory, Moscow 119992, Russian Federation*

e-mail: dusanka@phy.bg.ac.yu

The doping of the lead-telluride based alloys with the III-group impurities as In, Ga, Tl modifies substantially the electronic spectrum of the semiconductor. In $Pb_{1-x}Sn_xTe$ (In) solid solutions Fermi level is pinned at some position that does not depend on N_{In} [1]. The pinned Fermi level moves continuously from the conduction band to the valence band with increasing SnTe content, passing the band gap in the composition range $0.22 \le x \le 0.28$ at T = 4.2 K [2,3]. It shows metal (n-type) – insulator –metal (p-type) transition owing to x at low temperature. External IR illumination leads to substantial increment in material conductivity at T‹25K independently on the Fermi level pinning position.

Raman scattering spectra of $Pb_{0.85}Sn_{0.15}Te$ doped with Indium in temperature range 10 to 300 K are presented. As it is well known, $Pb_{1-x}Sn_xTe$ crystallizes in the cubic structure of the NaCl type (O_h space group symmetry) and the first-order Raman modes are not active. In the Raman spectra of doped sample, we registered impurity induced scattering on the phonons of the $Pb_{1-x}Sn_xTe$ lattice which tend to folow the host lattice density of state. We registered some broader modes as a consequence of electron transition between valence band and two impurity levels and between impurity levels. At the same time we registered three local modes of impurities. The position of these modes depends on impurity center charge.

[1] B. A. Volkov, L. I. Ryabova, D. R. Khokhlov, Physics-Uspekhi 45 (8) (2002) 819.

[2] D.R. Khokhlov, I.I. Ivanchik, S.N. Raines, D.M. Watson, and J.L. Pipher, Appl. Phys. Lett. 76 (2000) 2835.

[3] K.G. Kristovskii, A.E. Kozhanov, D.E. Dolzhenko, I.I. Ivanchik, D. Watson, and D.R. Khokhlov, Phys. Solid State 46 (2004) 122.

16:00 Poster A15

Resonant and non-resonant Raman spectra of CdTe/ZnTe self-assembled quantum dots

Nebojsa Romcevic[1], Maja Romcevic[1], Radmila Kostic[1], Dusanka Stojanovic[1], Grzegorz Karczewski[2], Robert Rafal Galazka[2]

1. *Institute of Physics (IF), Pregrevica 118, Belgrade 11080, Serbia*
2. *Polish Academy of Sciences, Institute of Physics, al. Lotników 32/46, Warszawa 02-668, Poland*

e-mail: romcevic@phy.bg.ac.yu

We present Raman scattering results of CdTe/ZnTe self assembled quantum dots (SAQD). Investigated samples were grown by molecular beam epitaxy on GaAs substrate. A CdTe buffer layer 4.5mm thick was deposited on the substrate. After a 1mm thick ZnTe layer, 3 monolayers (ml) of CdTe were deposited to form a random distribution of quantum dots. The dot layer was covered by 50 nm ZnTe capping layer.

Raman spectra were obtained in the backscattering geometry using lines of Ar-ion laser. Multiphonon (MP) resonant process can be described by the following equation: $E_{in}-K\hbar w=E$; E_{in} and E are the incident photon energy and electron transition energy, respectively. $\hbar w$ is the phonon energy and K is the MP order. MP emission is not registered at T=300K. One-phonon spectrum shows weak intensity line at 201.6 cm^{-1}. MP emission processes are registered at temperature below T=200K (for 2.41eV laser energy, K=4). However, one-phonon spectrum consists of two lines. Besides mentioned line at 201.6 cm^{-1} new line at 204.2 cm^{-1} appears and takes part in resonance process. Resonance with line at 201.6 cm^{-1} is not observed. At T=20K resonance order depend on excitation energy and its values are 2, 4, 5 and 7 for laser lines 2.41eV, 2.47eV, 2.49eV and 2.54eV, respectively. One phonon spectra is now more complicated. Besides mentioned, new lines are registered at 200.4, 210.3, 217 and 386 cm^{-1}.

We attribute the peak 204.2 cm^{-1} to confined longitudinal-optical (LO) phonons from bulk ZnTe (209 cm^{-1}). Raman features at 210.3 and 200.4 cm^{-1} are ascribed to the ZnTe LO modes confined by degenerate superlattices. We identified the peaks at 217 and 386 cm^{-1} as ZnTe (TA+LO) modes and (LO+TO(Γ)) modes, respectively. We connected mode at 201.6 cm^{-1} with specific structure of ZnTe in the isolated islands of CdTe neighbourhood.

16:00 Poster A16

Effect of Fe^{2+}(Fe^{3+}) doping on structural properties of CeO_2 nanocrystals

Marko Radović[1], Novica Paunović[1], Zorana D. Dohcevic-Mitrovic[1], Maja Šćepanović[1], Zoran V. Popovic[1], Branko Matović[2]

1. *Institute of Physics (IF), Pregrevica 118, Belgrade 11080, Serbia*
2. *VINCA Institute, POB 522, Belgrade 11001, Serbia*

e-mail: marrad@phy.bg.ac.yu

Raman spectroscopy at room temperature was used to investigate defect structure and mixed valence states of Fe^{2+}(Fe^{3+}) doped CeO_2 nanopowders. Existence of CeO_2 fluorite cubic structure was characteristic for all investigated samples whereas the presence of first order Raman modes of Fe_2O_3 and Fe_3O_4 structural phases were not observed. Additional modes at 720 cm^{-1}, 1320 cm^{-1} and 1600 cm^{-1} are observed for doped samples and can be assigned to maghemite (g-Fe_2O_3) cation deficient structure, to 2LO IR-allowed overtone and two magnon features, respectively. This implies that our powders are composed of mixed valence states and have defective structure.

16:00 Poster A17

Raman Scattering From ZnSe Nanolayers

Diana D. Nesheva[1], Maja J. Šćepanović[2], Sonja Aškrabić[2], Zelma Levi[1], Irina Bineva[1], Zoran V. Popovic[2]

1. *Institute of Solid State Physics, Bulgarian Academy of Sciences (ISSP-BAS), 72, Tzarigradsko Chaussee blvd., Sofia 1784, Bulgaria*
2. *Institute of Physics (IF), Pregrevica 118, Belgrade 11080, Serbia*

e-mail: nesheva@issp.bas.bg

Thin nanocrystalline semiconductor films are promising materials for gas sensor applications since in such layers the sensing surface is significantly larger than the geometric one. Therefore layer resistence may show significant changes upon exposure to some gases or vapours. In this study a series of ZnSe single layers were deposited on c-Si and glass substrates at room substrate temperature. Thermal evaporation of ZnSe powder in vacuum has been performed and the layer thickness of the produced films varied between 30 and 100 nm. Also, SiO_x/ZnSe periodic multilayers have been studied. Both kinds of layers (2 or 4 nm thick) were produced using the same deposition technique. Up to four maxima have been observed in the Raman spectra of all samples taken at 20 and 295 K, using the 442 nm (2.8 eV) line of a He-Cd laser as an excitation source. The observed spectral features have been related to multiple phonon (1LO to 4LO) light scattering and connected with the existence of crystalline ZnSe grains in both single layers and the ZnSe layers of multilayers. On the other hand, absorption results imply presence of amorphous ZnSe phase in the single layers, as well. Therefore, it has been assumed that as-deposited single layers contain two phases, amorphous and crystalline. In an attempt to improve the film crystallinity, series of Raman spectra have been obtained at 295 K on both ZnSe single layers and SiOx/ZnSe multilayers using the 488 nm line of an Ar^+/Kr^+ laser with a gradually increased laser beam power. The obtained results indicate an increased crystallinity at high illumination levels. The effect is better pronounced in the multilayers.

16:00 Poster A18

Raman spectroscopy of multiphonon emission process in Ni-doped PbTe

Nebojsa Romcevic[1], Branka Hadzic[1], Jelena Trajic[1], Tatyana G. Kuznetsova[2], Maja Romcevic[1], Zorica Lazarevic[1], Dusanka Stojanovic[1], Dmitry R. Khokhlov[2]

1. *Institute of Physics (IF), Pregrevica 118, Belgrade 11080, Serbia*
2. *M.V. Lomonosov Moscow State University, Vorobyevy gory, Moscow 119992, Russian Federation*

e-mail: jelena@phy.bg.ac.yu

The doping of $A^{IV}B^{VI}$ semiconducting compounds with transition metal impurities has significant scientific and practical interest. Lead telluride (PbTe) belongs to the $A^{IV}B^{VI}$ IR-sensitive narrow-gap semiconductors group, which acquire new properties in consequence of doping. Transition metals behave either as donors (Cr, Co, Ni) or neutrals (Mn).

In this paper, we present room temperature unpolarized Raman scattering spectra of Ni doped PbTe single crystal sample. Crystal of PbTe(Ni) was grown by the Bridgman method. The Ni concentration in the samples used here were $1\cdot10^{19}$ at.%./cm^3. Well resolved peaks appear at about 126, 143, 181, 362 and 724 cm^{-1}. The modes at 126 and 143 cm^{-1}, which are also observed in other telluride compounds, originate from vibrations in TeO_2. We assume that the mode at about 181 cm^{-1} is connected to excitations of a local phonon mode in the vicinity of an impurity atom (donor Ni^{3+} state). Modes at about 362 cm^{-1} and 724 cm^{-1} are the second and forth harmonic of a local phonon mode, registered here according to multiphonon emmission (MPE). Namely, in the PbTe(Ni), the equilibrium position of the ground donor level before the electron capture is in the upper half of the gap. After the capture of the electron, the lattice near the defect relaxes in such a way as to lower the equilibrium position of the level in the energy gap. Immediately after the capture of the electron the lattice is displaced far from the new equilibrium position and there will be a violent lattice vibration at the defect. The vibration will rapidly damp down to the amplitude of the thermal vibrations (ω_0) after a small number of vibrational periods. During the damping, the localized energy propagates away from the defects as phonons.

16:00 Poster A19

Chemical interactions of the polyaniline/fullerene composite with N-methyl pyrrolidinone evidenced by SERS spectroscopy

Ioan Baltog[1], Mihaela Baibarac[1], Serge Lefrant[2], Nicoleta Preda[1]

1. *National Institute for Materials Physics, Bucharest- Magurele 010555, Romania* **2.** *LPC, Institut des matériaux Jean Rouxel, BP 32229, Nantes 44322, France*

e-mail: ibaltog@infim.ro

Surface enhanced Raman scattering (SERS) spectroscopic studies reveal a particular chemical interaction of polyaniline/fullerene (PANI/C_{60}) composite with N-methyl pyrrolidinone (NMP). Chemical polymerization of aniline in the presence of sulfuric acid, potassium dichromate and fullerene has been used for the preparation of PANI doped with fullerene. The resulted composite material contains the polymer in the leucoemeraldine salt (LS) state. The interaction of this composite with NMP leads to a de-doping of PANI that appears as a transformation of the LS into leucoemeraldine base (LB). Besides, a gradually increase in the intensity of the Raman line with maximum at 1452 cm^{-1} associated to $A_g(2)$ pentagonal pinch mode of fullerene indicates formation of a charge transfer complex of the type fullerene-NMP. UV-VIS absorption spectroscopic studies regarding the kinetic of chemical interaction of the PANI/fullerene composite with NMP are also shown. After a storage of the PANI/fullerene composite in NMP, time of 19 days, a chemical treatment with iron chloride leads to a doped PANI having a protonated structure similar with the emeraldine salt. To evaluate the electrons number accepted of fullerene during of the above interactions, Raman studies on sample prepared by electrochemical polymerization of aniline on the fullerene film are presented, too.

16:00 Poster A20

Characterization of Diamond Films by Near-infrared Excited Raman Spectroscopy

Miklos Veres, Sára Tóth, Margit Koós

Hungarian Academy of Sciences, Research Institute for Solid State Physics and Optics (SZFKI), Konkoly Thege M. út 29-33, Budapest H-1121, Hungary

e-mail: vm@szfki.hu

Raman spectroscopy is an important and widely used characterization tool of different carbon containing materials, including nano- (NCD) and ultra-nanocrystalline diamond (UNCD) thin films. The spectrum of the diamond layers excited by visible light consists of up to five bands assigned to diamond peak, G and D bands of inter-granular amorphous carbon phase and to vibrations of trans-polyacetylene formed on the grain surfaces. While similar features would be expected in the Raman spectra of these materials excited using different excitation wavelengths (with some differences in the intensity ratios and positions), our near infrared excited micro-Raman spectroscopic investigations on series of NCD samples with grain sizes above 50 nm showed that a number of narrow well separable new bands appear in the spectrum. Beside the grain size the appearance of these peaks was found to be dependent on the excitation spot size too: the bands were observable when only a few grains were falling into the excitation volume.

The small width of the bands suggests that they are related to vibrations of well defined, probably molecular structural units of the films, located on the diamond crystallite surface (grain boundary). The peaks may vary from point to point on the sample surface, but the statistical analysis performed on a series of spectra measured in different points of the surface showed that there are characteristic peaks for a given sample, being present in most of the spectra.

For UNCD thin films with grain sizes below 50 nm the excitation volume should be lowered to a few nanometers in order to observe the narrow Raman peaks. This was realized by Surface-enhanced Raman spectroscopy (SERS), where colloidal gold nanoparticles (10 nm in diameter) were placed on the UNCD layer surface and the SERS spectra were recorded from the few nanometer surrounding of the Au particles.

This work was supported by Bolyai Janos Research Scholarship of the Hungarian Academy of Sciences.

16:00 Poster A21

A few molecules surface-enhanced Raman scattering studies on nickel-modified silver substrates

Andrzej Kudelski

University of Warsaw, Department of Chemistry, Pasteura 1, Warsaw, Warszawa 02-093, Poland

e-mail: akudel@chem.uw.edu.pl

A few clusters surface-enhanced Raman scattering (SERS) measurements on a substrate covered with a layer of practically SERS non-active metal were realized. We measured SERS spectra dominated by the contribution from only a few carbon clusters for hydrogenated carbon deposited on the nickel-modified silver substrate. It means that a few molecules SERS measurements on many catalytically important metals can be realised. In recorded spectra the contributions characteristic for various clusters could be identified (and hence presence of these clusters in the analysed mixture could be proved), even when contribution of many types of carbon clusters to the standard (averaged) SERS spectrum cannot be reliably identified.

16:00 Poster A22

As_nS_m Nanoclusters in the Structure of Amorphous Materials: Ab Initio and Raman Study

Roman Holomb[1], Vladimir Mitsa[1], Miklos Veres[2]

1. *Uzhgorod National University (UzhNU), Pidhirna str.46, Uzhgorod 88000, Ukraine* **2.** *Hungarian Academy of Sciences, Research Institute for Solid State Physics and Optics (SZFKI), Konkoly Thege M. út 29-33, Budapest H-1121, Hungary*

e-mail: vm@szfki.hu

The fundamental statements of topological-cluster structure of non-crystalline chalcogenide semiconductors related to the changes in the connectivity of the structural matrix and to the dependence of physical properties on the average coordination number were investigated by both experimental and theoretical methods.

We here present a study of different type As_nS_m nanoclusters (n=1-6; m=3-6, 8, 10, 12) which realization in the amorphous structure is possible. The differences in the topology (geometrical structure) and bonding of clusters causes changes in their physical and chemical properties. This work was aimed to analyze the formation energy, stability, electronic, optical, and vibrational properties of such clusters, calculated from the first-principles.

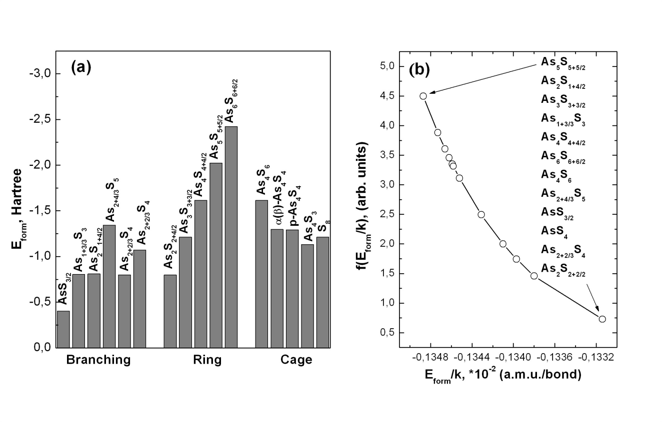

Fig. 1: (a) Formation energy (E_{form}) and (b) Boltzmann distribution of $E_{form.}/k$ (k is the number of bonds) values of $As_nS_m(S_8)$ clusters.

The experimental spectra of amorphous arsenic sulphides were interpreted by using the results of *abinitio* calculations of the vibration spectra of different As_nS_m nanoclusters, taking into account their relative stability. Physical and technological conditions under which the structure of the amorphous film reaches the structure of the corresponding bulk glass or essentially differs from it have been revealed.

16:00 Poster A23

Damage assessment in low doses Si^+-implanted GaAs

Ida-Dunja Desnica Frankovic, Krešimir Furić, Uros V. Desnica

RUDJER BOSKOVIĆ INSTITUTE, BIJENIČKA C. 54, Zagreb 10 000, Croatia

e-mail: ddesnica@irb.hr

Ion implantation is a widely used technique in device technology, and becoming even more important as the size of devices decreases. The studies of damage and introduced defects have been extensive and, although the overall development and annealing of the implantation damage is relatively well understood, many details remain unclear. Especially, not enough attention has been paid to the effects of very low doses, which are particularly important in controlling the threshold voltage of transistors in the fabrication of GaAs integrated circuits. The reason might be that the induced changes were very often below the detectivity limits of standard methods.

In this work, we present the results of the implantation induced disorder analysis, conducted on GaAs implanted with low ion doses. Czochralski grown, undoped, (100) oriented GaAs samples, with dislocation density in the $10^4/cm^2$ range, were implanted with 100 keV $^{30}Si^+$ ions, doses ranging from $3x10^{11}/cm^2$ - $3x10^{13}/cm^2$, at 21 ^oC. The damage assessment was done by applying Raman scattering and Rutherford backscattering ion channeling (RBS), connected by the inter-cascade distance model (ICD) and the results were then compared with the results of photoacoustic displacement technique (PAD).

We have shown that Raman scattering is very sensitive method even if applied on samples implanted with very low doses. Furthermore, the equivalency between the RS and RBS damage assessment, previously established for high doses *via* the ICD model, proved equally valid also for very low implantation doses, where implanted ions create disordered cascades that are far apart, and most of the layer is still undamaged.

16:00 Poster A24

Impact of Pd additive on phonon vibrations and element distribution in nickel silicide

Aliaksandra Karabko[1], Anatoly Dostanko[1], Jinfang Kong[2], Wenzhong Shen[2]

1. *Belarusian State University of Informatics and Radioelectronics (BSUIR), P.Brovka str. 6, Minsk 220000, Belarus* **2.** *Shanghai Jiao Tong University (SJTU), Shanghai 200030, China*

e-mail: alkorobko@gmail.com

Recently, the optimisation of nickel silicides by 3^{-rd} element additives has appeared to become an effective way to reduce agglomeration and to retard the formation of undesirable $NiSi_2$ phase. Nevertheless, it puts a question on adequate identification and investigation of possible changes of NiSi properties that could be tremendous for microelectronic applications.

In our experiments, pure Ni films and Ni films with the initial concentration of 10 % of Pd were deposited on *n*-Si by dc magnetron sputtering system and silicidated in two step annealing procedure in the range of temperatures 475–900 ˚C.

The results of Raman and Auger (AES) measurements have shown that the introduction of small amount of Pd in NiSi in comparison with pure NiSi films retards the formation of $NiSi_2$ by at least 100 ˚C and enhances the technology process window up to 900˚C. Although this is a major advantage for thermostability of NiSi there are some peculiarities to note. Firstly, the presence of Pd introduces the redshift to the positions of NiSi phonon peaks in Raman spectra, i.e. Pd increases the interatomic distance of the crystal lattice in the film. Performed calculations from the mass change point of view have proved that the redshift coincides with the amount of Pd present in NiSi. We have also noted extra Raman peaks at 322 and 434 cm^{-1} in NiPdSi spectra becoming more prominent with the increase of annealing temperature, which have not been reported before. We assume it is due to the disorder Raman effects, induced by Pd. Finally, we have investigated element distribution in NiSi at various temperatures and followed the diffusion of Pd element. AES spectra have shown that distribution of Pd in NiSi changes with exponential decay law at temperature increase. Although Raman spectroscopy unambiguously identifies NiSi phase, AES results indicate that there is a deviation from the equilibrium stoichiometry to the slight lack of silicon and excess of metal phase in the compound.

16:00 Poster A25

Kinetics of compound formation at the interface of the binary system Cr/Si during rapid thermal annealing.

Abdelali Merabet, Houria Benkherbache

University de Setif, Faculte des Sciences de l'Ingenieur, Laboratoire Physique et Mecanique des Materiaues, Sétif 19000, Algeria

e-mail: merabet_abdelali@yahoo.fr

The effect of the arsenic on the nature of the formed silicide in the annealed Cr/Si system is studied. The chromium layer is deposited by electron gun evaporation on the undoped and arsenic doped monocrystalline silicon (100). The samples are analysed by X-ray-diffraction (XRD) and Rutherford backscattering spectrometry (RBS). The electrical activity has been investigated by the method of the four point probes. The analysis by DXRD and RBS of the samples annealed at 500°C for different times during rapid thermal annealing (R.T.A.) showed the formation of CrSi2 disilicide for lower annealing times. The thickness of formed chromium silicide was practically the same for 30 and 60 seconds. The sheet resistance measurement in function of annealing time shows a sharp increasing in the beginning annealing. After that, it then rises slightly over time and stabilizes. The value of saturation is at around 125 and 180 for Cr / Si and Cr / Si (As), respectively. This result justifies the using of the arsenic in order to obtain ultra-shallow junctions and highly doped.

16:00 Poster A26

Intercalation of layered metal iodides with pyridine evidenced by Raman spectroscopy

Nicoleta Preda, Lucian Mihut, Mihaela Baibarac, Ioan Baltog, Marius Husanu

National Institute for Materials Physics, Bucharest- Magurele 010555, Romania

e-mail: nicol@infim.ro

Using Raman spectroscopy four layered metal iodides (PbI_2, BiI_3, CdI_2 and AgI) crystalline samples intercalated with pyridine have been studied. After intercalation, both Raman spectra of host material and guest molecule are modified. All as growth investigated samples are featured by specific Raman spectra situated in the 40-200 cm^{-1} range. The Raman spectra of the intercalated compounds reveal new bands, keeping the original crystal signature. Changes in the Raman spectrum of the guest molecules are also observed. The most significant, considered as an evidence of a chemical interaction between pyridine molecules and layered metal iodide, are the enhancement of the Raman lines situated at 1574-1598 cm^{-1} and the appearence of new Raman line at ~ 3066 cm^{-1}. Based on these data result that the intercalation process evolves in two steps: i) initially neutral pyridine molecules are inserted between the metal iodide layers and ii) afterwards due to the chemical interaction, between metal ion and nitrogen atom of the guest molecules, a coordinated complex is formed. Photoluminescence observed at liquid nitrogen temperature on intercalated compound sustains this mechanism.

16:00 Poster A27

First order Raman scattering in Bi_2Te_3 thin films on flexible substrate

Anabela G. Rolo[1], Luís M. Gonçalves[2], Pedro Alpuim[1]

1. *Centro de Física, Universidade do Minho, Campus de Gualtar, Braga 4710-057, Portugal* **2.** *University of Minho, Dept. of Industrial Electronics, Azurém, Guimarães 4800-058, Portugal*

e-mail: arolo@fisica.uminho.pt

Raman spectroscopy was used in the optimization of the thermal co-evaporation deposition process for n-type bismuth telluride (Bi_2Te_3) thin films for thermoelectric applications. Films were deposited with good adhesion onto glass and plastic (Kapton) substrates. The influence of deposition parameters on film composition and thermoelectric properties was studied for optimal thermoelectric performance. The film chemical composition and structure was studied by Energy-Dispersive X-ray spectroscopy, X-ray diffraction, X-ray photoelectron spectroscopy, Rutherford Backscattering Spectroscopy, Induced X-ray Emission and Raman spectroscopy.
Seebeck coefficient (up to 250 μVK^{-1}), in-plane electrical resistivity (≈10 $\mu\Omega m$), carrier concentration ($3x10^{19}$ - $20x10^{19}$ cm^{-3}) and Hall mobility (80 - 170 $cm^2V^{-1}s^{-1}$) were measured at room temperature in selected Bi_2Te_3 samples.
For Raman scattering experiments both 514.5 nm and 488 nm lines of an Ar^+ laser and 1064 nm line of an YAG:Nd laser were used for excitation. Raman spectra were obtained in a Jobin-Yvon T64000 spectrometer and from the infrared line in a Bruker RFS 100/S FT-Raman spectrometer. In all cases, Raman spectra were performed at room temperature, in a backscattering geometry with polarized incident light and without analyser.
Bulk Bi_2Te_3 is a semiconductor which at room temperature presents four Raman active modes. Three Raman active modes of Bi_2Te_3 were detected in our films. The Eg mode at a calculated low-frequency of 50.6 cm^{-1} was not observed probably due to its too weak intensity.
The agreement between the Raman and XRD results in the present work for films and bulk referenced ones allows us to conclude that the system is quite stoichiometric.

16:00 Poster A28

Ge nanocrystals embedded in alumina for non volatile memory applications

Anabela G. Rolo[1], Sara R. Pinto[1], Adil Chahboun[1,2], Maria J. Gomes[1]

1. *Centro de Física, Universidade do Minho, Campus de Gualtar, Braga 4710-057, Portugal* **2.** *Physics Department, Dhar Mehraz Sciences Faculty, Fes BP1796, Morocco*

e-mail: arolo@fisica.uminho.pt

Ge NCs have attracted considerable attention because of their potential applications in nonvolatile memory and integrated optoelectronics. A number of groups have already proposed integrate flash memories based on Ge NCs embedded SiO_2 matrix.
In this work Ge NCs embedded in alumina thin films were deposited over Si (111) substrates using RF co-sputtering technique. Annealing was performed in order to improve the cristallinity of the Ge phase in the films and achieve control over the NCs size [1]. Ge NCs of suitable size and good crystalline quality were obtained by different techniques, including X-ray diffraction, Raman spectroscopy and high resolution transmission electron microscopy. The NCs size was estimated from Raman spectra using Fauchet and Campbell model [2] and from X-ray diffraction using Debye-Scherrer equation. A good agreement between the three techniques for the size estimation was observed for smallest NCs. However, for larger NCs (> 20 nm) there is a discrepancy between XRD and Raman results. For this sample the TO Raman peak presents a blue shift relative Ge bulk and X-ray peaks are shifted for higher angles relative to the Ge diamond structure. A possible explanation for this shift is the compressive stress exerted on Ge NCs by the Al_2O_3 matrix [3]. Further detailed studies are in course in order to clarify both confinement and stress effects.

References:
[1] P. Caldelas et al, in press in Journal Nanoscience and Nanotechnology
[2] I. H. Campbell, F. M. Fauchet, Solid State Commun. 58, (1986) 739
[3] I. D. Sharp et al, Journal. Applied Physics 100, (2006) 114317, and references there in.

Acknowledgements
This work has been partially supported by FCT-Fundação para a Ciência e a Tecnologia-Portugal, and by the "Programa Operacional Ciência e Inovação 2010-POCI 2010" co-financed by FEDER through the Projects POCTI/FIS/56930/2004 and PTDC/FIS/70194/2006. SRCP thanks FCT for the financial support (grant SFRH/BD/29657/2006).

16:00 Poster A29

An array of ferroelectric $PbTiO_3$ nanorods by pulse laser deposition technique

Swati Shandilya[1], Kondepudy Sreenivas[1], Ram Katiyar[2], Vinay Gupta[1]

1. *Department of Physics and Astrophysics, University of Delhi, Delhi 110007, India* **2.** *Department of Physics,University of Puerto Rico, San Juan 00931, Puerto Rico*

e-mail: swatishandilya@rediffmail.com

In the past few years ferroelectric has been the most studied material because of its potential application in non linear optics, sensors, micro-electromechanical systems and non volatile memories. Among different ferroelectric materials, Lead Titanate (PT) found to be an attractive for pyroelectric, electro-optic and non linear optical applications because of its large polarization, high pyroelectric and electro-optic coefficients. It has also been considered promising materials for applications in modern nano-electronics, and MEMs. In today's world nanostructures are gaining lots of attention due to its unique and novel properties as compared to bulk counterpart. However less efforts have been made to grow ferroelectric nanostructures especially in the form of vertically aligned nanorods.

In this work nano-rods of ferroelectric lead titanate (PT) were fabricated on Si substrate by pulsed laser deposition using platinum layer as a catalytic template. The successive settlement of nano-particles one over the other results in the formation of elongated nano-rods under higher oxygen pressure. The diameter of nanorods was found to be 50-90nm. Raman scattering and SEM studies indicated that the fabricated PT nano-rods were of single phase and *a-axis* oriented. The temperature dependent Raman spectra confirming the ferroelectric nature of fabricated PT nano-rods, shows a shift in the soft phonon modes towards lower frequency with increasing temperature and disappear at about 523 K

16:00	Poster	A30

Fabrication and characterization of diameter controlled Ag and Ni nanowires for bio-sensing devices

Shoso Shingubara

Kansai University, Suita 3-3-35, Osaka 564-8680, Japan

e-mail: shingu@ipcku.kansai-u.ac.jp

We have developed a method to fabricated metallic nanowires with a well controlled length and a diameter between 5 and 50 nm. At first, pure Al film was deposited on a low resistivity Si substrate, then it was anodically oxidized at a constant voltage in an oxalic acid of 0.3 M. A well ordered nanohole array (AAO: Aluminum Anodic oxide) was formed by this method, and we further enhanced regularity of nanoholes arrangement by the use of nano-imprinting prior to anodic oxidation.

We formed Ag or Ni nanowires by DC pulse electroplating in AAO nanoholes. Metallic nanowires with an average diameter of 12 nm and 25 nm were obtained at anodic oxidation voltage of 10 and 20 V, respectively. One example of metal nanowires array formed within AAO nanoholes is shown in Fig.1, where polycrystalline Ni nanowire was formed in every hole. Metallic nanowires were separated each other by dissolving porous alumina matrix using NaOH solution. These nanowires are very promising materials for drug delivery or bio-molecular sensing, and further characterizations such as magnetic and SERS properties are in progress.

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16:00	Poster	A31

Fabrication and Raman Studies of Core-Shell Heteronanowires

Hyo Sung Kim, Hyoun Woo Kim

Inha University, School of Materials science and engineering, 253 Yong Hyun Dong, Nam Ku, Incheon 402-751, Korea, South

e-mail: hyosunglove@hanmail.net

Since the discovery of carbon nanotubes, one-dimensional (1D) nanoscale materials have drawn much attention due to their peculiar and interesting physical properties and potential device applications. Recently, coaxial nanocable-like 1D structures comprising different kinds of materials have been successfully synthesized for a variety of purposes, such as making nanometer scale electronic devices with a variety of functions and protecting the 1D structures from contamination or oxidation, etc. Furthermore, as the demand for fabricating special nanowire structures increases, to develop the method not only for synthesizing a wide variety of nanowires but also for modifying or improving the properties of as-synthesized nanowires becomes very important. In the present study, we have fabricated the core-shell heteronanowires and investigated comparatively the core/shell structures before and after coating, with respect to their morphological, structural and Raman characteristics. In addition, the effects of thermal annealing on the Raman spectra have also been scrutinized.

Transparent and Flexible Electronics: from Materials to Devices

Symposium B

Programme

Monday, 15 September

Opening & Plenary Session

Czochralski Award Ceremony
Monday morning, 15 September, 10:00
Small Hall (237)

Lunch break
Monday afternoon, 15 September, 12:30
Inner Courtyards

Transparent conducting oxides
Monday afternoon, 15 September, 14:00
Room 226
Chair: Prof. R. Martins and Prof. G. Kiriakidis

14:00 Invited oral

Electrical transport in zinc oxide based transparent window layers

Klaus Ellmer

Helmholtz Centre Berlin for Materials and Energy, Glienicker Str. 100, Berlin D-14109, Germany

e-mail: ellmer@helmholtz-berlin.de

Zinc oxide (ZnO) research relives a third renaissance since about 15 years, due to its prospective use for opto-electronic devices in the blue and ultra-violet spectral range. Here, one of the main research topics is the p-type doping of ZnO in order to build pn junctions. In order to tune the wavelength, ZnO alloys, for instance with magnesium or cadmium, are investigated. ZnO and its derivatives are also of interest for transparent, conductive electrodes, especially for thin film solar cells [1]. In this field alloying of ZnO is interesting for improving the band alignment in the heterojunction between the absorber and the window and contact layer. In this paper the transport properties of polycrystalline and epitaxial $ZnMe_xO_y$ films are summarized. The films habe been prepared by reactive magnetron sputtering from oxidic targets and by RF (13.56 and 27.12 MHz) plasma excitation. The carrier concentration in these films can be adjusted by small additions of oxygen or hydrogen to the Ar sputtering gas. X-ray diffraction was used to characterize the phases and the structural perfection (strain, grain sizes). By (temperature-dependent) Hall and conductivity measurements the electrical transport properties were analyzed. These data for epitaxial and polycrystalline $ZnMe_xO_y$ films are compared to data from literature and with the reported data of single crystalline ZnO [2]. By photoelectron spectroscopy (PES) the work functions φ of the different $ZnMe_xO_y$ layers have been measured. The expected decrease of φ by alloying with group II elements was observed. Its implications for a better band alignment in thin film solar cells will be discussed.

[1] "Transparent Conductive Zinc Oxide: Basics and Applications in Thin Film Solar Cells"; Edited by K. Ellmer, A. Klein and B. Rech (Springer, Berlin, 2008).

[2] K. Ellmer, J. Phys. D: Appl. Phys. 34 (2001) 3097.

14:30 Oral

p-type ZnO:N thin films fabricated by rf-sputtering in oxygen plasma from ZnN target

Vicky Kambilafka[1], Maria G. Androulidaki[1], Katerina Tsagaraki[1], Zacharias Viskadourakis[2], Elias Aperathitis[1]

1. *Microelectronics Research Group, Institute of Electronic Structure and Laser, Foundation for Research and Technology – Hellas, P.O. Box 1527, 71110 Heraklion, Crete, Greece, P.O. Box 1527, Heraklion 71110, Greece* **2.** *University of Crete, Materials Science and Technology Department, P.O. Box 2208, Heraklion 71003, Greece*

e-mail: eaper@physics.uoc.gr

ZnN is a relatively new material, and even though its physical properties are not well studied and there is a controversy concerning its optical band gap, it has been used for the fabrication of p-type ZnO:N films through oxidation at temperatures ≥400°C. Until now, ZnN thin films had been fabricated by rf-MBE, MOCVD, sputtering or ammonization of Zn and electrochemically. In a recent investigation we had fabricated zinc nitride thin films by rf-sputtering of a commercially available zinc nitride target in a mixture of $Ar-N_2$ plasma and examined the properties of the films [2,3]. These n-type zinc nitride films had been converted into p-type ZnO:N films by oxidation at 400°C [1,2].

In this investigation, we report on the properties of zinc nitride films fabricated from zinc nitride target by rf-sputtering in plasma containing a mixture of $Ar-O_2$ gases on unintentionally heated glass and Si substrates. The structural (X-ray diffraction, AFM), optical (UV-NIR trans. & refl. as well as PL emissions at 18K using a 325nm He–Cd laser) and electrical (Hall effect, Van der Pauw technique, Seebeck effect-thermoelectric power) properties of the films were examined as a function of the oxygen content in the plasma, just after deposition as well as after annealing in flowing nitrogen.

Films deposited in plasma containing 10-40% O_2 were p-type materials with resistivity 10^5 Ωcm. XRD analysis revealed that the films had the ZnO structure. The resistivity of these p-type ZnO:N films was decreased to around 10^3 Ωcm upon annealing in flowing N2.

The possibility of fabricating a p/n junction from the zinc nitride target, in one deposition run without breaking the sputtering vacuum, which is actually a transparent p/n ZnO/ZnN heterostructure, will be addressed.

[1] V. Kambilafka, et al, Superlattices and Microstructures 42 (2007) 55.

[2] V. Kambilafka, et al, Thin Solid Films 515 (2007) 273.

[3] P. Voulgaropoulou, et al, Thin Solid Films (2008) : doi: 10.1016/j.tsf.2008.04.025

14:45 Oral

Transparent p-type ZnO obtained by Ag doping

Eliana Kamińska[1], Iwona Pasternak[1], Piotr Boguslawski[2], Andrzej Jezierski[3], Elzbieta Dynowska[2], Rafał Jakieła[2], Ewa Przezdziecka[2], Emil Kowalczyk[1], Anna Piotrowska[1], Jacek Kossut[2]

1. *Instytut Technologii Elektronowej (ITE), al. Lotników 32/46, Warszawa 02-668, Poland* **2.** *Polish Academy of Sciences, Institute of Physics, al. Lotników 32/46, Warszawa 02-668, Poland* **3.** *Institute of Molecular Physics, Polish Academy of Sciences, Smoluchowskiego 17, Poznań 60-179, Poland*

e-mail: eliana@ite.waw.pl

The most often studied acceptors in ZnO are group-V N, As, and Sb atoms. However, stable and reproducible p-type material with high concentration and high mobility is yet to be achieved. Motivated by the recent reports [1,2] we have studied the efficiency of Ag as an acceptor.

Ag-doped ZnO thin films were fabricated in a two step process in which ZnO/Ag multilayer was first sputter-deposited on sapphire substrate and then heat treatment was performed to obtain a homogeneous distribution of dopant. The Ag content was 1-5 at. %. High-resolution X-ray diffraction, secondary mass spectrometry, and atomic force microscopy analyses assessed a good crystalline quality with a uniform composition. Transport measurement revealed that after moderate temperature (400-500^{o}C) anneals in N_2 flow ZnO:Ag is p-type with carrier concentration above 5x10^{18}cm^{-3}, which compares favorably with group V dopants. Mobility is few cm^{2}/Vs The transmittance of 500 nm thick p-ZnO films in the visible wavelength spectrum was >60%.

In parallel, acceptor level of Ag was calculated based on the density functional theory using the ESPRESSO code [3]. The calculated level of Ag is 0.2-0.25 eV above the top of the valence band. This confirms our experimental results, and shows that ionization energy of Ag is comparable to those of N, As, and Sb. Formation of Ag-related bands with the increasing Ag content was analysed using the Coherent Potential Approximation.

Part of the research was supported by the grant from the Polish Ministry of Science and Higher Education “Bandgap engineering of ZnO-based alloys” N50703131/0743 and the national scientific network (“New materials and sensors for optoelectronics, informatics, energetics and medicine) 72/E-67/SN-033/2006.

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[2] B. D. Ahn, H. S. Kang, J. H. Kim, Gun Hee Kim, H. W. Chang, S. Y. Lee, J. Appl. Phys. **100**, 093701 (2006)

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15:00 Oral

Exploring the optical and electrical properties of $SrCu_2O_2$: theoretical and experimental studies

Mircea Modreanu[1], Michael J. Nolan[1], Simon D. Elliott[1], Ekaterina Chikoidze[2], Bernard Servet[3], Olivier Durand[3,7], Guy Garry[3], Guido Huyberechts[5], Evie L. Papadopoulou[4], Elias Aperathitis[4], Odette Chaix-Pluchery[6], Jean-Luc Deschanvres[6]

1. *University College Cork, Tyndall National Institute (TYNDALL), Lee Maltings, Prospect Row, Cork, Ireland* **2.** *University of Versailles CNRS (GEMAC), 1, Place A. Briand, Meudon 92195, France* **3.** *Thales Research and Technology (TRT), Route Départementale 128, Palaiseau 91767, France* **4.** *Institute of Electronic Structure and Laser, FORTH,, P.O. Box 1527, Vassilika Vouton, Heraklion 71110, Greece* **5.** *Umicore Group Research and Development, Kasteelstraat 7 B-2250, Olen B-2250, Belgium* **6.** *Laboratoire des Matériaux et du Génie Physique, Minatec-Bâtiment INPG, BP 257, Grenoble 38016, France, Grenoble 38016, France* **7.** *Département Matériaux et Nanotechnologies UMR-FOTON, 20 av. des Buttes de Coësmes, Rennes CS14315, France*

e-mail: mircea.modreanu@tyndall.ie

In the framework of a European project, NATCO (Novel Advanced Transparent Conducting Oxides) we are working towards a deeper understanding of the optical properties and conduction mechanism of Cu based TCOs, which are currently the leading p-type TCO candidates. In this contribution, we review and correlate modelling studies and experimental results of optical and electrical properties of $SrCu_2O_2$. Using first principles modeling we have investigated point defects such as Cu and oxygen vacancies providing insights into the origin of p-type conduction. The experimental optical constants of both bulk and thin films of $SrCu_2O_2$ over a large spectral range have been inferred from spectroscopic ellipsometry and reflectance/transmission spectrophotometry measurements. Computed and experimental phonon modes obtained from Raman and Fourier Transform Infrared spectroscopy are reported for the tetragonal $SrCu_2O_2$ phase. In conjunction with XRD and FTIR, Raman measurements provide a more comprehensive understanding of the $SrCu_2O_2$ thin films crystalline structure. The correlation between optical and microstructural properties and the assignment of infrared and Raman active modes for $SrCu_2O_2$ in thin films deposited by Pulsed Laser deposition and MOCVD is discussed. Temperature-resolved optical and electrical properties of $SrCu_2O_2$ thin films will be also presented.

15:15 Oral

Thermochromic VO_2 films with enhanced luminous transparency and solar modulation

Nuru R. Mlyuka, Gunnar A. Niklasson, Claes Granqvist

Uppsala University, Department of Engineering Sciences, The Angstrom Laboratory, Uppsala SE-75121, Sweden

e-mail: nmlyuka@yahoo.com

Vanadium dioxide (VO_2) shows an abrupt change in optical and electrical properties when its temperature is raised beyond a critical point of ~68ºC. Films made from such materials have a potential to be used in smart windows with dynamic throughput of solar radiation. Two of the drawbacks of this material have been its low luminous transmittance and small solar transmittance modulation during switching. In this work we report calculations and experiments on multilayers of VO_2 and TiO_2 films produced by reactive magnetron sputtering, that significantly improve the luminous transmittance and solar modulation of the films during switching.

15:30 Oral

High Conductivity and Light Trapping Surfaces of Lithium and Fluorine-Codoped SnO_2 Films for Dye-Sensitized Solar Cell Applications

Chin-Ching Lin, Mei-Ching Chiang, Chia-Hsin Lin

Industrial Technology Research Institute (ITRI), Q200, UCL/ITRI, No.321 Kuang Fu Road Sec.2, Hsinchu 300, Taiwan

e-mail: chinchinglin@itri.org.tw

High conductivity and transparent tin oxide films have been prepared by temperature controlled spray pyrolysis technique. The codoped films were deposited on glass at temperatures ranging between 300°C and 400°C by ultrasonic spraying a water solution of stannous chloride. Dopants used were lithium chloride and ammonium fluoride for lithium and fluorine codoped tin oxide films. Among undoped tin oxide films, the least resistivity was found to be 4.0 x10^{-3} Ω-cm for a molar concentration of 0.4 M. In case of fluorine doped films it was found to be 6×10^{-4} Ω-cm for a doping percentage of 30 at% of fluorine in 0.4M solution and in case of lithium codoped films minimum resistivity value was found to be 3 x 10^{-4} Ω-cm for a film with (Li/Sn) = 0.03, deposited at 385°C. The corresponding values of the carrier concentrations were found to be $1.8 \times 10^{20}/\text{cm}^3$ and $8.1 \times 10^{20}/\text{cm}^3$, respectively. The electrical property and surface morphology of these films were studied as a function of both doping concentration and deposited temperature. Controllable surface morphologies of high conductivity SnO_2 films could obviously improve the efficiency of light trapping and then enhance the energy conversion efficiency of the DSSCs from 6.5 to 8.0 %. Codoping percentage of lithium and fluorine in the spray solution has been optimized for achieving a minimum electrical resistivity and maximum optical transmittance. The detailed interaction of lithium and fluorine in SnO_2 films will be further studied in future at electron-hole compensation behavior and increasing the solubility of fluorine doping in SnO_2 matrix.

Joint Poster Session I

Flexible and Transparent Electronics I
Monday afternoon, 15 September, 16:00
Main Hall (Monday & Wednesday)

Tuesday, 16 September

New Materials I

Tuesday morning, 16 September, 9:00
Room 226
Chair: Prof. K. Ellmer and Prof. M. Hirano

9:00 Invited oral

Next Generation Transparent Conducting Oxides for Solar Cell Applications

David S. Ginley, Joseph Berry, Christopher Gorrie, Matthew S. White, Matthew Dabney, Dana Olson, Nikos Kopidakis, John Perkins

National Renewable Energy Laboratory (NREL), 1617 Cole Blvd, Denver 80401, United States

e-mail: david_ginley@nrel.gov

In a large variety of opto-electronic devices including solar cells, displays, and OLEDs the transparent contact is becoming an increasingly important part of the devices with many critical parameters beyond transparency and conductivity are important including deposition temperature, work function, smoothness and processibility. We will discuss recent results on some recently emerging TCOs that are beginning to be investigated for PV and related applications. This includes amorphous InZnO a low temperature TCO deposited by DC magnetron sputtering with excellent thermal stability, smoothness and processibility. Conductivities as high as 5000 S/cm have been reported for films and recent results indicate it may be chemically more stable in use in CIS cells than conventional materials. We also investigate Ga doped ZnO which has shown conductivities to 10,000 S/cm by PLD but these have not easily been replicated by sputtering. The material has shown excellent results in OLEDs in place of InSnO. ZnO is also a key element in hybrid OPV devices. We will report on the use of sub-monolayer and monolayer TiO_2 to significantly improve the interfacial properties of ZnO/P3HT solar cell devices and Mg substitution to significantly improve the Voc. Finally we discuss the potential of Nb:TiO2 as a novel new TCO material with a much higher refractive index than conventional TCO materials.

9:30 Oral

Oxide acceptor layers with doping gradients as electron acceptors in polymer/oxide bilayer photovoltaic devices.

Matthew S. White[1,2], Joseph Berry[1], Nikos Kopidakis[1], Dana Olson[1], David S. Ginley[1]

1. *National Renewable Energy Laboratory (NREL), 1617 Cole Blvd, Golden, CO 80401, United States* **2.** *University of Colorado, Boulder, CO 80309, United States*

e-mail: matthew_white@nrel.gov

Hybrid organic/inorganic photovoltaic (h-OPV) devices have emerged as an interesting class of solid-state organic devices. Oxides offer several customizable properties, such as morphology, band offset, dielectric constant, and doping level that make them desirable from both a scientific and a manufacturing standpoint. By simply varying the oxide from ZnO to TiO2, or by depositing thin layers of TiO2 onto ZnO, it is possible to increase the VOC in a device by roughly a factor of 2 from ~350mV to ~600mV. JSC is somewhat diminished in devices with TiO2, but the fill factor of the devices is often abnormally low, due to a double-diode characteristic. The fill factor is greatly influenced by the dielectric constant of the bulk oxide and the doping level. This study utilizes pulsed laser deposition (PLD) to deposit oxide films, with doping gradients through the film thickness, as electron acceptor layers in bilayer h-OPV devices with P3HT donor layers. PLD films are deposited at less than a monolayer per pulse, which allows for a high degree of control in the doping levels. Doping in the oxide layer largely determines recombination kinetics of geminate electron-hole pairs at the donor-acceptor interface.

9:45 Oral

Balanced electron and hole mobility in organic/inorganic hybrid materials

Maria Hammer[1], Daniel Rauh[2], Carsten Deibel[1], Vladimir Dyakonov[1,2]

1. *University of Würzburg, Experimental Physics VI, Am Hubland, Würzburg 97074, Germany* **2.** *ZAE Bayern, Bavarian Centre for Applied Energy Research, Am Hubland, Würzburg 97074, Germany*

e-mail: maria.hammer@physik.uni-wuerzburg.de

The efficiency of bulk heterojunction solar cells is known to suffer from unbalanced electron and hole transport within the donor and acceptor material. Using an inorganic component offers the possibility of setting up its transport properties namely mobility, conductivity and charge carrier density and adjusting it to an optimum for the combined performance with the organic material. Our measurements on field effect transistors made of the organic semiconductor poly(3-hexylthiophene) and the variedly doped inorganic Al-doped Zinc Oxide nanoparticles allow the determination of charge carrier mobility in dependence of the accumulated charge carrier densities and temperature. With respect to the morphology, we survey the properties of the transport in disordered systems, organic and inorganic, considering the underlying transport models. Furthermore we compare the effect of doping induced and accumulation induced increase in charge carrier density. Whereby the former goes along with additional defect states and the latter remains at a constant trap density. We show that by doping Zinc Oxide nanoparticles it is possible to adjust a balanced electron and hole transport in the hybrid material.

10:00 Invited oral

Recent Progress in ZnO-based Transparent Electronics

David J. Rogers, Ferechteh Hosseini Teherani

Nanovation, 103 bis rue de Versailles, Orsay, Orsay 91400, France

e-mail: d.j.rogers@nanovation.com

This talk reviews the recent progress in the development of transparent electronics based on ZnO.

Wurtzite ZnO is a wide bandgap material (~3.34eV) with an intrinsically high transparency in the visible range and a resistivity that can be tuned from semi-insulating right through to semi-metallic. Compared with other Transparent Conduction Oxides (TCOs), ZnO has the lowest toxicity, the lowest cost and is the most amenable to chemical etching. When doped with fluorine, it also has the highest optical transparency and the lowest plasma frequency. Moreover, ZnO can be readily fabricated in crystalline form at relatively low temperatures using large-area deposition techniques [1]. These properties have led to the adoption of ZnO for a number of TCO applications, such as coatings for UV filtering and contacts for use in flat panel displays, solar cells and LEDs.

Recently, there has been a surge of activity in the development of next-generation Transparent Thin Film Transistors (TTFT) for use in applications such as electronic paper and flexible organic LED panels. Amongst the TCOs attracting the most interest at present are wurtzite ZnO and amorphous $InGaZnO_4$ (a-IGZO). This is due mainly to increases in the carrier mobilities which can be achieved with these materials. Indeed, typical mobilities for TTFTs made with state-of-the-art ZnO and a-IGZO are $250cm^2/Vs$ and $100cm^2/Vs$, respectively, as compared with values of $100cm^2/Vs$ and $1cm^2/Vs$ for the polycrystalline and amorphous Si TTFTs, used in today's LCD displays.

Currently, there is also a lot of work into the development of p-type ZnO. If these efforts succeed, we can expect a further generation of transparent electronics which moves on from discrete TTFTs to transparent integrated circuits and completely transparent electronic products [2].

[1] R. G. Gordon, MRS Bulletin, August (2000) 52

[2] http://techon.nikkeibp.co.jp/article/HONSHI/20071024/141211/

Coffee break

Tuesday morning, 16 September, 10:30
Main Hall

New Materials II

Tuesday morning, 16 September, 11:00
Room 226
Chair: Dr. D. Rogers and Prof D. Ginley

11:00 Invited oral

Smart Windows using Thermochromic VO_2 Films as an Environmental Technology

Yuzo Shigesato

Aoyama Gakuin University, Graduate School of Science and Engineering, 5-10-1 Fuchinobe, Sagamihara 229-8558, Japan

e-mail: yuzo@chem.aoyama.ac.jp

There are so many interesting materials which can be applied for energy-efficient windows. (1) Vanadium dioxide (VO_2) is one of the most attractive thermochromic materials, which shows large changes in optical and electrical properties at around 68°C, nearly room temperature. This thermochromic behavior has been explained in terms of the Mott-Hubbard transition from a high-temperature rutile structure (metal phase) to a low-temperature monoclinic structure (semiconductor phase). We already reported that r.f. magnetron sputtering using V_2O_3 or V_2O_5 targets enable us to deposit polycrystalline thermochromic VO_2 films with high reproducibility by introduction of oxygen gas ($O_2/Ar+O_2=1$□1.5%) or hydrogen gas ($H_2/Ar+H_2=2.5$□10%), respectively, as reactive gases. (2) However, the thickness of the VO_2 films should be larger than 400 nm because stoichiometry x of the VO_x film deposited on glass substrate was higher than 2 (slightly over-oxidation state) in the early stages of the film growth. In this study, ZnO polycrystalline films were deposited as a buffer layer between the VO_2 film and glass substrate also by r.f. magnetron sputtering, which have been known to exhibit <001> preferred orientation in the wide range of the deposition conditions. Very thin thermochromic VO_2 films with thickness of 70 nm were successfully deposited on the ZnO coated glass substrate because of the heteroepitaxial relationship of $VO_2(010)[100]//ZnO(001)[100],[010],[\bar{1}\bar{1}0]$. (3) Such thin VO_2 films could be applied for the “smart windows” of the high total energy efficiency in various architectures or automobiles.

11:30 Oral

Diffusion profiles of transition metals (TM= Co or Mn) in ZnO and GaN incorporated by annealing of thin TM film

Mac Mugumaoderha Cubaka[1], Jacques A. Dumont, Jacques Ghijsen[1], Wolfgang Drube, Bogdan J. Kowalski[2], Cathérine Moisson[4], Laurent Houssiau[1], Robert Sporken[1,3]

1. *University of Namur (FUNDP), rue de Bruxelles 61, Namur 5000, Belgium* **2.** *Polish Academy of Sciences, Institute of Physics, al. Lotników 32/46, Warszawa 02-668, Poland* **3.** *University of Illinois at Chicago, Chicago, Il 60607, United States* **4.** *NOVASiC Savoie Technolac, Le Bourget du Lac 73375, France*

e-mail: mac.mugumaoderhacubaka@fundp.ac.be

Injecting spin-polarized carriers electrically into a spintronic device remains a challenge that could be solved using Diluted Magnetic

Semiconductors (DMS). Room temperature ferromagnetism can be achieved in DMS based on wide bandgap semiconductors (eg. GaN or ZnO). Nevertheless the structural and electronic properties of these wide bandgap DMS must be further studied in other to explain the origin of this ferromagnetic character.

The aim of this work was to investigate the structural and electronic properties of (Zn,TM)O and (Ga,TM)N layers obtained by thermal diffusion of thin films (≤ 2nm) of TM (TM = Mn or Co) into ZnO and GaN single crystals.

The samples were characterised in-situ by scanning tunnelling microscopy (STM), Auger electron spectroscopy (AES), low energy electron diffraction (LEED), High energy X-ray Photoemission Spectroscopy (XPS) and ex-situ by time of flight secondary ion mass spectroscopy (ToF-SIMS). The present abstract will mainly refer to AES results. From the evolution of the intensity of TM, Zn, O, Ga, and N Auger lines upon annealing, and thanks to modelling of the attenuation of Auger lines by matter we could describe the diffusion profile of TM into ZnO and GaN under various conditions. The results of the model were then compared to ToF-SIMS depth profiles.

Upon annealing, coalescence of the TM film into 3D islands is observed followed by diffusion and substitution.

In the case of TM/ZnO, the (Zn$_{1-x}$,TM$_x$)O layer is very thin (~6.6 nm), with x~0.5. According to High energy XPS on Co/ZnO system, at 800 K oxidation of Co into CoO is complete.

In case of the Mn/ZnO system, a Moiré structure is observed on the LEED pattern. From the Auger data, Mn seems to remain at the surface of ZnO in the form of a stable oxide layer.

For Mn/GaN, Ga atoms substituted by Mn segregate towards the surface. Annealing the system up to 910K induces formation of a (Ga$_{0.8}$,TM$_{0.2}$)N layer with thickness of ~ 18.6 nm.

11:45 Oral

Study of the influence of crystal orientation and bond polarity on the potentiometric response of III-N surfaces

Nikoletta G. Sofikiti[1], George Tsiakatouras[2], Eleftherios Iliopoulos[2], Alexandros Georgakilas[2], Nikos Chaniotakis[1]

1. *University of Crete, Chemistry Department, Voutes P.O Box 2208, Heraklion 71003, Greece* **2.** *Microelectronics Research Group, Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas, and University of Crete, Physics Department (MRG), Heraklion 71110, Greece*

e-mail: niksof@chemistry.uoc.gr

GaN has shown to be a very unique material for the development of chemical sensors and biosensors, mainly due to its semiconductor properties and its increased chemical stability.

We have shown previously that GaN (0001) grown on sapphire can be used as sensor element, or transducer, for the development of electrochemical sensors. In particular, we developed an all solid-state GaN-based sensor that shows anion sensitivity. Potentiometric and impedance spectroscopy proved that the observed electrochemical sensitivity originates from the direct interaction of the anions in the solution with the acidic gallium (III) on the surface of the GaN (0001) crystal. This is also supported by the fact that the gallium atoms are electron deficient due to the induced polarity of the Ga to the N bond, enhancing the electrostatic interaction between the Lewis basic anions. It has thus been concluded that the mode of response originate from the direct interaction of the reactive Lewis acidic gallium atoms with the Lewis bases in solution (OH$^-$, Cl$^-$ etc) and not with Lewis acis (H$^+$, K$^+$ etc).

Moving one step forward, in this work we will present our recent study in which we investigate how crystal orientation and/or induced polarity of the outer surface atom influence the potentiometric response of these III-N surfaces. More particular, in this work two differently crystal oriented GaN surfaces (c-plane, Ga-face and a-plane) as well as InN (In-face) surface are examined and compared. According to the observed results it is shown that crystal orientation has little or any effect on the potentiometric response of these materials, while the bond polarity and thus the electron deficiency of the outer atom of these surfaces has a greater influence on their potentiometric response.

12:00 Oral

Synthesis and Characterization of host-guest materials with charge transfer complexes of Coumarin:TCNQ inserted into hydrotalcite for LED applications.

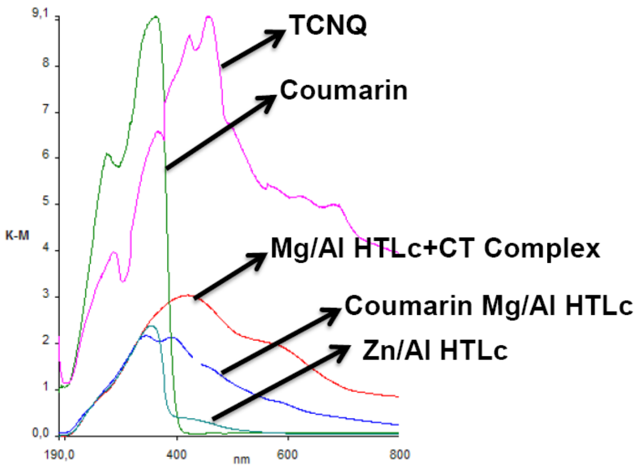
Sumeet Kumar, Leonardo Marchese, Marco Milanesio, Enrico Boccaleri

Università degli Studi del Piemonte Orientale and NANO-Sistemi Interdisciplinary Centre (DISTA), Via V. Bellini 25/G, Alessandria 15100, Italy

e-mail: sumeet.kumar.iitk@gmail.com

Recent study of charge transfer (CT) effects on hole injection and device stability in an Organic thin film transistor (OTFT)[1]and its stability supposedly by the complex formation of poly(9,9-dioctylfluorene-alt-bithiophene) doped with an 8 % of electron-acceptor 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane, study of photo-physical features[2] and further organization of chromophores into layered double hydrotalcite (LDH) like materials[3] motivated us to follow a similar approach.The possible interactions between CT pairs with the LDH host have been investigated. We present the work done in synthesizing luminescent materials based on coumarin-3-carboxylic acid (3CCA) and 7,7,8,8-tetracyanoquinodimethane (TCNQ). An in situ hydrothermal synthesis is carried out to intercalate the 3CCA alone at first and then the CT complex into the LDH Hydrotalcite, following a one-pot synthesis approach. In fact the organic-inorganic hybrid materials have been obtained by dissolving 5 mmol each of 3CCA and TCNQ with 10 mmol of hydrated Aluminium nitrate and 20 mmol of (Zn/Mg) nitrate hydrate salts with at a controlled pH of 7.5±0.5 and CO$_2$ free water solvent. A LDH sample with empirical composition:

[M(II)$_{0.65}$ M(III)$_{0.35}$ (OH)$_2$](A$^-$)$_{0.175}$.nH$_2$0], where MII = (Mg^{2+}or Zn^{2+}), MIII = Al^{3+}, and A$^-$= anionic CT complex was obtained. The effect of the M(II) cations was studied by synthesizing Mg/Al HTLc and Zn/AlHTLc [M(II)/M(III) = 2.0]. Finally the samples were washed with decarbonised water, dried at 60 °C and characterized by XRPD/FTIR/IR/FT Raman/UV Vis/TGA techniques. A clear absorption edge with DR-UV-Vis Lambda 900 is observed for the Mg/Al HTLc with 3CCA and with its CT complex with TCNQ (See figure). The [Mg/Al HTLc + CT complex/or 3CCA alone] also shows luminescence in the visible.



Ref:
[1] Hong-Ku et al. / J. Mater. Chem., 2007, 17, 1416-1420.
[2] U. Costantino et al. / J. Mater. Chem., 2002, 12, 3316-3323.
[3] L. Latterini et al. / Inorganica Chimica Acta 360, 2007, 728-740.

12:15 Oral

Photo- and electroluminescence properties of hybrid nanocomposites based on conjugated polymers

Oleg Posudievsky, Vitaly Pokhodenko

L.V.Pisarzhevsky Institute of Physical Chemistry of the National Academy of Sciences of Ukraine, prospect Nauki 31, Kiev 03028, Ukraine

e-mail: posol@inphyschem-nas.kiev.ua

The objectives of the present work was the preparation of new hybrid guest-host nanocomposites based on semiconductive conjugated polymers, creation on their basis of materials for light-emitting diodes, analysis of photo- and electroluminescence properties of the polymers in confinement conditions.

In the present report the results connected with preparation and research of the structure of hybrid nanocomposites based on polymers of polyphenylenevinylene type and also mesoporous silicon dioxide and molybdenum oxide with the layered structure are presented. The possibility of forming nanocomposites possessing guest-host structure, when the macromolecules of the conjugated polymers are localized inside nanosized galleries or channels of the oxide matrix, is shown.

Considerable difference in spectra of optical absorption, photo- and electroluminescence of the prepared hybrid nanocomposites from similar properties of the neat conjugated polymers is established. The obtained results are interpreted on the basis of mainly straightened conformation of the polymer chains and weakening of intermolecular interaction due to the confinement influence of the inorganic matrix. The presented data testify to possibility of creation of light-emitting diodes on the basis of the hybrid nanocomposites materials characterized, in comparison with individual polymer analogues, by increased luminescence intensity and higher environmental stability.

Lunch break

Tuesday afternoon, 16 September, 12:30
Inner Courtyards

Applications I

Tuesday afternoon, 16 September, 14:00
Room 226
Chair: Prof. Y. Shigesato and Prof. G. Kiriakidis

14:00 Invited oral

Prospects for Flexible and/or Transparent Electronics

John F. Wager

Oregon State University School of EECS, 4091 Kelley Engineering Center, Corvallis 97331-5501, United States

e-mail: jfw@ece.orst.edu

The development of transparent thin-film transistors (TTFTs) leads to the possibility of invisible circuits and electronic systems. If TTFTs can be fabricated on bendable, see-through substrates, the realization of flexible transparent electronics is a possibility. However, accomplishing this commercially will be challenging. The purpose of this presentation is to first provide an introductory overview of transparent electronics, and to then assess challenges and opportunities for its advance and merger with flexible electronics.

14:30 Oral

OWLS See in the Darkness: a Label Free Microbiological Detection Method with SiTiO and InSnO Coated Planar Waveguide Sensor

Károly Somogyi, Istvan Szendro, Katalin Erdélyi, Zsolt Puskás, Márk Fábián

MicroVacuum, Kerékgyarto u. 10, Budapest H-1147, Hungary

e-mail: karoly.somogyi@microvacuum.com

The surface sensitivity of an optical waveguide is higher in the case of thin planar waveguides with a greater specific surface. The evanescent field of the light will detect the surface coating. Such optical waveguide lightmode sensors were developed on the basis of transparent $Si_xTi_{1-x}O_2$ layers with the necessary grating and can be successfully operated both in inorganic chemistry and in life sciences as label free biosensors. On the other hand, voltammetric and/or potentiometric electrochemical measurements also play paramount importance in the same and similar investigations. Since the optical waveguide lightmode detection method allows a label free approach in microbiological investigations with high sensitivity, presently the need of the combination of these mentioned two methods is of vital importance.

$Si_xTi_{1-x}O_2$ is a dielectric and the electrochemical measurements require a conducting electrode, thus, optically transparent, but conductive thin layer must be deposited on the grated optical sensor. Basically indium-tin-oxide (ITO) nanolayer covered chips were developed. At about 10 nm thick ITO layers show sufficiently good electrical conductivity and their good optical transparency corresponds to the requirements of the optical sensing. Outstanding sensibility of the ITO coated sensor chips on any surface modifications allows a highly attracting application of these layers.

It was demonstrated that the presence of the electrical field in an electrochemical cuvette incorporated into an integrated measuring instrument affects both the transport and the adsorption/desorption processes of the investigated species at the surface of the sensor. Lactic acid bacteria were adsorbed in native form on the surface of the sensor chips by ensuring polarizing potential (1 V) and were exposed to various chemical stressors and the behaviour of bacteria was monitored.

14:45 Oral

Electrical and optical properties of $Li_xNi_{1-x}O_2$/In:$Mg_xZn_{1-x}O$ heteroepitaxial junction grown on TiN buffered Si

Hon Fai Wong, Chun Hei Lau, Kin Hung Wong

Department of Applied Physics and Materials Research Centre,The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong 00-852, China

e-mail: 07900999r@polyu.edu.hk

P-type Li doped NiO (LNO) and n-type In doped cubic $Mg_xZn_{1-x}O$ (In:MZO) thin films were grown on TiN buffered Si(100) substrates by pulsed laser deposition. X-ray diffraction characterization revealed a heteroepitaxial relationship of $(001)_{LNO}||(001)_{MZO:In}||(001)_{TiN}||(001)_{Si}$. These heterojunctions showed reasonable rectifying current-voltage characteristics. The typical current turn-on voltage at room temperature was about 2.3V. It decreased to 2.1V at 100°C. Spectral responses of these heterojunctions were measured in the near UV region. Photocurrent as a function of irradiation intensity was evaluated using a He-Cd laser with 325 nm wavelength. Our results have suggested that LNO/In:MZO heterojunction is a potential candidate for photovoltaic UV detection.

15:00 Oral

Wide Band Gap Conducting Polymer

Alexei N. Lachinov[1], Victor M. Kornilov[1], Sergei N. Salazkin[2]

1. *Institute of Molecules and Crystal Physics, Ufa Scientific Centre of Russian Academy of Sciences, 151 Prospekt Oktyabrya, Ufa 450075, Russian Federation* **2.** *Institute of Organoelement Compounds RAS, 28 Vavilov St., Moscow 119991, Russian Federation*

e-mail: lachinov@anrb.ru

The paper presents review of experimental results on the charge transport study in the polymer materials, possessed charge instability [1]. The base of these materials is noncojugated polyaromatic compounds [2]. Characteristic feature these materials is a wide of band gap up to 4.3 eV and the value of first ionization potential about 6 eV. Electronic energetic parameters like these are typical for insulator materials. However it was established that there are not only hopping mechanism of charge transport possible but coherent too in such organic systems. Wide band gap organic material capable to transport charge carrier effectively under certain conditions and the same time conductivity can reach 10^5 $(\text{Ohm}\cdot\text{cm})^{-1}$value and current density up to 10^6 A/cm^2 and more. Transformation to conducting phase may occur with different fields and influences, such as electric field, magnet field, pressure, temperature and others. These transformations are reversible as a rule.

The common point of view on high conductivity mechanism in wide band polymer is absent now.

It is possible to create metal like conductivity in organic material during the polymer film formation. This phenomenon was used for preparing full organic transparent conductive adhesive (OTCA). All components of the OTCA are soluble organic compounds. High level conductivity is a result of insulator to metal transition, which occur during curing procedure. Conductivity reach up to 10^5 (Ohm cm)$^{-1}$ and transparency to 95% after the curing. The OTCA has a high anisotropy of conductivity. The paper discusses different areas of application for new flexible, transparent conducting polymer materials.

References

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15:15 Oral

Tandem Dye Sensitised Solar Cells

Udo Bach, Andrew Nattestad, Yi-Bing Cheng

School of Physics and Materials Engineering, Monash University, Australia, Melbourne, Australia

e-mail: udo.bach@sci.monash.edu.au

Tandem solar cell concepts are currently successfully applied in conventional pn-junction solar cells with enhanced energy conversion efficiencies of up to 40 %. Several tandem concepts have recently been introduced in the area of dye-sensitized solar cells, such as stacking of preassembled dye-sensitized solar cells, the combination of complete dye-sensitized solar cells with CdTe inorganic solar cells as well as the combination of dye-sensitized photocathodes with dye-sensitized photoanodes (pnDSSCs). The latter is of particular interest as it requires only marginally higher fabrication costs, compared to other concepts that involve stacking of complete preassembled cells, which de facto results in a doubling of manufacturing costs. In this work we will present a more detailed analysis of dye-sensitized p-type nano-structured nickel(II)oxide electrodes as a model system for dye-sensitized photocathodes. We presented a novel preparation method to fabricate nanostructured NiO electrodes based on a preformed NiO nanopowder. Critical properties such as pore-size distribution, crystallinity and internal surface area of the resulting films were optimised for their application as dye-sensitised photocathodes. Film preparation conditions were found to strongly influence the nanostructure and photovoltaic performance of dye-sensitised nanostructured NiO photocathodes. Under optimised conditions NiO based cells show photon-to-electron conversion efficiencies beyond 50%, suggesting that there are no fundamental limitations to achieving photocathodes that can match the photocurrent outputs of conventional dye-sensitized photoanodes. This work shows that there should be no fundamental limitations for the development of novel efficient dye-sensitised tandem solar cells. Further advancements will require the identification of nanostructured p-type semiconductor materials with optimised band positions for their use in conjunction with dye-sensitised TiO2 photoanodes.

Coffee break

Tuesday afternoon, 16 September, 15:30
Main Hall

Oxides

Tuesday afternoon, 16 September, 16:00
Room 226
Chair: Dr. H. Kumomi and Dr. D. Rogers

16:00 Invited oral

Transparent Integrated Circuit with ZnO TFT and TCO

Cs Hwang[1], Sang-Hee K. Park[1], Chun-Won Byun[1], Min-Ki Ryu[1], Jaeheon Shin[1], Woo-Seok Cheong[1], Doo-Hee Cho[1], Sung Min Yoon[1], Sung Mook Chung[1], Jeong Ik Lee[1], Hye Yong Chu[1], Ik-Seok Yang[2], Oh-Kyong Kwon[2]

1. *Electronics and Telecommunication Research Institute (ETRI), 161 Gajeong-Dong, Daejeon 305-350, Korea, South* **2.** *Hanyang University, 14-509, Heangdang-Dong, Seong-dong-Gu, Seoul 133-791, Korea, South*

e-mail: hwang-cs@etri.re.kr

Transparent oxide semiconductor materials make it possible to realize transparent electronic devices. In 2006, we reported for the first time the possibility of transparent AMOLED with ZnO TFT backplane in SID. Some companies also presented transparent AMOLED panel since 2007. But, the number of transistors for unit pixel of AMOLED is small. To realize true transparent electronics, we should integrate many TFTs together with transparent electrodes. In this meeting, highly transparent and practically integrated circuit (e.g. 47-stage ring oscillator) with ZnO TFT and TCO will be presented.

The control of threshold voltage of TFT is one of the basic conditions for integration of many TFTs. For the oxide TFT with top gate structure, we could control the threshold voltage with optimizing the back-channel interface.

To minimize the area of integrated circuit and improve the characteristics of integrated circuit, the decrease of channel length is imperative. We propose the scale down of thickness in oxide TFT could be a general solution for this problem. With the advantage of ALD process, accurate control of the thickness of deposited thin film, we could optimize the thickness of various films in the ZnO TFT for the application of constructing integrated circuit.

The resistance of transparent electrode is another big issue for maximize the transparency of integrated circuit. Actually, the metal layer has been included partially in the presented transparent AMOLED panel. The structured transparent electrode layer with the combination of oxide and thin metal layer showed that maintaining transparent and decreasing apparent sheet resistance as low as 2~5 ohm/sheet is possible.

The realization of practical transparent electronics seems likely to happen in the near future with well controlled and scale-downed oxide TFT and transparent electrode having conductivity comparable with metal layer.

16:30 Oral

In situ interferometry characterization of MOCVD grown ZnO on (100)-silicon

Jens-Peter Biethan, Laurence Considine, Dimitris Pavlidis

Darmstadt University of Technology, Department of High Frequency Electronics, Merckstr. 25, Darmstadt 64283, Germany

e-mail: biethan@hfe.tu-darmstadt.de

ZnO is an attractive transparent semiconductor material for electronic and optoelectronic applications. Compared to GaN, one of the major competitors of ZnO, ZnO has a higher binding energy, higher saturation velocity and exhibits better radiation hardness. ZnO has been already deposited on various substrates such as sapphire, glass or GaN, but only few reports exist on its deposition on silicon. The use of silicon as a substrate presents major advantages compared with other substrates. First, high quality silicon wafers can easily be obtained at low cost and second their resistivity can be relatively low.

Here we report the successful growth of ZnO on (100)-silicon wafers using an Aixtron 200 MOCVD system. To achieve good crystal quality and to address the issue of difference in crystal structure between the layers and the substrate, a low temperature nucleation buffer layer was first deposited on the silicon surface. Oxygen and DEZ were used as precursors while the carrier gas was selected to be nitrogen. The layer features were monitored using a homemade in situ laser interferometer. A red and a green laser were used for this purpose. To drastically minimise parasitic noise a notch filter was placed in front of a photodetector. A typical nucleation layer involves a two stage growth process where island formation results in reduction of reflectivity, followed by growth of either flat top areas covering the islands or of a planar layer leading to the start of an oscillation. A slight reduction of the reflected light intensity was observed shortly after DEZ was introduced. This effect could be described by diffusion scattering in the established Vollmer-Weber growth of islands. The subsequent increasing intensity of the laser signal marks the point were ZnO planar growth starts. High temperature ZnO layer growth starts following a heating step. Here typical well known thickness oscillations are observed by interfero-

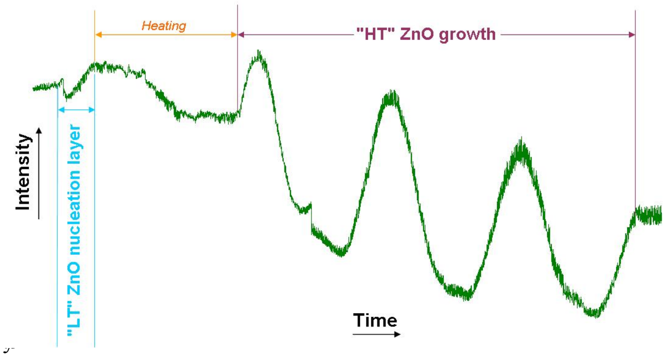

Fig. 1: Interferometer data LT and HT growth

16:45 Oral

Atomically-flat $ScAlMgO_4$ single-crystalline films fabricated by reactive solid-phase epitaxy; Effects on growth of ZnO and GaN

Takayoshi Katase[1], Kenji Nomura[2], Hiromichi Ohta[2,3], Hiroshi Yanagi[1], Toshio Kamiya[1,2], Masahiro Hirano[2,4], Hideo Hosono[1,2,4]

1. *Materials and Structures Laboratory, Tokyo Institute of Technology (TOKYOTECH), R3-1, 4259 Nagatsuta, Midori-ku, Yokohama, JAPAN, Kanagawa 226-8503, Japan* **2.** *ERATO-SORST, Japan Science and Technology Agency, in Tokyo Institute of Technology, Mailbox S2-13, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan* **3.** *Garaduate School of Enginnering, Nagoya University (NAGOYAU), Nagoya university, Furo-cyo, Chikusa-ku, Nagoya 464-8603, Japan* **4.** *Frontier Reserch Center, Tokyo Institute of Technology (FRC), R3-1, 4259 Nagatsuta, Midori-ku, Yokohama, Kanagawa 226-8503, Japan*

e-mail: katase@lucid.msl.titech.ac.jp

ZnO and GaN have been investigated for optoelectronic devices including UV-LEDs and TFTs. However, they are, in general, grown on c-sapphire or YSZ single crystal substrates but these have large lattice mismatchings with ZnO and GaN (Da/a > 10 %), which leads to a three-dimensional spiral grain growth and high-density defects. Therefore a lattice matched substrate or buffer layer is important to reduce the defects and to improve carrier transport properties [1]. Homologous series compounds such as $ScAlMgO_4$ (SCAM) with the chemical formula of $RMO_3(AO)_3$ have good lattice matching with ZnO and GaN (Da/a ~ 0.1 %).

Here we report the fabrication of single-crystalline thin films of SCAM on (111)-oriented YSZ single crystals by PLD and their application to buffer layers for ZnO and GaN. The SCAM films were fabricated by reactive-solid phase epitaxy (R-SPE) using bilayer composed of amorphous-SCAM / thin epitaxial ZnO template (~10 nm) [2].

In preliminarily experiments, it was found that 20mol% excess addition of Sc_2O_3 was necessary to obtain pure SCAM films. To obtain atomically-flat SCAM films, 40% Zn was added with respect to Mg in the PLD target. Finally, step-and-terraced epitaxial films were obtained with the relationships of $[000l]_{SCAM}$ // $[111]_{YSZ}$ in out-of-plane and $[11\text{-}20]_{SCAM}$ // $[1\text{-}10]_{YSZ}$ in in-plane. The SCAM layers were applied to buffer layers for growing ZnO and GaN films. The SCAM buffer layer enhanced the lateral growth of the ZnO layer to > 1 micrometer and resulted in step and flow growth at 800 ^oC. For GaN films grown by N_2 source RF-MBE on the SCAM, residual carrier concentration was reduced to ~ 4.0×10^{17} cm^{-3} and Hall mobility was increased to ~140 cm^2/Vs compared to ~2.0×10^{18} cm^{-3} and ~120 cm^2/Vs for GaN on Al_2O_3 (0001) a low temperature GaN buffer layer.

[1] A. Ohtomo et al., *Appl.Phys.Lett.*75, 17 (1999). [2] H. Ohta et al., *Adv.Funct. Mater.*13, 2 (2003).

17:00 Oral

Co-sputtered dielectrics for transparent electronics

Luis Pereira[1], Pedro Barquinha[1], Gonçalo Gonçalves[1], Anna Vila[2], Joan R. Morante[2], Elvira Fortunato[1], Rodrigo F. Martins[1]

1. *Materials Science Department, CENIMAT-IxN and CEMOP-UNINOVA, FCT-UNL, Campus da Caparica, Caparica, Caparica 2829-516, Portugal* **2.** *Electronics Department, University of Barcelona, C\ Martí i Franqu?s, Barcelona 08028, Spain*

e-mail: lmnp@fct.unl.pt

In this work it is presented a study on the structural, compositional and electrical properties of HfO_2, HfO_2/SiO_2 and HfO_2/Al_2O_3 dielectric layers deposited by sputtering without any intentional substrate heating. The films were deposited from 2 inches ceramic targets of HfO_2, SiO_2 and Al_2O_3 using argon (Ar) and oxygen (O_2). The incorporation of SiO_2 and Al_2O_3 was obtained by co-sputtering and it was controlled by adjusting the r.f. power ratio on the targets.

The HfO_x films present a microcrystalline structure even when deposited at room temperature. The average grain size determined by the Scherrer formula may overcome 100 nm depending on the processing conditions. The crystallinity decreases with the oxygen flow due to a reduction on the energy of the species reaching the substrate, associated with the decrease on the deposition rate. However, the lowest leakage current in crystalline silicon MIS structures (below 10^9 Acm^{-2} at 10V on films with a thickness around 180 nm) was obtained for a ratio Ar/O_2 of 14/1 sccm, indicating higher oxygen flow does not lead to further improvement on the electrical characteristics.

The co-deposition of SiO_2 has a strong influence on the structure since the films become amorphous. Also the roughness is decreased where the values determined by spectroscopic ellipsometry are less than an half of those obtained for HfO_x films. The refractive index stays between the values for pure HfO_2 and SiO_2 and the gap increases more than 0.4 eV, confirming the incorporation of silicon oxide. The leakage in MIS structures is reduced by a factor of 2. Only the dielectric constant is negatively affected due to the lower value for the SiO_2. The same structural effect is observed when using Al_2O_3 instead of SiO_2. Again, the refractive index and the band gap confirm that HfO_x films are incorporating aluminum oxide. The reduction on the dielectric constant may be minimized since the value for pure Al_2O_3 is around 9.

17:15 Oral

Incorporation of CdTe nanocrystals into metal oxide matrices: An inorganic technique for nano-composit material preparation

Elena V. Frolova, Vladimir Lesnyak, Tobias Otto, Nikolai Gaponik, Alexander Eychmüller

Physical Chemistry and Electrochemistry TU Dresden (TU), Bergstraße 66b, Dresden 01062, Germany

e-mail: elena.frolova@chemie.tu-dresden.de

Semiconductor nanocrystals (NCs) dispersed in optically transparent metal oxides have promising applications for optical switching, optical filters, waveguides and solar cells. Optical losses in thin film solar cells arise e.g. from reflections at interfaces where dielectric discontinuities may be significant, such as at the interface between glass and transparent conducting oxide (TCO) or between the TCO and semiconductor NC layers. Advanced optical engineering approaches like the incorporation of semiconductor NCs into the TCO are necessary to minimize such losses. A few works have been performed on the incorporation of CdSe and/or CdTe NCs into SiO_2, TiO_2 and SiO_2-ZrO_2 matrices, respectively. The main problem in these systems is the degradation of the optical properties of the NCs as a result of the incorporation process. In this work we report on a fully inorganic incorporation technique of NCs into sol-gel prepared metal oxide and TCO matrices. Optimal synthetic and incorporation parameters have been found to secure the PL of the NCs in Al_2O_3 and Al_2O_3-SnO_2 systems. The optical and structural properties of these systems as well as the incorporation mechanism will be discussed.

Wednesday, 17 September

Applications II

Wednesday morning, 17 September, 9:00
Room 226
Chair: Prof C. Hwang and Prof. C. Granqvist

9:00 Invited oral

Flexible Electronic Paper Driven by Transparent Amorphous Oxide TFT

Manabu Ito

Toppan Printing Co., Ltd, 4-2-3 Takanodai-Minami, Sugito, Saitama 345-8508, Japan

e-mail: manabu.ito@toppan.co.jp

Transparent amorphous oxide material has attracted tremendous attention since the first report of amorphous InGaZnO based TFT by Nomura et.al., in 2004. Unique features of transparent amorphous oxide material compared with conventional amorphous Si are their high performance, low process temperature and transparency. Here, we focus attention on the low process temperature of the amorphous oxide TFT and demonstrate the potentiality of transparent amorphous oxide TFT in flat panel display application.

Applicability of low process temperature is fully compatible with plastic substrates, which leads to flexible display. We demonstrate a flexible *a*-IGZO TFT array by sputtering technique onto PEN substrate at room temperature. Flexible TFT array was combined with Vizplex Imaging Film, which is a flexible frontplane of the electrophoretic display supplied by E Ink Corporation. 5.35 inch flexible electronic paper with high resolution of 150 ppi was successfully driven by a-IGZO TFT array.

9:30 Oral

Blue and Yellow Light Emitting Diodes using IZO as anode

Edivaldo L. Queiroz[2], Gonçalo Gonçalves[1], Pedro Barquinha[1], Luis Pereira[1], Rodrigo F. Martins[1], Elvira Fortunato[1], Roberto M. Faria[2]

1. *Materials Science Department, CENIMAT-IxN and CEMOP-UNINOVA, FCT-UNL, Campus da Caparica, Caparica, Caparica 2829-516, Portugal* **2.** *University São Paulo Institue of physics of São Carlos, Sao Carlos 0000, Brazil*

e-mail: gpg@fct.unl.pt

Current-voltage, impendance, absorption and emission measurements have been carried out with ITO/LP/metal and IZO/LP/metal (LP – Luminescent Polymers) with the objective to compare the performance of IZO with that of ITO. We use as active LP layers in the electroluminescent devices two different polymeric films: poly[2-methoxy, 5-(2-ethylhexoxy)-1,4-phenylene vinylene], and a blend of composed by two derivatives of polyfluorene, (poly(2,7-9,9'-di-n-hexilfluorene) and poly(9,9–di-hexilfluorenediilvynilene-1,4-phenylenevynilene). The deposited thin films, by spin-coating process, were optically characterized before to build the devices. An investigation of the electrical properties of IZO shows that it can be used as transparent anode to replace the commonly used ITO. In addition, we developed a detail study on current-voltage characteristics and real and imaginary part of the impedance. Fitting of the experimental results were obtained by the Random-Free Barrier model that assumes, based on the disordered structure of the polymer film, a random distribution of energetic barriers, for carriers, that should be surpassed by hopping or by tunneling activated by phonons.

9:45 Oral

Resistance switching properties of epitaxial $Pr_{0.7}Ca_{0.3}MnO_3$ thin film with different electrodes

Hon Kit Lau, Yuk Kwan Chan, Wai Fai Cheung, Chi Wah Leung

Department of Applied Physics and Materials Research Centre,The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong 00-852, China

e-mail: ckcklau@gmail.com

$Pr_{0.7}Ca_{0.3}MnO_3$(PCMO) thin films were prepared on (001) oriented $LaAlO_3$ substrate using pulsed laser deposition. Epitaxial PCMO films were grown on the substrate at 650□ in a-150m Torr oxygen atmosphere. Resistance switching characteristics caused by electric field were investigated by using different metal electrodes, including Al, Pt, Au, Ti. The PCMO thin films exhibited switching characteristics upon changing polarity of voltage, especially with Al electrodes. The PCMO film with Al electrode showed non-linear, hysteresis current-voltage loop by applying a continuous dc voltage source and show resistance switching effect where other metals do not. We found that the total resistance of the film is dominated by interface resistance and the switching phenomenon is mainly due to the Al electrode. Such a structure can find applications in non-volatile memory devices.

10:00 Oral

Towards Roll to Roll Printed Organic Magnetic Sensor

Sayani Majumdar[1,2], Himadri S. Majumdar[1], Daniel Tobjörk, Reino Laiho, Ronald Österbacka

1. *Abo Akademi University, Department of Physics, Porthansgatan 3, Turku 20500, Finland* **2.** *Wihuri Physical Laboratory, University of Turku (UTU), Vesilinnantie 5, Turku 20014, Finland*

e-mail: sayani.majumdar@utu.fi

Organic magnetoresistance (OMAR) is a universal magnetic field effect in organic semiconductor based devices with non-magnetic electrode where the device show a substantial change in electrical current under low magnetic field of few milliTeslas.[1] At room temperature, the maximum change in current observed is of the order of 15 - 20% for most organic small molecules and polymers having hydrogen molecules in their side chains and this effect is the highest reported so far for any non-magnetic material. This universality of OMAR, apart from being very intriguing from the physical point of view, gives rise to tremendous prospect for application of these devices in magnetic sensors and also magnetically controlled opto-electronic devices.

We have made inkjet printed organic diodes on flexible plastic substrates (PET-505) and thoroughly investigated their magnetoresistance (MR) properties. The bottom electrode was evaporated or sputtered and the semiconductor and the top electrodes were inkjetted from a Dimatix^{TM} printer. Preliminary results show that depending on the materials and operating conditions of the device both increase or decrease in electrical current (i.e. negative or positive MR) can be achieved from these diode devices under a magnetic field which can be used for magnetic field sensing purposes. A detailed discussion of different physical aspects of OMAR will be presented and a comparison will be made between results from the spin-coated and ink-jet printed devices to understand the role of different fabrication techniques on the device properties and also the prospect of roll to roll fabricated magnetic sensors in near future.

References:

[1] Ö. Mermer, G. Veeraraghavan, T. L. Francis, Y. Sheng, D. T. Nyugen, M. Wohlgenannt, A. Köhler, M. K. Al-Suti, and M. S. Khan, Phys. Rev. B **72**, 205202 (2005).

10:15 Oral

Improvement of light extraction efficiency in n-ZnO:Ga/p-Si heterojunction light emitting diodes by SiO_2 current-blocking layer

Won Suk Han, Young Yi Kim, Cheol Hyoun Ahn, Hyung Koun Cho

School of Advanced Materials Science and Engineering Sungkyunkwan University (SKKU), 300 Cheoncheon-dong, Jangan-gu, Suwon, Suwon 440-746, Korea, South

e-mail: wshan1@skku.edu

ZnO, with a large band gap (~3.37 eV) and exciton binding energy (~60 meV), is suitable for optoelectronic applications such as ultraviolet light emitting diodes (LEDs) and detectors. However, the ZnO-based p-n homojunction is not readily available because it is difficult to fabricate reproducible *p*-type ZnO with high hall concentration and mobility. In order to solve this problem, there have been numerous attempts to develop *p-n* heterojunction LEDs with ZnO as the *n*-type layer. Among those structures, *n*-ZnO/*p*-Si heterojunction is a good candidate due to its price competitiveness and lower driving voltage of LED. Recently, the electroluminescence (EL) of the *n*-ZnO/*p*-Si was repoted by several groups. The EL was achieved from vertical-injection ZnO-based LEDs. These structures have been attractive for high-power and high-efficiency devices. However, the LED using vertical-injection structures shows much lower extraction efficiency, because it has small top contact and large backside contact. In these structures, the injected current from the top contact enters the active region underneath the top contact. Thus, the emitted light is hindered by the opaque top contact. This problem can be solved by using a current-blocking layer (CBL) that prevents the current injection into the active region below the top contact.

In this work, the ZnO:Ga film was grown on the SiO_2-patterned *p*-Si (100) substrates using RF magnetron sputtering method. The SiO_2 layer was deposited to investigate the effect of the CBL. At the same time, the normal *p*-Si wafer was used as the substrate for the deposition of ZnO:Ga film in order to compare with the LED performance of *n*-ZnO:Ga/*p*-Si structure using the CBL. The current-voltage characteristics revealed that both LEDs showed nonlinear and rectifying behavior, although the LED using the CBL exhibited the soft turn on. On the contrary, the EL showed higher light extraction intensity in *n*-ZnO/*p*-Si LED structure with the CBL.

Coffee break

Wednesday morning, 17 September, 10:30
Main Hall

TFTs

Wednesday morning, 17 September, 11:00
Room 226
Chair: Prof. J. Wager and Prof. M. Ito

11:00 Invited oral

Device structures for amorphous oxide semiconductor TFTs

Hideya Kumomi

Canon Inc., 3-30-2 Shimomaruko, Ohta-ku, Tokyo 146-8501, Japan

e-mail: kumomi.hideya@canon.co.jp

Amorphous oxide semiconductor (AOS) TFTs (thin film transistors) have attracted keen attention mainly for their application to flat-panel devices. The first AOS TFT[1] was demonstrated with a device structure of top-gate top-contact configuration using ITO (indium tin oxide) source and drain (SD) electrodes. Since then, various device structures have been reported with various insulator and SD materials, including types of top/bottom/double gate, top/bottom contact, back-channel etch (BCE), etch-stop, and homojunction coplanar[2]. While the device structure has to be selected in view of the application and fabrication processes, there has not been sufficient discussion in terms of TFT characteristics.

The most critical condition to the device structure arises from the selection of the SD electrodes which are limited to a few materials such as Ti, Mo, and transparent oxide conductors (TCO) for good ohmic contact and low contact resistance. There is no problem in patterning them for a bottom-contact configuration, but the deposition of the AOS layer can cause contact problems through the oxidation of the SD surfaces. For the top-contact configuration fabricated with BCE process, only Mo is available so far for patterning the SD electrodes by etching techniques. In any top-contact TFTs, it is not easy to lower the contact resistance when the AOS layer is deposited as being highly resistive. It will be shown in this paper that BCE TFTs fabricated with deposition of low-resistivity AOS and homojunction coplanar TFTs yield parasitic resistivity as low as 10-20 ohm cm along with high mobility of 12 cm^{2}V^{-1}s^{-1}, small subthreshold swing of 0.15 Vdec^{-1}, and their operation is almost close to ideal MOSFETs.

[1] K. Nomura, *et al.*, Nature **432**, 488 (2004).

[2] R. Hayashi, *et al.*, Digest of Technical Papers, SID'08, p.621.

11:30 Oral

Oxide based TFTs with high-k multicomponent dielectrics

Pedro Barquinha, Luis Pereira, Gonçalo Gonçalves, Rodrigo F. Martins, Elvira Fortunato

Materials Science Department, CENIMAT-IxN and CEMOP-UNINOVA, FCT-UNL, Campus da Caparica, Caparica, Caparica 2829-516, Portugal

e-mail: pmcb@fct.unl.pt

During the last years, a large number of publications related with oxide based TFTs have appeared. Polycrystalline binary oxides, like ZnO or SnO_2, or more recently multicomponent amorphous oxides, like IZO or GIZO, have been the semiconductors responsible for the excellent performance of these TFTs. However, little attention has been given to the dielectric layer development, being most of the TFTs based on "standard" dielectrics, like thermal SiO_2 or PECVD SiN_x. In this work several high-k gate dielectrics produced without intentional heating by r.f. magnetron sputtering are explored and used to produce TFTs based on GIZO semiconductor. Binary oxides, like Ta_2O_5 and HfO_2, lead to good performing devices: for example, with Ta_2O_5 high field-effect mobility (μ_{FE}) and low threshold voltage (V_T) are obtained, ≈40 cm^2/Vs and ≈1 V respectively, at the cost of an undesirably high gate leakage current (I_G), that can reach 1 μA at V_D=V_G=15 V, even when 300 nm thick dielectrics are used. The high I_G should be related with a non-favorable band offset between GIZO and Ta_2O_5 (or HfO_2) and dielectric crystallization (mainly HfO_2). In order to decrease I_G, mixtures of the binary oxides referred above with amorphous and high bandgap dielectrics, like SiO_2 or Al_2O_3, are produced by co-sputtering. The TFTs based on these multicomponent dielectrics still present high μ_{FE} and low V_T: values like 15-30 cm^2/Vs and 1.5-3.0 V, respectively, are obtained depending on the composition of the multicomponent dielectric, which is controlled by the r.f. power applied to the SiO_2 or Al_2O_3 target. However, I_G decreases considerably, being now possible to obtain values as low as 1 pA at V_D=V_G=15 V. Top and bottom-gate structures are analyzed, but generally the former leads to worse properties, which is mainly ascribed to the high bombardment at which the GIZO surface (hence, the GIZO/dielectric interface) is exposed during the dielectric deposition in top-gate structures.

11:45 Oral

High mobility Cu_2O epitaxial films and the application to p-channel thin film transistor

Kosuke Matsuzaki[1], Kenji Nomura[2], Hiroshi Yanagi[1], Toshio Kamiya[1,2], Masahiro Hirano[2,3], Hideo Hosono[1,2,3]

1. *Materials and Structures Laboratory, Tokyo Institute of Technology, Mailbox R3-1, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan* **2.** *ERATO-SORST, Japan Science and Technology Agency, in Tokyo Institute of Technology, Mailbox S2-13, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan* **3.** *Frontier Research Center, Tokyo Institute of Technology, Mailbox S2-13, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan*

e-mail: matsuzaki@lucid.msl.titech.ac.jp

Cuprous oxide (Cu_2O) is a *p*-type oxide semiconductor expected as active layers of optoelectronic devices such as solar cells and thin film transistors (TFTs) because it has a large hole mobility ~100 cm^2 V^{-1}s^{-1} for single crystal [1]. However, it is in general difficult to grow high quality Cu_2O thin films exhibiting large mobility because the chemical stoichiometry is easily changed by growth conditions. Here, we report the epitaxial film growth of high mobility Cu_2O films on MgO (110) single crystal substrates. We also succeeded in *p*-channel operation of Cu_2O channel TFTs.

The Cu_2O films were prepared by a pulsed laser deposition technique using a Cu metal target. The substrate temperature (T_{sub}= 650 – 800 ^{o}C) and the oxygen partial pressure (Po_2= 10^{-3} – 10^0 Pa) were varied. Hole mobility (m_h) and carrier concentration (N_h) were measured by Hall effect using the van der Paw configuration. TFTs with amorphous Al_2O_3 gate insulators were fabricated by a standard photolithography and lift-off process.

It was found that pure semiconducting Cu_2O films were obtained in growth conditions of T_{sub}= 650 – 700 ^{o}C and Po_2= 0.30 – 1.0 Pa, while Cu impurity was observed at Po_2 <0.30 Pa and Cu_2O films were polycrystalline insulating at T_{sub}≥ 730 ^{o}C. The high-resolution X-ray diffraction measurements revealed that the pure semiconducting Cu_2O films were grown epitaxially with the relationship of [110] Cu_2O // [110] MgO in out-of-plane and [1-10] Cu_2O // [1-10] MgO in in-plane. The tilting and twisting angles of the crystallites were 0.25 and 0.20 degrees, respectively, indicating that the films have high crystalline quality. 650-nm-thick Cu_2O films showed large hole mobilities up to m_h ~ 90 cm^2 V^{-1}s^{-1} (N_h ~ 1.6×10^{14} cm^{-3}), which is comparable to that of a single crystal.

The TFTs using Cu_2O channels exhibited typical *p*-channel behavior in a depilation mode. The field-effect mobility was estimated to be ~0.25 cm^2 V^{-1}s^{-1}.

[1] E. Fortin *et al.*,Can. J. Phys., **44**, 1551 (1966).

12:00 Oral

Flexible field-effect transistors based on liquid crystalline phenylterthiophene derivatives

Masahiro Funahashi, Fapei Zhang, Nobuyuki Tamaoki

The University of Tokyo, Bunkyo-ku, Tokyo 113-8655, Japan

e-mail: funahashi@chembio.t.u-tokyo.ac.jp

Liquid-crystalline semiconductors exhibit the high carrier mobility comparable to those of molecular crystals as well as solubility in common organic solvents. We have already reported the fabrication of field-effect transistors (FET's) using liquid-crystalline phenylterthiophene derivatives with the spin-coating method [1,2]. The FET devices fabricated on Si/SiO_2 substrates exhibited p-type operation with a field-effect mobility of 0.042 cm^2/Vs and an on/off ratio of 10^7. This good performance of the FET devices should be attributed to the close molecular packing within the smectic layers and the low defect density in the smectic phase.

In this study, the FET devices are fabricated on flexible polymer sheets aimed for the application to electronic papers. The liquid crystalline semiconductor 5-propyl-5''-(4-pentylphenyl)-2,2':5',2'-terthiophene was synthesized. On a polyimide sheet with the thickness of 0.3 mm, a gold gate electrode was deposited under vacuum. Then a dielectric layer made from PVA was fabricated by the spin-coating of the PVA/H_2O solution and baked in vacuum. The chlorobenzene solution of this compound was spun on the PVA layer to form the liquid crystalline layer, finally gold source and drain electrodes were vacuum-deposited on it to produce defined top-contact FETs.

The FET devices exhibit a p-type operation with the mobility of 0.01 cm^2/Vs and the on/off ratio of 10^4. These characteristics keep almost constant even when the strain (bending the substrate) reached 2.7 %. It is superior to conventional OFETs using the polycrystalline thin films, in which the performances degrade remarkably when the strain exceeds 1 %. The soft and flexible structure of the liquid crystalline semiconductor results in this good mechanical flexibility of the FET devices.

[1] M. Funahashi, F. Zhang, and N. Tamaoki, *Adv. Mater.*, **19**, 353 (2007).

[2] F. Zhang, M. Funahashi, and N. Tamaoki, *Appl. Phys. Lett.*, **91**, 063515 (2007).

Lunch break

Wednesday afternoon, 17 September, 12:30
Inner Courtyards

Coffee break

Wednesday afternoon, 17 September, 15:30
Main Hall

Joint Poster Session 2

Wednesday afternoon, 17 September, 16:00
Main Hall

Posters

Monday, 15 September

Joint Poster Session I

Flexible and Transparent Electronics I
Monday afternoon, 15 September, 16:00
Main Hall (Monday & Wednesday)

16:00 Poster B01

Comparable study of ZnInO & ZnN as channel layers for transparent transistors

Elias Aperathitis[1], Vicky Kambilafka[1], Mircea Modreanu[4], Roussos Skervelakis[3], George Kiriakidis[2,3]

1. *Microelectronics Research Group, Institute of Electronic Structure and Laser, Foundation for Research and Technology – Hellas, P.O. Box 1527, 71110 Heraklion, Crete, Greece, P.O. Box 1527, Heraklion 71110, Greece* **2.** *University of Crete, Iraclion 71409, Greece* **3.** *Institute of Electronic Structure and Laser, FORTH,, P.O. Box 1527, Vassilika Vouton, Heraklion 71110, Greece* **4.** *University College Cork, Tyndall National Institute (TYNDALL), Lee Maltings, Prospect Row, Cork, Ireland*

e-mail: eaper@physics.uoc.gr

Fig.1 Source-drain current as a function of
source-drain voltage for gate voltages up to 20V.

ZnO is a wide band gap semiconductor (Eg ~ 3.3eV) with high exciton binding energy (~60 meV), has good transparency and its conductivity approaches that of the widely used n-type indium-tin-oxide (ITO). As a result, ZnO is the ideal material for many applications in the emerging field of transparent electronics and optoelectronics. While achieving p-type ZnO in a controllable, reproducible and reliable manner remains difficult, amorphous ZnO has been used as channel layer in the fabrication of transparent thin film transistors (TTFTs).

ZnO-based TTFTs have been fabricated with promising results in replacing a-Si TFTs for many transparent applications (flat panel displays, oscillators, flexible electronics, etc).The ZnO-based materials which have been reported as channel layer in these TTFTs are: ZnO, ZnO:N and Zn-M-O where M=In, Ga, Sn.

In this investigation we report on the fabrication of TTFT having ZnN and ZnInO of varying Indium and Oxygen content as channel and source-drain materials. The gate-bottom TFTs were fabricated on silica substrates, having rf-sputtered ITO as gate and HfO_2 or SiO_2 as the dielectric. The n-type ZnN channel layer was deposited by rf-sputtering from a zinc nitride target whereas the ZnInO layer was deposited by dc-magnetron sputtering utilizing a metallic ZnIn target in a varying oxygen plasma.

Typical I_{DS}-vs-V_{DS} characteristic of the normally off transistor (after annealing at 410^{o}C in flowing nitrogen) having ZnN channel, HfO_2 dielectric and metallic (Ti/Au) source and drain is seen in Fig.1. A direct comparison of the required annealing on the output characteristics of the devices as well as the material transport characteristics will be addressed along with target and processing flow for the TTFT fabrication.

16:00 Poster B02

Tin monooxide as a 5s based p-type oxide semiconductor: Epitaxial film growth and thin film transistor

Yoichi Ogo[1], Hidenori Hiramatsu[2], Kenji Nomura[2], Hiroshi Yanagi[1], Toshio Kamiya[1,2], Masahiro Hirano[2,3], Hideo Hosono[1,2,3]

1. *Materials and Structures Laboratory, Tokyo Institute of Technology, Mailbox R3-1, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan* **2.** *ERATO-SORST, Japan Science and Technology Agency, in Tokyo Institute of Technology, Mailbox S2-13, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan* **3.** *Frontier Research Center, Tokyo Institute of Technology, Mailbox S2-13, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan*

e-mail: y-ogo@lucid.msl.titech.ac.jp

Tin dioxide SnO_2 is an eminent n-type conductive oxide with a wide bandgap and a high conductivity, and therefore extensive investigations have been carried out to apply them for transparent electrodes, gas sensors, and thin film transistors (TFTs). TFTs using oxide channels have been limited to n-channel type because there are a few materials system known as p-type semiconductors. Tin monoxide, SnO, is a unique and interesting material in this aspect; SnO films show p-type conduction (1), which is thought to originate from the fact that the hole transport paths are made from the closed-shell $5s^2$ orbitals of Sn^{2+} ions. Nevertheless, there have been few reports even on transport and optical properties of SnO. Here, we report epitaxial film growth of SnO and its electronic and optical properties. We have succeeded in operating p-channel TFTs with reasonable mobilities as well.

The epitaxial SnO films were deposited by PLD on YSZ(001) substrates. The substrate temperature and the oxygen partial pressure were varied from 400-700□ and 10^{-4} ~10^{-1} Pa, respectively. The epitaxial relationships were (001)SnO//(001)YSZ in out-of-plane and (100)SnO//(1-10)YSZ in in-plane. Hall effect measurements indicated that the film had a hole density of 2.5 x 10^{17} cm^{-3} and a hole mobility of 2.4 cm^{2}(Vs)$^{-1}$ at RT. 20 nm thick SnO layers were employed as channels of top gate type TFTs (W/L = 300/50 μm). 210nm thick amorphous almina layers were deposited by PLD as gate insulators. Finally, the TFTs were annealed by RTA in vacuum at 200 ^{o}C for 5 min to reduce the gate leakage current. The TFTs operated in a p-type depletion mode with a threshold voltage of ~5V and an on/off ratio of ~10^{2}. Field effect mobility and saturation mobility were 1.2 cm^{2}(Vs)$^{-1}$ and 0.7 cm^{2}(Vs)$^{-1}$, respectively.

(1)X. Q. Pan et. al., J. Electroceram. **7**, 35 (2001).

16:00 Poster B03

Comparison of ITO by capacitive RF magnetron sputtering and facing target DC sputtering as an anode on the organic light emitting diode

Jun Tak Kim[1], Chul Yoon[1], Sang Ho Kim[1], Hee Taek Shin[2]

1. *Korea University of Technology and Education, Cheonan 330-708, Korea, South* **2.** *BOWON light metal, BongDam DongHwa-ri 397-2, Hwasung 445-893, Korea, South*

e-mail: taks@kut.ac.kr

ITO is being used widely as a transparent conducting electrode for OLED. Surface roughness and microstructure of ITO have been known to give important influence on the OLED performance. However the effect of the both couldn't be separated with ITO made by same method. In this study, 4 ITOs deposited using a conventional capacitive

RF magnetron sputtering, a new facing target DC sputtering and two post-annealed of these samples were compared.

The grain structure, surface roughness, electrical and optical property of the ITO were investigated by XRD, FESEM, AFM, 4 point probe and UV spectrophotometer, and those are related to the resultant I-V-L characteristic of OLED.The grain structure of ITO by capacitive RF magnetron sputtering was almost columnar, on the while that by facing target DC sputtering was equi axed at the as deposited condition. By the post annealing, the grain structure by capacitive RF magnetron sputtering changed to the totally columnar but that by facing target DC sputtering maintained an equi axed only just with some grain growth. The RMS surface roughness of the ITO was 0.9nm and 0.2nm, respectively at the as deposited condition. After the post-annealing, that was increased by 5.4nm and 1.5nm. Both ITO films showed amorphous structure at the as deposited condition were crystallized with a same (400) preferred growth orientation and the transparency was improved by post annealing.

From the I-V-L characteristic, we could see that the threshold voltage and luminescence of the OLED was better with ITO of annealed facing target DC sputtering that sustains a compact and fine equi axed grains with appropriate surface roughness. This result means that there is a lower limit of RMS surface roughness about 1 to 1.5nm to give an effective carrier injection and above the limit the compact equi axed grain structure become more effective for good OLED. With ITO of annealed facing target DC sputtering, OLED with V_{th} of less than 6 volts was obtained.

16:00 Poster B04

Fabrication of Single Walled Carbon Nanotubes Flexible Transparent Conducting Films

Sellaperumal Manivannan, Il Ok Jeong, Je Hwang Ryu, Kyuchang Park

Kyung Hee University, Dongdaemoon-Ku, Seoul 130-701, Korea, South

e-mail: ksmaniphysics@yahoo.com

Carbon Nanotubes (CNTs) are attractive materials and potential alternatives to transparent (inorganic) oxide semiconductors (TOSs) that are employed in a variety of device architectures in display and optoelectronics applications. Transparent conductive indium tin oxide (ITO) has enjoyed widespread use for the past three decades which can be readily obtained on glass and although even on plastics, the inherent brittleness of ITO severely limits film flexibility. We describe an extremely simple method by which one can obtain strongly adherent thin films of single-walled carbon nanotubes (SWNTs) on flexible, transparent substrates such as polyethylene napthalate (PEN). In the present investigation, we purified the commercially available arc discharged SWNTs by dry oxidation and acid treatments and used to fabricate films on UV-O_3 treated PEN. We obtained highly transparent (>83 %@550nm) with robust flexibility and low sheet resistance (130 Ω/□) films from the dispersed SWNTs using a conventional spin coating method after effective wetting by post treatment. The films can be bent while retaining electrical properties without sacrificing their optical transparency. The hardness/adhesion test of the SWNTs on flexible PEN after passing laboratory scotch tape analysis reveals variation in sheet resistance 5-10 Ω/□ (<10%) with no remarkable change in optical transmittance. The purity, morphology and effect of post treatment on films were characterized by thermogravimetry (TG), micro Raman, Fourier Transform infrared (FT-IR) and scanning electron microscope (SEM). This approach provides a systematic way of fabrication films with reasonable film performance compared to other related works. The low sheet resistance can meet the criteria of transparent conducting films for touch screen applications which require ~500 Ω/□ for 85% optical transmittance and may replace the conventional ITO with high flexibility.

16:00 Poster B05

Polyurethane nano-composites with luminescence properties for optics and optoelectronics applications.

Ewelina A. Zawadzak[1], Joanna Ryszkowska[1], Dariusz Hreniak[2], Wiesław Stręk[2], Krzysztof J. Kurzydlowski[1]

1. *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland*
2. *Polish Academy of Sciences, Institute of Low Temperature and Structure Research (INTiBS), Okólna 2, Wrocław 50-422, Poland*

e-mail: ewelina205@wp.pl

The physical and chemical properties of polyurethane nano-composites have attracted much attention due to their promising applications in optoelectronictechnologies. Thin films of polyurethane nano-composites with luminescent properties could be used as potential materials for document protection. The materials for optoelectronic applications should fulfill specific requirements such as: high intensity of photoemission and high transmittance. Both characteristics depend on the quantity and good dispersion of luminophores in polymer matrix. Inorganic nanofillers have a strong inclination to agglomeration in polymers because of physical interaction between organic polymer matrix and inorganic filler.

The aim of this study was to evaluate the influence of nanofiller type on the structure and properties of the polyurethane composites.

For polyurethane synthesis the following chemicals were used: polycaprolactone diol, 4,4'-dicyclohexymethane diisocyanates and two chain extenders. As a nanofiller yttrium-aluminum-garnet (YAG) doped with 10mol.% of Tb^{3+} was used. The fillers were prepared using two different methods: the Pechinie method and the thermal decomposition. The filler was added to the polyurethane matrix in the proportion 0.1 wt. %. Nanocomposites were synthesized by prepolymer method.

A series of nano-composites with various amounts of nano-filler were obtained which exhibited high luminescence and intensity of emissions. The microstructure of these composites was investigated via Atomic Force Microscopy in a Tapping Mode and High Resolution Scanning Electron Microscopy (HRSEM). The size analysis of nanofillers was performed with HRSEM and TEM. The mechanical and electro-optical properties of the specimens have been correlated to their microstructure.

16:00 Poster B06

Microwave response of TCO coated glass analysed via transmission and reflectivity measurements

Antonio Cunha, Carla Rubinger, Fabio Vinagre, Luís C. Costa

Physics Department (UA), Campus Universitario, Aveiro 3810-193, Portugal

e-mail: kady@ua.pt

TCO's are widely used in the display and in thin film solar cell industries among others. We are now exploring the possibility of using TCO coated glass in microwave oven doors. This would have the advantage of better transparency than present day door designs.

Having that in mind we are studying the microwave response of TCO coated glasses through transmission and reflectivity measurements and correlating the behaviour to the properties of the TCO film nature and electrical DC properties.

In this work we report the results of our microwave transmission/reflectivity studies. We have compared the response of a typical microwave oven door with that of glass coated with commercial ITO and with in-house deposited FTO with varying DC conductivities. We have seen that the TCO coated glass analysed compares quite favourably with the response of an actual oven door although some improvements are still required. We have not seen significant differences between the responses of ITO and FTO coated glasses. Nevertheless we believe FTO has advantages over ITO because of its superior thermal stability and also because it does use In, which is an expensive element.

16:00 Poster B07

Thickness and dc magnetron sputtering growth temperature influence on ZnO thin films optical properties

Mirela Suchea[1,3], Savas Christoulakis[1,2], Theophanis Kitsopoulos[1,3], George Kiriakidis[1,2]

1. *PEML IESL (FORTH), 100, N. Plastira str, Heraklion 70013, Greece* **2.** *Physics Dpt, Univ. of Crete, PO Box 1527, Heraklion 71409, Greece* **3.** *Chemistry Dpt, Univ. of Crete, PO Box 1527, Heraklion 71409, Greece*

e-mail: kiriakid@iesl.forth.gr

Zinc oxide transparent conductive thin films with different thickness were grown by dc magnetron sputtering technique at different growth temperatures onto silicon and Corning glass substrates. X-ray diffraction characterization showed that all the ZnO films are polycrystalline, highly textured with the c axis perpendicular to the substrate surface. The dependence of their optical and electrical properties on the thickness and the growth temperature was investigated. In all cases, the films were found to be highly transparent in the visible wavelength region with an average transmittance of 90%, with a fall-off for wavelengths shorter than 380 nm, characteristics of high quality ZnO films. The position and the shape of the absorption edge observed for wavelengths below 380 nm were found depending on the film thickness and growth temperature. Moreover, an additional absorption band centred near 360 nm was clearly recorded, for all growth temperatures and thicknesses larger than 40 nm. Although a similar absorption band attributed to excitonic resonances as those related to the exciton/LO phonons has been reported by other researchers, this study focuses on a coherent study of dc magnetron sputtering growth parameters effect on the position and intensity of this absorption local.

16:00 Poster B08

Direct current magnetron sputtering deposition parameters effect on the properties of Silicon doped Aluminum Zinc Oxide thin films

George Kiriakidis[1,2], Mirela Suchea[1,3], Savas Christoulakis[1,2], Theophanis Kitsopoulos[1,3]

1. *PEML IESL (FORTH), 100, N. Plastira str, Heraklion 70013, Greece* **2.** *Physics Dpt, Univ. of Crete, PO Box 1527, Heraklion 71409, Greece* **3.** *Chemistry Dpt, Univ. of Crete, PO Box 1527, Heraklion 71409, Greece*

e-mail: kiriakid@iesl.forth.gr

The surface topology, crystallinity and optical transmission of 100nm thick films grown from a Si-doped Aluminum Zinc Oxide (Si:ZAO) commercial ceramic target (composed of 2% Al_2O_3 and 1000 ppm Si) by dc magnetron sputtering technique have been investigated for various oxygen partial pressures in the sputtering atmosphere at two different plasma currents. The effect of Si co-doping of the target reflected on a decrease of deposition rate of about 25% and in an increase of dust formation during growth leading in some cases to an unstable deposition process and growth rate fluctuations.

The thickness variation effect on the physical properties of these films compared with results from an undoped ZAO ceramic target has also been studied. X-ray diffraction (XRD), atomic force microscopy (AFM), and UV-VIS transmission studies have been applied in order to investigate the physical and transport properties of the deposited films as a function of deposition parameters.

Film surface characterization by AFM showed a tendency for grain agglomeration unlike the case of pure ZAO leading to increased surface roughness from 0.3 nm to ~21 nm for thickness variation from 100nm to 1μm while their preferential crystalline growth orientation revealed by X-ray diffraction remained always the (002) as in the case of undoped ZnO thin films with a slight increase on peak intensity. On the other hand, Si doping of the ZAO target lead to a small decrease of optical transmission compared with thin films grown from an undoped ceramic ZAO target. Decrease of the argon/oxygen ratio in the plasma caused a small decrease in the films' transmission and a very slightly improvement of conductivity. Si:ZAO thin films deposited by dc planar magnetron sputtering exhibited surface structural and morphological properties which were enhanced significantly by the control of the film deposition parameters.

16:00 Poster B09

Synthesized ZnO micro-rods present strong exciton emission centered at 390 nm and null visible emission under UV photon excitation

Francisco Ramos-Brito[1,2], Manuel García-Hipólito[3], Enrique Camarillo[1], José M. Hernández[1], Ciro Falcony[4], Hector O. Murrieta[1]

1. *Universidad Nacional Autónoma de México-Instituto de Física (IFUNAM), Circuito exterior s/n ciudad universitaria, México 04330, Mexico* **2.** *Laboratorio de Materiales Optoelectrónicos-Centro de Ciencias de Sinaloa, Av. de las Américas 2771, Culiacán 80010, Mexico* **3.** *Universidad Nacional Autónoma de México, Instituto de Investigaciones en Materiales (UNAM), Circuito Exterior S/N Cd. Universitaria Coyoacan Mexico D.F. Mexico, México 70-360, Mexico* **4.** *Departamento de Física, Centro de Investigación y de Estudios Avanzados del IPN, A.P. 14-740,, México 07360, Mexico*

e-mail: murrieta@fisica.unam.mx

Employing a simple chemical synthesis method, hexagonal shaped zinc oxide microrods with lattice parameters: a = 3.2498 and c = 5.2066 Å were deposited on pyrex glass and aluminum substrates. PL results revealed best optical quality for ZnO on pyrex glass. Their principal optical and physical characteristics were: a) very uniform wide and large sizes of around 1 and 10 μm, respectively, b) preferred crystalline growth in [1010] and [0001] directions, c) strong exciton photoluminescent emission centered at 390 nm with a FWHM of 70 meV at room temperature, d) an energy band gap of 3.32 eV, e) almost null photoluminescent emission in the visible region of the electromagnetic spectrum due to poor existence of structural defects, f) good emission efficiency supported by the not required high energy densities to obtain strong exciton emission and g) good ZnO stoichiometry endorsed by photoluminescent and chemical composition results. ZnO microstructures obtained in this work are evidence that the grow mechanism of microrods strongly depends on the substrate employed. Pyrex glass substrate resulted better than aluminum for deposition of microrods, enhancing its optical properties. They presented good optical quality to future applications in photonics.

16:00 Poster B10

Investigation of flat-band voltage distributions over the gate area of Al-SiO_2-Si structures

Krzysztof Piskorski, Henryk M. Przewłocki

Institute of Electron Technology (ITE), al. Lotników 32/46, Warszawa 02-668, Poland

e-mail: kpisk@ite.waw.pl

Extraction of MOS system parameters is very important in modeling and device optimization for modern integrated circuits. Having a possibility to make very accurate measurements of some electrical parameters of MOS systems, it is possible to use these results as a diagnostic tool on technological line for control purposes.

In this research we have developed a new, high precision photoelectric measurement method of the local flat-band voltage V_{FB} values in MOS structures. This method, called SLPT (Scanning Light Pulse Technique) consists in scanning the whole gate area with the small light spot, which allows determination of the local V_{FB} value distribution over the gate area. It was found that in Al-SiO_2-Si structures the local values of V_{FB} in the central part of the metal gate are higher than at gate corners. This characteristic non-uniform, dome-like shape of $V_{FB}(x,y)$ distribution over the gate area was obtained for many MOS structures made in different technological processes.

To confirm these results the measurements of the V_{FB} voltage by classical C(V) characteristics method (without any illumination) were performed. It turned out that V_{FB} values (for the entire gate area) decrease monotonically with the R-ratio of the gate perimeter to gate area. Such behavior confirms that local V_{FB} values in the vicinity of gate edges are lower than in the central part of the gate.

In our previous investigations we proved that the effective contact potential difference f_{MS}, and the barrier height at the metal gate – dielectric interface E_{BG}, both have a similar dome-like shapes of distributions over the gate area. It supports our hypothesis that the mechanical stress existing in the oxide under the metal gate has a dominating influence on the shape of distributions of the above mentioned electrical parameters.

16:00 Poster B11

Structural and photoluminescence studies of erbium doped nanocrystalline silicon thin films

Pedro Alpuim[1], Sergej A. Filonovich[1], Fátima Cerqueira[1], Anabela G. Rolo[1], Eduardo Alves[2], Jorge Soares[3]

1. *Centro de Física, Universidade do Minho, Campus de Gualtar, Braga 4710-057, Portugal* **2.** *Instituto Técnológico Nuclear, Sacavém 2686, Portugal* **3.** *Departamento de Física, Universidade de Aveiro, Campus de Santiago, Aveiro 3810-193, Portugal*

e-mail: arolo@fisica.uminho.pt

Semiconductor nano-structures of typical size<10*nm* systems are of considerable current interest because of the new physics involved and potential device applications. The achievement of an efficient room-temperature light emission from Si is a crucial step toward the fully integrated Si-based optoelectronics. Er-doped silicon has special importance for optical communication systems due to the emission line at 1.54 μm.

In this work we will compare the Er^{3+} emission in Erbium doped nanocrystalline silicon thin films grown with different procedures, namely in situ doped by reactive magnetron sputtering on glass substrates under several different conditions (RF power, Er content and gas mixture composition), Hot Wire (HWCVD) and rf-PECVD with different hydrogen dilution and substrate temperature, in order to obtain different microstructures. The film structure was studied using X-ray diffractometry and Raman spectroscopy. The chemical composition was determined using RBS technique. The undoped as-grown samples have been doped by implantation with two doses and a Gaussian profile around 50 nm. We have performed different temperatures annellaling in order to evaluate if the initial microstrutures will be important for the final state (recovering the initial size and crystalline fraction). Our samples show sharp photoluminescence (PL) spectra of Er centers with the strongest peak positioned at the wavelength 1.536 μm. We have studied also the photoluminescence behaviour with temperature and we have verified that at temperature increasing from 5K to 300K the PL measured decreases less as comparing to that usually observable in monocrystalline silicon. Our results indicate that the kind of matrix where the nanocrystals are embedded (more or less oxygen) influences strongly the erbium emission.

16:00 Poster B12

Some Optical Effects on the Electrical Conductivity of ITO Nanoscale Layers

Károly Somogyi, Katalin Erdélyi, Istvan Szendro

MicroVacuum, Kerékgyarto u. 10, Budapest H-1147, Hungary

e-mail: karoly.somogyi@microvacuum.com

The as grown indium tin oxide ($InSnO_2$, ITO) layers have high resistivity and the transparency is also very limited though ITO is known as a transparent oxide with n-type electrical conductivity. In this work ITO layers were deposited by evaporation and then underwent a post-growth annealing. Annealing leads to low electrical resistivity and to an enhanced transparency. Annealed samples really show n-type conductivity. In this work ITO coating layers are envisaged for measurements where the layer conductivity plays an important role. One of such cases is when the optical sensitivity can be combined with specific advantages of the electrochemical processes.

ITO layers of typically 10 nm thickness were deposited onto OWLS sensor chips and on $Si_{1-x}Ti_xO$ covered glass substrates. The basic measurement after the annealing was the conductivity determination. On sensor chips also the angle dependent photocurrent spectra were evaluated. This allows the selection of the chips. The electrical conductivity was estimated first by two point direct resistance measurements, then by van der Pauw configuration and by collinear four point probe method. W needles and Sn containing mechanical contacts were used. All types of contacts proved to be applicable. Contact resistance was determined separately. Also the repetitivity of the technological processes was controlled partly by electrical measurements.

Storage time dependent stability and light sensitivity were studied. It is demonstrated that the resistance decreases due to the illumination, but in a very small extent. The decrease depends on the wavelength and the process is very slow (tens of minutes, up to hours). The recovery is also slow and also some drift in resistance is observed under continuous repetitive measurements.

16:00 Poster B13

The effect of thermal treatment conditions employed in sol-gel method on the structure of ZnO thin films

Takashi Ehara, Takafumi Otsuki, Junya Abe, Takaaki Ueno, Masahiro Ito, Takafumi Hirayama

Ishinomaki Senshu University, Ishinomaki 986-8580, Japan

e-mail: ehara@isenshu-u.ac.jp

We have prepared the ZnO thin films by the sol-gel method from a 2-methoxyethanol solution of zinc acetate dihydrate stabilized by 2-aminoethanol on SiO_2 substrates. The structure of the films showed a significant dependency on thermal treatment temperature, not only in the final thermal-annealing process at several hundreds of degrees, but also in the heat-treatment after spin coating at lower temperature to evaporate the solvent in the films. The intensity of the (0002) peak in X-ray diffraction showed significant dependence on the heat treatment conditions after spin coating which ranged from 100ºC to 300ºC. The temperature employed in the initial 10 min of the heat treatment was found to be important in determining the structure of the film. The results indicate that the elimination condition of the organic components is important in achieving the high crystallinity.

16:00 Poster B14

Surface morphology and film structure of poly[3-(4-octyloxyphenyl) thiophene (POOPT) thin films obtained by thermal annealing during Matrix Assisted Pulsed Laser Evaporation (MAPLE)

Valeria Califano[1], Francesco Bloisi[1,2], Luciano Vicari[1,2], Antonio Cassinese[1,2], Mario Barra[1], Antonio Carella[3], Antonio Roviello[3]

1. *INFM - Coherentia, Via Cinthia, Napoli 80125, Italy* **2.** *University of Naples "Federico II", Department of Physical Sciences, Napoli, Italy* **3.** *Department of Chemistry, University of Naples Federico II, Via Cintia, Napoli 80124, Italy*

e-mail: valeriacalifano@hotmail.com

Among other materials semiconducting conjugated polymers are used in several organic electronic devices (OED) such as field effect transistors (FET), light emitting diodes (LED), photovoltaic cells (PC). Polythiophenes are attracting some attention for their chemical stability and structural versatility. Furthermore, alkyl-substituted polythiophenes have self-p-stacking ability, and p-stacking structures are essential for the optical and electrical properties of these polymers.

The morphology and the structure of a polymeric thin film can highly affect its properties and, therefore, the behaviour of the OED. Since morphology and structure are affected by temperature, post-deposition annealing/quenching has been used to enhance the performance of OEDs.

Currently organic or polymeric thin films are successfully deposited using Matrix Assisted Pulsed Laser Evaporation (MAPLE), an evolution of Pulsed Laser Deposition (PLD) reducing the risk of photochemical decomposition produced by direct interaction of laser radiation with the material since the target, reached by the laser beam, is a dilute frozen solution of the polymer in a volatile solvent.

We have already successfully used MAPLE technique in order to deposit POOPT thin films on glass substrate and here we examine the effect of substrate temperature during depositions (deposition/annealing), comparing the results with annealing applied after MAPLE deposition (post-annealing).

16:00 Poster B15

Optical and electrical properties of oriented $SrCu_2O_2$ thin films grown by pulsed laser deposition

Bernard Servet[1], René Bisaro[1], Guy Garry[1], Mircea Modreanu[2], Ekaterina Chikoidze[3], Guido Huyberechts[4]

1. *Thales Research and Technology (TRT), Route Départementale 128, Palaiseau 91767, France* **2.** *University College Cork, Tyndall National Institute (TYNDALL), Lee Maltings, Prospect Row, Cork, Ireland* **3.** *University of Versailles CNRS (GEMAC), 1, Place A. Briand, Meudon 92195, France* **4.** *Umicore Group Research and Development, Kasteelstraat 7 B-2250, Olen B-2250, Belgium*

e-mail: mircea.modreanu@tyndall.ie

$SrCu_2O_2$ is found to be a promising p-type transparent conductive oxide (TCO). Here, we report on a study of $SrCu_2O_2$ thin films grown by pulsed laser deposition (PLD) on crystalline substrates (sapphire, Ge). The stoichiometric phase can be obtained under thermodynamical growth conditions, *e.g.* deposition temperature of 500°C and oxygen pressure of 10^{-5} mbar, according to the phase diagram of bulk strontium-copper-oxygen. The lattice constants and texture of the oriented $SrCu_2O_2$ films are determined by X-ray diffraction (XRD) using a four-circle diffractometer so as to deduce the contact plane and the orientation of *a* and *b* axes (*i.e.*, axes of high conductivity). The film orientation is also determined by Raman scattering and IR absorption measurements according to the theoretical vibrational analysis based on first-principle calculations. Then, the films are post annealed under a controlled oxygen pressure and their electrical properties (conductivity, hole concentration and mobility) are measured and interpreted in terms of anisotropy of conductivity in the crystal structure of $SrCu_2O_2$ and of stoichiometry provided by electron probe microanalysis (EPMA).

16:00 Poster B16

Characterization of organic light emitting diodes by spectroscopic ellipsometry

Emmanuel S. Nolot, Agathe André, Henri Doyeux, David Vaufrey

CEA-LETI-MINATEC (MINATEC), 17 rue des Martyrs, Grenoble 38054, France

e-mail: emmanuel.nolot@cea.fr

Organic light emitting diodes (OLEDs) are developed to be used in next-generation flat panel displays like TV sets, and more generally in display devices like cell phones, PDA... In a multi-layer OLED device (Fig.1), multiple reflections of emitted electroluminescence (EL) light from interfaces generate optical interferences that can strongly reduce the external quantum efficiency of EL. Determination of both thickness and optical constants of each individual layer is compulsory for optimizing the display performance.

To comply with the requirement of on-line optical characterization and monitoring of individual organic layers in the 190-1000 nm spectral range, we developed the following procedure on a Woollam M2000 rotating-compensator spectroscopic ellipsometer.

First, the analysis was limited to a spectral region where the layer is optically transparent (500nm-1000nm typically) to determine its thickness and refractive index in this limited range, using a Cauchy model. Then, at a fixed thickness, both refractive index and extinction coefficient were calculated at each wavelength of the investigated spectral range. Finally, based on this mathematical approximation, an oscillator-based model, Kramers-Kronig consistent, was built to fully describe the optical dispersion of the layer, including position and shape of the numerous absorption peaks in the UV range (Fig.2).

Figure 1 : Schematic view of multilayer OLED stack

Figure 2 : Optical dispersion of Alq3 organic layer in the 190-1000nm spectral range

16:00 Poster B17

Carbon coating manufactured in RF and MW/RF plasma for detectors and electronic devices

Witold Z. Kaczorowski[1], Piotr Niedzielski[2], Jacek D. Grabarczyk[1], Marian Cłapa, Stanislaw F. Mitura[2]

1. *Technical University of Lodz, Institute of Materials Science and Engineering, 1/15 Stefanowskiego, Łódź 90-924, Poland* **2.** *Technical University of Łódź, Institute of Materials Engineering, Stefanowskiego 1/15, Łódź 90-924, Poland*

e-mail: witold.kaczorowski@gmail.com

Carbon has a very interesting characteristic: high hardness and wear resistance, low friction coefficient and good electrical properties. The combination of these properties makes carbon films a very attractive material for use in many fields of the industry, especially in detectors and other electronic devices. In this work carbon coatings were deposited using RF PACVD and MW/RF PACVD methods. Descriptions of applied plasmo-chemical technologies and surface preparation methodology are presented. Deposited layers were investigated on SEM and AFM. Mechanical properties such as nanohardness, Young's modulus adhesion and friction coefficient were measured with use of the nanointendation techniques. Thickness of manufactured layers was determined using elipsometric and profilometer techniques. Electrical parameters was examined. The analysis of the influence of the main process parameters on the thickness of obtained layers was made. It was noticed that due to microwave plasma application very thick, about 20 micrometers thick layers can be deposited. The most interesting investigation results were obtained during the blocking potential tests conducted in different temperatures. Acquired results suggests that carbon coatings deposited in dual mode microwave and radio frequency plasma are a very perspective material especially for high power devices.

16:00 Poster B18

ITO and BST Thin Films for Transparent Transistors

Magdalena Nistor[1], Florin Gherendi[1], Nicolae Bogdan Mandache[1], Jacques Perriere[2], Daniel Defourneau[2], Wilfrid Seiler[3]

1. *National Institute for Lasers, Plasma and Radiation Physics (INFLPR), Bucharest- Magurele 077125, Romania* **2.** *Institut des nanosciences de Paris (INSP), 140 rue de Lourmel, Paris 75015, France* **3.** *Ecole Nationale Supérieure d'Arts et Métiers (ENSAM), 151, boulevard de l'Hôpital, Paris 75013, France*

e-mail: florin.gherendi@infim.ro

The fabrication of transparent thin film transistors (TTFT) requires the growth of high quality thin films with specific properties in order to have different functionalities as channel materials, transparent electrodes and gate dielectrics. In this work indium tin oxide (ITO) and barium strontium titanate (BST, Ba/Sr=0.25) were studied for transparent electrode and high-k gate insulator of a TTFT. ITO and BST thin films were grown on various substrates (quartz and single crystals) at different temperatures by the pulsed electron beam deposition method (PED). The latter is a low cost growth technique of oxides thin films with high quality surface morphology even at low processing temperatures. The composition, structure and surface morphology of ITO and BST thin films were determined by Rutherford Backscattering Spectrometry, X-ray diffraction and Scanning Electron Microscopy measurements. These characterizations showed that the films are stoichiometric, crystalline, smooth and dense. The quality of ITO thin films depends strongly on the growth conditions. Electrical properties of ITO thin films (resistivity, charge carrier density and mobility) were investigated by temperature-dependent conductivity and Hall effect measurements in the van der Pauw geometry, for different growth conditions. Dielectric measurements were performed for the BST thin films. Optical absorption spectra were measured in UV to near IR for ITO and BST thin films. These results will be presented and discussed in the frame of applications in transparent electronics.

16:00 Poster B19

Test ZnO Nanostructures Synthesis Conditions and Methods on ZnO Thin Film for Use in SAW Sensors

Sina Baghbani kordmahale[1], Fatemeh Dehghan Nayeri[2], Hasan Ghafouri Fard[1], Ebrahim Asl Soleimani[2], Shamsoddin Mohajerzadeh[2]

1. *Amirkabir University of Technology (AUT), Hafez, Tehran 15914, Iran* **2.** *University of Tehran (UT), North-Kargar, Tehran 14395-731, Iran*

e-mail: sina_baq.k@aut.ac.ir

Using ZnO Nanostructures is a very attractive in the field of optoelectronics and sensors .growth of ZnO Nanostructures on ZnO film prepared by RF Sputtering is an efficient method in achieving aligned NWs.In the ways that thin films of ZnO(>1000nm that we used)save their piezoelectric properties during the process of NWs synthesis ,we can use these thin films to fabricate ultra sensitive SAW sensors.SEM,XRD,Four-point probe and surface profile measuring system are used to characterization thin films.We chose Si(100)and deposited ZnO on Si by RF Sputtering.We repeated ZnO deposition on oxided Si(100)(with 250 nm dry oxide) .We used this wafers to test nanostructure synthesis conditions in VLS process(temperature and gas flow)on ZnO film. Our VLS process occur in a atmospheric CVD.We have tested both high temperature VLS(using graphite /ZnO mixture and Ar gas flow)and low temperature VLS(using Zn and O2 gas flow).we have noticed that in the ZnO/SiO2/Si samples with increase of temperature the structure of ZnO became worse .they lose their (002)orientation and the grain size became larger. Although their resistances decrease by increasing temperature that can increase power consumption in saw devices. Interestingly in ZnO/Si samples the Nanostructure synthesis condition act as annealing and can improve the structure. On these samples increasing temperature didn't affect on bulk resistance and increase(002)peak in XRD test.we tested some types of VLS and chemical methods on ZnO thin films and we have showed that, for ZnO/SiO2/Si samples chemical methods and low temperature VLS processes(T~500-600c) like Zinc powder evaporation are better, because in the temperatures above 500c the bulk resistance decrease from 150kohm to 100kohm.In ZnO/Si samples we didn't see any decrease in bulk resistance at high temperatures and the bulk resistance is about 200kohm. We expected that fabricated ZnO NWs on ZnO/Si samples with suggested methods are suitable for the SAW sensors.

16:00 Poster B20

Hydrothermal synthesis of vanadia-based whiskers for application as flexible cathode material

Sergey V. Balakhonov

M.V. Lomonosov Moscow State University, Vorobyevy gory, Moscow 119992, Russian Federation

e-mail: Balakhonov@inorg.chem.msu.ru

Recently, evolution of nanoelectronics shows the tendency of size reduction of digital microdevices. The main problem in this field is complexity of reduction of battery size without decline of their electrochemical properties. The decision is use of closed volumes of devices. Electrode “paper” of a new type whiskers based on V_2O_5 due to excellent electrochemical and mechanical characteristics is capable to fill closed spaces of devices.

The aim of the present study - development of a hydrothermal technique of V_2O_5 based whiskers preparation and investigation of their physical and chemical properties for subsequent use as a cathode material in lithium-ion batteries.
$V_2O_5 \cdot nH_2O$ xerogel was applied as precursor for preparing of whiskers. The xerogel was received by addition of V_2O_5 powder to H_2O_2 (15 % water solution). Then it was mixed with $Ba(NO_3)_2$ water solution. Ba-whiskers were prepared by hydrothermal treatment of Ba-replaced xerogel. H-whiskers were obtained at the same conditions but using initial non-replaced xerogel.

According to SEM and TEM data, whiskers had 50-100 nm thickness and about 3-4 mm length (aspect ratio reached up 40000/1).

Element composition of whiskers was established by EDX analysis. XPS data has shown, that H-whiskers contains only V^{5+}, while during Ba^{2+} ion exchange oxidation state of vanadium ions are partially reduced to 4+.
Thermal stability of Ba-whiskers was investigated by TG and XRD methods. Structure of samples due to water less is transformed up to ~280°C. At more high temperature phase transformation occurs and V_2O_5 is formed.

Electrochemical properties of Ba-whiskers were investigated by charge-discharge curves and cycle voltammogramm data. The main advantage of prepared whiskers is high (~140 mAh/g) discharge capacity which does not change during process. UV-vis spectrometry data shows that whiskers are semiconductors with gap energy 1 eV (Ba-whiskers) and 2.5 eV (H-whiskers).
This work was supported by RFBR (grant No. 07-03-00654).

16:00 Poster B21

Nanoscale patterning of metal-dielectric overlayers: from surface ripples to nanowires

Francesco Buatier de Mongeot[1,2], Andrea Toma[1,2], Daniele Chiappe[1,2], Corrado Boragno[1,2], Ugo Valbusa[1], Barbara Šetina[3], Matjas Godec[3], Monika Jenko[3]

1. *Dipartimento di Fisica (DIFI), Via Dodecaneso, 33, Genova 16146, Italy* **2.** *CNISM Unità di Genova (CNISM), Via Dodecaneso, 33, Genova 16146, Italy* **3.** *Insitute of metals and technology (IMT), Lepi pot 11, Ljubljana 1000, Slovenia*

e-mail: buatier@fisica.unige.it

Thin solid films appear most commonly in polycrystalline form, which means that they have highly constrained single-crystalline grains. Polycrystalline films are used in a large variety of devices, such as magnetic storage media, catalytic and thermal elements, protective coatings. It is thus desirable to extend to polycrystalline films, the approaches which have been developed for the self-organized formation of nanostructures on single-crystalline metal substrates [1].

We report on the formation of periodic metal nanostructures induced by self-organized sputtering processes of polycrystalline metal films supported on dielectric substrates. These results qualitatively agree with the behaviour reported for off–normal sputtering experiments on single-crystal metals where periodic ripples endowed with wavelengths in the 10 nm range are observed [2].

At variance with the latter case, we found that a non-singular starting surface morphology does plays a critical role in guiding self-organization during the early stages, where the hierarchical distribution of polycrystalline grains imposes a non-stochastic spatial modulation of the ion impact sites.

We also discuss the role of grain boundaries in this self-organization process: although providing an additional bias for diffusion of mobile defects ona 100 nm scale, they do not limit the propagation of nanoscale ripples which extend for several micrometers across the individual grains .

[1] U. Valbusa et al., J. Phys. Condens. Matter 14 (2002) 8153

[2]A. Toma, D. Chiappe, B. Šetina Batič, M. Godec, M. Jenko, F. Buatier de Mongeot, submitted

16:00 Poster B22

A novel method to decrease sheet resistance of ITO thin films using current source

Ehsan Davoodi, Ebrahim Asl Soleimani

University of Tehran (UT), North-Kargar, Tehran 14395-731, Iran

e-mail: e.davoodi@gmail.com

ITO (Indium Tin Oxide) and AZO (Aluminum doped Zinc Oxide) are common semiconducting metal oxide thin films. Reducing the sheet resistance of these films while having trancparency is the main issue. For ITO layers reducing the sheet resistance is usually done by annealing in 300-600 °C after deposition. We have found that applying optimum current through layer results in the reduction of sheet resistance. This method is much faster and costs less than annealing.

ITO thin films are widely used as transparent semiconductor. LCDs and Solar Cells are some of the devices in which ITO layers are used. In our work, current is passed through ITO layer after deposition. The optimum current source does not depend on layer length ;however the voltage does. The best current is related to current cross section area (mainly thickness of layer).

22mA is the suitable current for optimum conductance with 500nm thickness for deposited ITO layer on glass substrate. More current will result in damaging the layer and less will not lead to optimum conductance. This method is suggested where annealing is not possible or current source can easily be applied to sample. Especially for solar cells current probes can put on fingers or busbars.

16:00 Poster B23

Physical properties of AZO thin film deposited on flexible substrate by RF-sputtering method

Fatemeh Dehghan Nayeri[1], Manoochehr Hoseini[1], Ehsan Davoodi[1], Ebrahim Asl Soleimani[1], Mohammad Reza Ketabdari[2], Shamsoddin Mohajerzadeh[1]

1. *University of Tehran (UT), North-Kargar, Tehran 14395-731, Iran* **2.** *Atomic Energy Organization of Iran, Tehran 45786, Iran*

e-mail: f.d.nayeri@gmail.com

Common semiconducting metal oxide thin films include ITO thin films, ATO thin films, and AZO thin films. Recently, increasing research interest on the AZO thin films is not only due to the low resistivity but also the optical characteristics. AZO thin film exhibits a sharp UV cut-off and a high refractive index in the IR range, and is transparent in the visible light. AZO thin films can be deposited by various methods of deposition. However among the methods of deposition, sputtering is a promising technique to grow AZO thin film at lower temperature with better adhesion and higher density. We have recently investigated the effect of annealing on properties of sputtered AZO thin films on glass [1]. In this paper we report high quality AZO thin films could be deposited on unheated polymer substrate by RF sputtering technique. The high quality AZO thin film could be obtained by changing films deposition process parameters such as pressure and RF power. The spurting was carried out in an Ar gas atmosphere with varying RF power ranging from 50 to 300 W. since PET substrates are very temperature sensitive, the deposition was performed at slow rate. The surface morphology and the crystallinity of the films were investigated by X-ray diffractometry and scanning electron microscopy. The thin film AZO deposited on Kapton substrate indicated that thin film deposited with RF power o 280W are strongly c-axis oriented. As well as structural properties, influence of RF power on optical properties of AZO film was investigated. The as grown AZO films deposited with RF powers of 150W exhibited an average transmittance of about 70% in the visible spectra. However, by raising the power of deposition the transmittance of the films decreased to 62%.

1. M.Hoseini, F. Dehghan Nayeri, E.Asl Soleimani, M.R. Ketabdari,& S.Mohajerzadeh, *IUMRS-ICEM, Hilton Sydney, Sydney, Australia - 28th July to 1st August 2008*

16:00 Poster B24

High-performance low-temperature transparent Ta2O5 thin film deposited on glass substrate by RF-sputtering

Fatemeh Dehghan Nayeri, Shahram Kazemi, Sasan Seyed Zamani, Jamshid Sabbaghzadeh

Laser Resaerch Center Paya Partov Co., Tehran 14665576, Iran

e-mail: f.d.nayeri@gmail.com

Tantalum pentaoxide (Ta2O5) dielectric films are of interest for applications in optical waveguides, antireflection coatings and MOS devices. Ta2O5 thin films of 120 nm thicknesses were prepared at room temperature by RF sputtering from a Tantalum Pentaoxide target. Deposition was performed in Argon 99.99% ambient on unheated glass substrate and without substrate heating which was either stationary in front of the target or in constant motion at RF power ranging from 50 to 350W and effect of plasma power on the surface morphology, optical properties, internal stress, refractive index and absorption of the layers was studied directly after deposition. Ta2O5 films showed different surface morphologies and surface roughness under different deposition conditions. X-ray diffraction technique (XRD) was employed to analyze the effect of deposition conditions on the structure of the films. The experimental results show that films with good qualities of surface morphology, transmittance and internal stress can be grown by the RF sputtering method on glass. Ta2O5/SiO2 multilayer coatings had smaller average compressive stress than single-layer Ta2O5 film.

16:00 Poster B26

Effect of annealing on electrical, structural and optical properties of sol gel ITO thin films

Talaat M. Hammad

Al-Azhar University (AZHR), El-Thalteen, Gaza 1277, Palestinian Territory

e-mail: talaath55@yahoo.com

The ITO thin films (In : Sn = 90 : 10) were prepared by the sol gel dip-coating process on glass substrates, followed by annealing in air. The effect of annealing in the temperature range of 150–550^{o}C on the electrical, optical and structural properties of ITO thin films has been studied. The electrical resistivity of ITO thin films was decreased by increasing annealing temperature. XRD pattern showed that increasing annealing temperature increased the crystallinity of thin films and at 550^{o}C high quality crystalline thin films with preferentially oriented in the (111) direction. The UV-vis transmittance spectra were also confirmed that the annealing temperature has significant effect on the transparency of thin films. The highest transparency at wavelength 520 nm of spectrum 92.3% obtained at 550^{o}C on annealing temperature. The allowed direct band gap at temperature range 150^{o}C-550^{o}C was estimated 3.32 eV – 4.15 eV. It was observed that the direct energy gap increases as the annealing temperature increases.

16:00 Poster B27

Antireflective properties of silica films formed in sol-gel processes

Janusz Jaglarz[1], Paweł Karasiński[2]

1. *Cracow University of Technology, Institute of Physics (PK), Podchorążych 1, Kraków 30-084, Poland* **2.** *Silesian University of Technology, Institute of Physics, Department of Microelectronics, Krzywoustego 2, Gliwice 44-100, Poland*

e-mail: pujaglar@cyfronet.krakow.pl

Sol-gel technology offers huge potential capabilities involving the fabrication of low refractive index layers which the refractive index can change within the range n=1.1 – 2.3, depending on the composition and the applied technological process. Therefore, basing on the silica films we can fabricate multilayer structures with a preset refractive index which can offer high application possibilities. In planar optoelectronics the silica films, depending on their optical and geometrical parameters, can be used as waveguide films, masking layers, and when supplied with an indicator they can be used as sensitive layers. The inhomogeneouity of these films may be also used as ARC (antireflective coatings).

The work presents silica films of the refractive index 1.12 to1.21 silica films of high Basic fabrication technology was presented as well as the applied measurement methods of refractive index and thickness. The paper provides examples for the application of the elaborated technology for the fabrication of waveguide films.
Basic fabrication technology was presented as well as the applied measurement methods of refractive index and thickness. The paper

provides examples for the application of the elaborated technology for the fabrication of sensitive layers

16:00 Poster B28

Effect of phosphorus incorporation in hydrogenated amorphous silicon

Amer Brighet[1], Rabah Cherfi[1], Mohamed Kechouane[1], Abdelmadjid Abdelmoumen[1,2]

1. *Laboratoire "Couches Minces et Semiconducteurs" - USTHB - Faculté de Physique -, BP 32 El-Alia - Bab-Ezzouar, Alger 16111, Algeria* **2.** *Centre de Developpement des Technologies Avancées (CDTA), BP17, Lot. 20 Aout 1956, Baba Hassen, Alger 16000, Algeria*

e-mail: kechouanem@yahoo.fr

The effects of the phosphorus incorporation on physical, chemical, optical and electric properties of phosphorus-doped hydrogenated amorphous silicon thin films (a-Si:H(P)) are presented. Doping was carried out from the use of a nontoxic phosphorus liquid source based on hydrocarbons (trimethylphosphine: TMP, (P (CH_3)) introduced into the deposit chamber by using hydrogen as carrying gas.

The a-Si:H films (0.7-1.0 mm thick) were deposited by the DC magnetron sputtering of a silicon target under hydrogen and argon plasma at various TMP partial pressures between 0 to 9.10^{-5} mbar. The a-Si:H(P) were characterized by secondary ion mass spectrometry (SIMS), infrared absorption, optical transmission and electrical conductivity measurements.
The infrared absorption at 670 cm^{-1} can be attributed to the P-H bonds. The effect of TMP partial pressure can be observed through the broadening of the 2000 cm^{-1} band and a displacement towards the high frequencies. The phosphorus incorporation in a-Si:H matrix was confirmed by secondary ion mass spectrometry (SIMS) measurements.

Optical transmission measurements are used in order to determine the refractive index n_S and the optical gap E_T. The increase of E_T can be explained by carbon/silicon alloy effect and the variation in refractive index is indicative of material structure change.

The effect of annealing temperature on electrical conductivity was also studied. The results concerning the variation of electrical conductivity under darkness and photoconductivity, respectively σ_d and σ_{ph}, according to the annealing temperature T_a clearly evidenced an increase in conductivity with T_a in the range of 130 - 225° C. The increase of conductivity with annealing can be explained by the increase in the doping effectiveness through the activation of the phosphorus atoms in the silicon matrix. The decrease of E_a can be related to the shift of the Fermi level towards the conduction band due to phosphorus doping.

16:00 Poster B29

Effects of boron and phosphorus incorporation in hydrogenated amorphous silicon

Amer Brighet[1], Nabil Khelifati[1], Rabah Cherfi[1], Mohamed Kechouane[1], Abla Rahal[1], Abdelmadjid Abdelmoumen[1], Aissa Keffous[2], Moussa Aoucher[1]

1. *Laboratoire "Couches Minces et Semiconducteurs" - USTHB - Faculté de Physique -, BP 32 El-Alia - Bab-Ezzouar, Alger 16111, Algeria* **2.** *Unité de Développement de la Technologie du Silicium (UDTS), 02 Boulevard Frantz Fanon, BP 140, Alger-7merveilles, Alger 16100, Algeria*

e-mail: kechouanem@yahoo.fr

The effects of boron and phosphorus incorporation on physical, chemical, optical and electric properties of boron and phosphorus-doped hydrogenated amorphous silicon thin films (a-Si:H(B), a-Si:H(B)) are presented. Boron was incorporated into the host material by a DC magnetron co-sputtering technique. Phosphorus doping was carried out from of a non-toxic phosphorus liquid source based on hydrocarbons (trimethylphosphine: TMP, (P (CH_3)) by using hydrogen as carrying gas.

a-Si:H(B) and a-Si:H(P) films at various hydrogen and TMP partial pressures were characterized by secondary ion mass spectrometry (SIMS), infrared absorption, optical transmission and electrical conductivity measurements.

SIMS measurements clearly showed evidence for boron incorporation. This boron incorporation induced an increase of the refractive index and a decrease of the optical gap. The infra-red analysis showed that hydrogen lies preferentially to silicon that with boron.

For a-Si:H(B) films, the increase of the hydrogen partial pressure induced an increase of the Si-H stretching and wagging band at 2000 and 640 cm^{-1} followed by a decrease of the Si-B and/or B-B stretching band at 700-900 cm^{-1}, accompanied by an increase of the optical gap and by an important reduction of electrical conductivity under darkness. The hydrogen is crucial for stability of the films; it plays the role as passivator for boron atoms where electrical activation takes place for the annealing temperature range between 200 and 350°C.

For a-Si:H(P) films, the infrared absorption at 670 cm^{-1} can be attributed to the P-H bonds. The effect of TMP partial pressure can be observed through the broadening of the 2000 cm^{-1} band. The increase of optical gap is related to carbon/silicon alloy effect and the variation of refractive index is indicative of material structure change. The conductivity increase with annealing is related to an increase of the doping effectiveness through the phosphorus activation in the silicon matrix.

16:00 Poster B30

Comparison among Mg-based photocathodes prepared by ns, ps and fs PLD for the production of high brightness electron beams

Paola Miglietta[1], Luca Cultrera[2], Alessio Perrone[1], Camelia Cojanu[3], Evie L. Papadopoulou[4]

1. *University of Lecce, Physics Department, Lecce 73100, Italy* **2.** *°Laboratori Nazionali Frascati INFN (INFN), Via E. Fermi 40, Frascati 00044, Italy* **3.** *National Institute for Lasers, Plasma and Radiation Physics (INFLPR), Bucharest- Magurele 077125, Romania* **4.** *IESL, FORTH, P.O. Box 1527, Vassilika Vouton, Heraklion 71110, Greece*

e-mail: paola.miglietta@le.infn.it

Mg-based photocathodes are attractive for the production of high brightness electron beams for future FELs, plasma acceleration experiments and high brillance linear colliders due to their respectable quantum efficiency.
The aim of this paper is to investigate the photoelectron performances and the surface morphology of Mg-based thin films prepared by pulsed laser deposition (PLD) using excimer lasers with different pulse duration: ns, ps and fs.
XeCl excimer laser (λ=308 nm) with pulse duration of 30 ns and KrF excimer laser (λ=248 nm) with 5 ps and 450 fs pulse duration were used for growing Mg films onto Si and Cu substrates in ultrahigh vacuum of 10^{-5} Pa at room temperature.

The photoelectron performances were tested in a DC photodiode cell. In order to increase the quantum efficiency, *in situ* laser cleaning treatments were applied to samples surface in order to remove oxidized or polluted layers.

Sacnning Electron Microscope (SEM) was used to characterize the morphology of the films deposited and the oxidation level of Mg was studied by Energy Dispersive X-Ray spectroscopy (EDX).

Comparison among Mg-based photocathodes prepared by ns, ps and fs PLD for the production of high brightness electron beams will be presented and discussed

16:00 Poster B31

Photoluminescence and Electrical properties of Epitaxial Al-doped ZnO thin film

Jun Hong Noh, Jae-Sul An, Chin Moo Cho, Hyun Soo Han, In-Sun Cho, Kug Sun Hong

Seoul National University, Department of Materials Science and Engineering (MSE, SNU), San 56-1, Sillim-dong, Gwanak-gu, Seoul 151-744, Korea, South

e-mail: perfect3@snu.ac.kr

Undoped and Al-doped ZnO (AZO) thin films were epitaxial grown on *c*-sapphire substrate by pulsed laser deposition. Photoluminescence and electrical properties of the as-deposited, 450 ^{o}C-air annealed, and 450 ^{o}C-subsequent hydrogen annealed films were measured. Near band edge (NBE) emission of AZO is far less than that of undoped ZnO. Further, the NBE emission of AZO reduced after 450 ^{o}C air annealing. However, subsequent hydrogen annealed AZO show more intense NBE emission than the as deposited film. In addition, electrical properties such as carrier concentration and Hall mobility were reversible changed as an oxidizing and a reducing annealing. In this study, temperature dependent photoluminescence properties of AZO as transparent conducting oxide which annealed in oxidizing and reducing atmosphere discussed combining their electrical properties.

16:00 Poster B32

Structured oxide films preparation by sol-gel method

Armen R. Poghosyan, Ira A. Ghambaryan, Stepan G. Grigoryan, Albert G. Hayrapetyan, Aleksandr L. Manukyan

Institute for Physical Research (IPR), IPR-2, Ashtarak-2 378410, Armenia

e-mail: arp@ipr.sci.am

The integrated optical elements prepared on ferroelectric thin films (in particular, lithium niobate films) are the most promising for optoelectronics applications. A key stage in production of the integrated optics devices is forming of microtopography on crystalline films. The current methods generally comprise two separate steps: producing of thin film and creation a topographical pattern on it. But use of these traditional methods to form the patterned lithium niobate films is very complicated due to difficulties of lithium niobate etching by mask.

Here we present new approach based on the development of the modified sol-gel technology. In this case, the photolithography is used on the stage of dried gel whereupon the direct crystallization of patterned precursor film allows to obtain structured oxide single crystal thin film without subsequent etching of crystalline film.

The precursor (dried gel) thin film patterns were prepared by two new related methods: from photosensitive sol-gel solution and by etching precursor film using photoresist. We have developed appropriate photosensitive precursors (amorphous film of the metal complex) for patterned lithium niobate film preparation and studied photosensitive characteristics of gel, film exposition and etching parameters. Unlike crystalline lithium niobate, the precursor films are easily etched. When grown on a sapphire substrate and properly annealed, the patterned precursor material becomes structured single crystal thin film with high aspect ratio topographic features. The developed method of preparation of structured oxide thin films could be the basis for future integrated optical devices.

16:00 Poster B33

The enhanced interface formation by low energy ion beam irradiation for the application of the fabrication process for flexible audible display device

Ie Sangyub, ByungTack Bea, JiWon Choi, WonKook Choi

Korea Institute of Science and Technology, Material Science and Technology Division, 39-1 Hawolgok-dong, Wolsong-gil 5, Seongbuk-gu, Seoul 136-791, Korea, South

e-mail: phantom7@empal.com

With the noble method of making the hydrophilic surface of polymer substrate before vacuum roll to roll process, the flexible audible display (FAD) device was studied. Our vacuum coated indium tin oxides (ITOs) electrodes on flexible polymer substrate, polyvinylidene difluoride (PVDF) showed the amorphous crystalline property and very robust mechanical properties. On the strongly textured polymer substrate of PVDF, the amorphous crystalline state was carefully characterized through XRD and TEM analysis. For the mechanical strength and the corresponding electrical property change analysis, we used the bending test with electrical property measurement. Our ITO layers showed the very little electrical conductance changes within a few percent after the bending condition over the several hundred times, of which test condition is asked by many industrial needs. Compared to the conventional other plasma or chemical treatment, ion beam irradiation technique is known to make an effective functional group near the targeted surface without any “damages or degradation” during the process. Without any degradation or chemical damages on the interface of ITOs and PVDF, the fully-dry process with laser ablation was considered to make the pattern for the device fabrication of OLED and film speaker. The FAD device after the process, showed two functions independently: light-emitting and sound generation. Especially, our film speaker device with the robust ITO layers on both sides of piezoelectric polymer worked at bended condition, which showed the adhesion enhanced effect of ITO/PVDF system. In the range of audible frequencies, FAD also showed the independent working performances as expected by our schematics of “two devices on one skin (flexible polymer substrate)”. From these results, the use of ion beam treatment for surface modification and the concepts of combinational flexible electronic device system with functional polymer substrate by dry process could be suggested.

16:00 Poster B34

Semimagnetic semiconductor oxides as materials for transparent electronics and spintronics

Andriy I. Savchuk, Victor P. Makhniy, Volodymyr I. Fediv, Gennadiy I. Kleto, Serhiy A. Savchuk

Chernivtsi National University (ChNU), 2 Kotsubinsky Str., Chernivtsi 58012, Ukraine

e-mail: savchuk@chnu.cv.ua

For ZnO doped with transition metals (TM) in addition to well known material properties new functionality and application in field of spintronics can be occurred. This application aspect especially has enhanced after theoretical prediction of room temperature ferromagnetism in ZnO doped with Mn [T. Dietl et al., Science, 287 (2000) 1019]. In our work TM (Fe, Co, Mn) doped ZnO thin films and nanocrystals are fabricated and their transport, magnetic, optical, magneto-optical properties are studied. The doped thin films were grown by pulsed laser deposition and ZnCoO nanocrystalline samples were prepared by chemical method. The most remarkable findings concerning to high-temperature ferromagnetic ordering was observed in case of $Zn_{0.97}Co_{0.03}O$ thin films and nanocrystals. It was found that kind of magnetism is very sensitive to growth conditions, carrier concentration, impurity concentration and kind of available defects. In addition, probability of occurrence of the ferromagnetism is higher for oxide nanometric layers and nanoparticles than in case of bulk crystals. Obviously, this is suggestion of exhibition of surface effects. From point of view possible application the studied materials are considered as an active component in sensing and detecting devices, in which can combine usual semiconductor properties with both quantum confinement and spin-exchange interaction effects. In particular, it was studied multilayer structure consisting of ZnMnO and ZnO layers. This structure was used for analysis of spin injection and detection in external magnetic field by magneto-optical technique. The revealed features give new insight into controversial magnetic behavior of semimagnetic semiconductor oxides and their possible applications in transparent and spin electronics. The work was supported by grant from Ministry of Education and Science of Ukraine.

Smart Materials for Smart Devices and Structures

Symposium C

Welcome

Dear Participants of Symposium on *Smart Materials for Smart Devices and Structures*

It has been a tradition of the E MRS Fall Meeting to organize Symposia on the hottest topics which currently excite the materials community.

Smart Materials are recognised as those that can respond to environmental stimuli with particular changes in some variables such as mechanical and physical properties, structure, composition or functions. Growing interest in their development is driven by emerging applications and integrations of smart materials into industrial systems including civilian, industrial, medical and military applications.

Among the variety of materials represented in the Symposium one can mention multiferroic materials, exhibiting two or more ferroic features, piezoelectric materials, shape memory and magnetic shape memory alloys, magnetorheological fluids and elastomers, and many others.

The Symposium highlights advances in the development of smart materials with a special focus on numerical modelling, fabrication methods, technologies, and properties, sensing and processing capabilities, in the light of their potential applications in smart structures, devices and systems.

Among the relevant scopes of the Symposium are new capabilities or a remarkable performance enhancement or cost reduction, new ideas and directions for future development.

The Symposium brings together researchers from various fields, including contributions from materials engineering, mechanical engineering, theoretical and applied mechanics, electronics, electromechanics and manufacturing.

I would like to take the opportunity of thanking everyone involved in the organization of this Symposium: the Organizing Committee, Scientific Committee, Invited Speakers and all the Participations whose contributions assure the high scientific level of this Conference.

Marcin Leonowicz

Organisers

Marcin LEONOWICZ, Faculty of Materials Science and Engineering, Warsaw University of Technology; mkl@inmat.pw.edu.pl

Mike R.J. GIBBS, Department of Engineering Materials, Sheffield University; m.r.gibbs@sheffield.ac.uk

Eckhard QUANDT, Institute for Materials Science, Faculty of Engineering, Kiel University; eq@tf.uni-kiel.de

Larisa KOZLOVA, Institute of Magnetism, NASU; kozlova@imag.kiev.ua

Laurent LEBRUN, Laboratoire de Génie Electrique et Ferroélectricité; laurent.lebrun@insa-lyon.fr

Dariusz OLESZAK, Faculty of Materials Science and Engineering, Warsaw University of Technology; daol@inmat.pw.edu.pl

Marzena SPYRA, Faculty of Materials Science and Engineering, Warsaw University of Technology; mspyra@inmat.pw.edu.pl

Proceedings

The manuscripts submitted to this symposium and accepted on the basis of the referee procedure adopted for regular papers will be published in the international scientific journal **"Solid State Phenomena".**

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Programme

Monday, 15 September

Opening & Plenary Session

Czochralski Award Ceremony
Monday morning, 15 September, 10:00
Small Hall (237)

Lunch break
Monday afternoon, 15 September, 12:30
Inner Courtyards

No session
Monday afternoon, 15 September, 14:00

Coffee break
Monday afternoon, 15 September, 15:30
Main Hall

Joint Poster Session 1

Monday & Wednesday
Monday afternoon, 15 September, 16:00
Main Hall

Tuesday, 16 September

Session 1
Tuesday morning, 16 September, 9:00
Room 231
Chair: Rouquette, Jerome

9:00 Invited oral

The remarkable electronic and mechanical properties of graphene.

Ernie W. Hill, Andre K. Geim

The University of Manchester, Centre for Mesoscience and Nanotechnology (CMN), Oxford Road, Manchester M13-9PL, United Kingdom

e-mail: e.w.hill@manchester.ac.uk

Graphene is the bright and still rapidly rising star on the horizon of materials science and condensed matter physics, revealing a cornucopia of new physical effects and potential applications. Graphene is the thinnest material known to man. It is a mono atomically thin 2-D film of Carbon atoms arranged laterally in a honeycomb benzene ring like structure. It was previously considered to be a physically unstable form until it was shown to exist in the free state by the team at Manchester. This conceptual material is widely used to describe the crystal structure and properties of graphite, large fullerenes and carbon nanotubes. Indeed, as a first approximation, graphite is made of graphene layers relatively loosely stacked on top of each other. In the case of carbon nanotubes, they are usually thought of as graphene layers rolled into hollow cylinders.

Graphene is a zero gap semiconductor, where the charge carriers have a linear dispersion relation near the Dirac point essentially giving them zero effective mass. Room temperature carrier mobilities of the order of 25,000 cm^2/Vs are routinely observed with mobilities up to approximately 200,000 cm^2/Vs ultimately achievable. Transport in this system is ballistic and carriers can travel sub-micrometer distances (typically300nm) without scattering giving it many applications for fast electronics. It is extremely transparent, yet highly conductive making it an ideal electrode material in LCD displays and solar cells. We will also show that micrometre-size sensors made from graphene are capable of detecting individual events when a gas molecule attaches to or detaches from graphene's surface. As a suspended membrane it is sufficiently electron transparent to allow individual metallic atoms to be imaged on its surface which together with its ruggedness provides an ideal support membrane for TEM studies. These remarkable electronic and mechanical properties will be discussed together with its potential applications.

9:30 Invited oral

Rapid prototyping methodologies for Smart Material micro components

Paul R. Chalker, Adam T. Clare, Kaj Berggreen, Jetinder Singh, Christopher J. Sutcliffe

The University of Liverpool (UOL), Engineering, Brownlow Hill, Liverpool L693GH, United Kingdom

e-mail: pchalker@liv.ac.uk

The development of Smart Materials is largely being driven by emerging applications in control and environmental monitoring. To be useful, manufacturing processes must be available that are capable of forming micro-scale components with complex shapes and three dimensional geometries which can fully exploit the properties of these smart materials. In this paper, we consider the rapid prototyping of micro components using selective laser - and the so-called 'digital light' - processing methodologies.

The selective laser sintering of barium titanate components directly from powder beds and from spin-coated suspensions in a carrier photoresist is discussed. The laser processing conditions and ambient environment are critical in achieving sintering. Peak laser power is found to be more influential than laser exposure time. The partial pressure of oxygen in the sintering environment is also critical in avoiding detrimental degradation of the ceramic.

Selective laser melting has been used to build high aspect ratio, three-dimensional NiTi components. The influence of laser dwell time and raster pitch on the density of NiTi shape memory alloy parts and their resolvable feature sizes is considered. The response of shape memory springs produced by this method is discussed.

Lastly the digital light processing of polymeric materials is reviewed as a potential route for the fabrication of piezoelectric polymer components. The use of mixtures of polymers such as an acrylic host combined with a piezoelectric constituent such as polyvinylidene fluoride is considered. The role of the UV photo sensitizer and its influence of the component performance will be reviewed.

10:00 Oral

Formation of Metal Silicide Nanodots on Ultrathin SiO_2 for Floating Gate Application

Seiichi Miyazaki, Mitsuhisa Ikeda, Katsunori Makihara, Kazuhiro Simanoe

Hiroshima University, Graduate School of Advanced Sciences of Matter (HU-ADSM), Higashi-Hiroshima 1-3-1, Higashi-Hiroshima 739-8530, Japan

e-mail: semiya@hiroshima-u.ac.jp

Charge storage in metallic nanodots embedded into a dielectric layer has received much attention because of their potential advantages in storage capacity in comparison to semiconducting quantum dots (QD). Uniform formation of metallic nanodots with an areal density over $\sim 10^{11} cm^{-2}$ without degrading gate oxide reliability caused seriously by metal diffusion is one of major technological challenges. We have developed a new fabrication method of nanometer-scale metal dots on thermally-grown SiO_2 with a fairly uniform size distribution and a high areal density, in which ultrathin films of Ni, Pt and Pd are exposed to remote H_2 plasma at room temperature [1].

In this work, we extended our research to form metal silicide dots showing good thermal stability compared with elemental metal dots.

Si-QDs with a dot density of $\sim 2x10^{11} cm^{-2}$ were first self-assembled on ultrathin SiO_2 by controlling the early stages of LPCVD using SiH_4. Subsequently, Ni or Pt evaporation on Si-QDs was performed and followed by remote H_2 plasma treatment without additional heating.

AFM measurements at each process step confirm uniform formation of Si-QDs on SiO_2 before metal evaporation, conformal coverage with a very thin metal layer just after evaporation and an increase in the dot height without no change in the dot density after the H_2 plasma treatment. By using an electrically-baised AFM tip, we have also verified that electrical separation among nanodots on SiO_2 is restored by the H_2 plasma treatment. The silicidation of Si-QDs was confirmed from changes in core lines and valence band spectra and photoemission cut-off energy as detected by high-resolution XPS. In addition, the temporal decay in the surface potential after charge injection to the dots shows that retention characteristics of silicide dots is superior to Si-QDs with almost the same size as expected in a deeper potential well for electrons in silicide dots than pure Si-QDs.

[1] K. Makihara et al., JJAP, 47 (2008) 3099.

10:15 Oral

Thermochromic VO_2 Films with Enhanced Luminous Transparency and Solar Modulation

Nuru R. Mlyuka[1,2], Gunnar A. Niklasson[1], Claes Granqvist[1]

1. *Uppsala University, Department of Engineering Sciences, The Angstrom Laboratory, Uppsala SE-75121, Sweden* **2.** *University of Dar es Salaam, Physics Department, Dar es Salaam 35063, Tanzania*

e-mail: nmlyuka@yahoo.com

Vanadium dioxide (VO_2) shows an abrupt change in optical and electrical properties when its temperature is raised beyond a critical point of ~68 ^{o}C. Films made from such materials have a potential to be used in smart windows with dynamic throughput of solar radiation. Two of the drawbacks of this material have been its low luminous transmittance and small solar transmittance modulation during switching. In this work we report calculations and experiments on multilayers of VO_2 and TiO_2 films, produced by reactive magnetron sputtering, that significantly improve the luminous transmittance and solar modulation of the films during switching.

Coffee break

Tuesday morning, 16 September, 10:30
Main Hall

Session 2

Tuesday morning, 16 September, 11:00
Room 231
Chair: Reaney, Ian M.

11:00 Invited oral

MagMEMS - increased functionality to traditional MEMS platforms

Mike Gibbs

University of Sheffield, Department of Engineering Materials, Mappin Street, Sheffield S1 3JD, United Kingdom

e-mail: m.r.gibbs@sheffield.ac.uk

MEMS are currently seeing significant market penetration in such areas as sensors for car air bags. Pick-off is typically achieved using piezoresistive elements to which electrical contact must be made. This presentation will demonstrate that the use of piezomagnetic materials in place of the piezoelectrics offers increased functionality. We coin the term MagMEMS for MEMS that contain magnetic components. The primary benefit of MagMEMS is that pick-off can now be by wireless techniques offering deployment in hostile or remore locations. Using simple structures, cantilevers and membranes, examples will be given of technology platforms. In exploring the benefits of piezomagnetic materials in MEMS the simplification to the whole sensor system will be discussed when the ΔE effect is used. This is the field dependence of Young's modulus that be be made to dominate the mechanical response of MagMEMS. Key materials for use in MagMEMS will also be discussed, along with some potential areas of commercial exploitation.

11:30 Invited oral

Creating Objects from the Inside-Out

Siavash Mahdavi

University College London (UCL), 20 Gordon Street, London WC1H, United Kingdom

e-mail: sia@complexmatters.com

This paper will detail the work that Complex Matters has achieved in the design and use of smart materials. The principals of the bio-inspired algorithms and the problems faced with using these algorithms on real world problems will be overviewed.

These algorithms have been successfully implemented in several industries. These range from products design, fashion and sportswear to aerospace, F1 and orthopedics.

12:00 Oral

3D magnetovision scanner as a tool for investigation of magnetomechanical principles

Daniel Lewandowski, Jerzy Kaleta, Przemysław Wiewiórski

Wroclaw University of Technology, Institute of Materials Science and Applied Mechanics (PWr - IMMT), Smoluchowskiego 25, Wrocław 50-370, Poland

e-mail: daniel.lewandowski@pwr.wroc.pl

The study was aimed at designing a system for measuring the distribution of magnetic field around different magnetic objects including Smart Magnetic Materials. A new type of 3D scanner for monitoring the magnetic field intensity was constructed. The measurement principle is based on internal magnetics properties of materials and the reverse magnetostriction effect (also called the Villari effect). No external magnetizing field is assumed; the entire magnetic effect is due to magnetomechanical principles.

The new generation of Honeywell magnetosensors were applied to measure filed intensity in 3D. Small size of measurement area (1.5 mm^3) allows quasi-local measurement of magnetic field. The aim of this stage of research was to constructed the set for measurement of strength of very weak magnetic field (10 A/m) around the magnetic objects. In scanner construction three axis for displacement in directions consistent with sensor axis were applied. It allows measure magnetic field vector in geometrical coordination. Specialized software for data acquisition, processing and visualization of magnetic field vector has been written.

In preliminary parts of work magnetic scanner system allows determination of correspondence between mechanical, electric and magnetic quantities. As a main application for this type of system are: reverse magnetostriction and magnetostriction in smart magnetic materials and composites, martensistic transformation induces plastic strain in shape memory alloys, NDT investigation, identification of local plastic deformation and texture of ferromagnetic materials.

12:15 Oral

Finite element model of polyelectrolyte hydrogels swelling-comparison with experiments

Robert A. Paxton, Ahmed Al-Jumaily

Institute of Biomedical Technologies, Auckland University of Technology (AUT), AUT City Campus, Auckland 1142, New Zealand

e-mail: ahmed.al-jumaily@aut.ac.nz

During the past few years we been extensively studying the swelling dynamics of polymer hydrogels, for use as a novel type of changeable focal length lens. It is anticipated that the "volume phase transition", inherent to all polymer hydrogels, can be utilised to create a lens with multiple focal distances. While hydrogel swelling can be triggered by a wide variety of stimuli, for the present purposes, electrical stimulation was seen as the optimum choice. Using MATLAB, a finite element model (FEM) was developed that could describe the swelling of a poly (acrylic acid) hydrogel under the influence of an applied electric field. The model is highly customisable, and essentially all results are available to the end user. The modular design of the model also permits each piece of the model to be improved individually, and then recombined back into the overall model. To verify this FEM model, gel swelling experiments were conducted on poly(acrylic acid) hydrogel disks under the influence of an externally-applied DC source. The deformation of the upper surface of the gels was recorded, and then compared to the theoretically predicted deformation. It must be stressed that this is the first version of this model, and it was not expected that the model would perfectly predict the swelling of the polymer hydrogel. However, experimental validation was necessary at this stage to identify parts of the model that required further improvement.

Lunch break

Tuesday afternoon, 16 September, 12:30
Inner Courtyards

Session 3

Tuesday afternoon, 16 September, 14:00
Room 231
Chair: Gibbs, Mike

14:00 Invited oral

Structure, domain structure and piezoelectricity in perovskite and related ceramics

Ian M. Reaney

Sheffield University, Brook Hill, Sheffield S37HF, United Kingdom

e-mail: I.M.Reaney@sheffield.ac.uk

Perovskites and related compounds constitute the majority of commercial piezoelectric ceramics. Typically, most publications note the structure, grain size and properties of piezoelectrics but often very little is reported about their domain and domain wall structure. In many commercial systems, it is the motion or vibration of the domain wall which dominate the piezoelectric and electromechanical coupling coefficients, the so-called extrinsic contribution. This article discusses mechanisms relating to structure and domain wall structure which either suppress or enhance extrinsic contributions. Consideration is given to the multiferroic nature of some systems in which octahedral tilt in addition to ferroelectric phase transitions occur. The domain structure at and adjacent to the morphotropic phase boundary in several well known systems is also discussed.

14:30 Invited oral

P-T studies of $Pb(Zr_{1-x}Ti_x)O_3$ Ferroelectric Materials

Jerome Rouquette, Guillaume Fraysse, Ali Al-Zein, Veronique Bornand, Marie Pintard, Papet Philippe, Julien Haines

e-mail: jerome@lpmc.univ-montp2.fr

Due to their exceptional ferroelectric properties, $PbZr_{1-x}Ti_xO_3$ (PZT) ceramics have been the subject of numerous studies. Dielectric susceptibility and piezoelectric properties are dependent on 3 variables: applied electric field, temperature and mechanical stress σ_{ij}. In spite of the high sensitivity of the physical properties of PZT to hydrostatic pressure, its effect has been studied only recently. However, large stress fields can be observed in miniaturized components or in ferroelectric dots. In the literature, experiments and theoretical calculations have indicated the existence of an intrinsic short range dynamical disorder over nearly the entire PZT solid solution. In order to determine the phase transition sequence of this disordered material, we reported resonance Raman Spectroscopy of a self-trapped exciton emission oxygen deficient complex (Ti_{Ti}'-V_O··) was performed to probe titanium displacements as a function of the temperature[1]. Recently, note also for example that careful Rietveld refinements yield significantly better agreement factors using monoclinic models for the long-range structure of $PbZr_{0.60}Ti_{0.40}O_3$, with a *Cc* space group at low temperature and with a *Cm* space group at high temperature, rather than the widely accepted rhombohedral symmetry[2].

Based on neutron diffraction, X-ray diffraction, resonance Raman spectroscopy and X-Ray absorption Spectroscopy, we will present an overview of our new results on structure and dynamics of $Pb(Zr_{1-x}Ti_x)O_3$ solid solution as a function of P and T[3]. These new important features have to be considered in the fundamental understanding of the ferroelectric-to-ferroelectric and ferroelectric-to-paraelectric phase transitions of such an important technological material.

[1] J. Rouquette, J. Haines, V. Bornand, M. Pintard, Ph. Papet, J.L. Sauvajol, Phys. Rev. B **73**, 224118, (2006).

[2] G. Fraysse, J. Haines, V. Bornand, J. Rouquette, M. Pintard, Ph. Papet, S. Hull, , Phys. Rev. B **77**, 064109 (2008).

[3] (to be published).

15:00 Oral

Simultaneous growth of MWCNTs at different temperatures in a variable gradient furnace

Valentina Grossi, Alessandro Urbani, Andrea Giugni, Sandro Santucci, Maurizio Passacantando

Università dell'Aquila, Dipartimento di Fisica, Via Vetoio, L'Aquila I-67010, Italy

e-mail: valentina.grossi@aquila.infn.it

Multi-walled carbon nanotubes (MWCNTs) have been grown, simultaneously at different temperatures, by thermal chemical vapour deposition (CVD) of acetylene (C_2H_2) gas, in ammonia (NH_3) atmosphere. The reactor for the CVD growth is a horizontal quartz tube mounted inside a furnace. An accurate calibration of the temperature, at various distances from the tube mean position has been performed by a thermocouple. Silicon oxide substrates, coated with 3 nm of nickel (Ni) film, have been placed at different positions in the reactor and the

CNTs have been grown at different temperatures: 750 °C, 725 °C, 700 °C and 600 °C. The tube has been heated by radiation, in an argon (Ar) flux, up to 980 °C (temperature in the middle of the reactor). In order to obtain the Ni nanoclusters, only a NH_3 gas has been introduced into the quartz tube for 20 min at 980 °C. The CNT growth has been performed at 980 °C for 1 hour introducing C_2H_2 and NH_3 gasses with the flux ratio (C_2H_2:NH_3) of 1:5. Scanning electron microscopy (SEM) images show a uniform and a highly dense distribution of CNTs. But, as the growth temperature of substrate increases, the CNT average diameter and density distribution decrease. There is a temperature limit (725 °C) for the CNT growth. At 750 °C we obtain only the Ni clusters with the amorphous carbon. The Raman spectra show that we produce the MWCNTs. The presence of the D-peak indicates that the CNTs have the structural defects to respect to the high crystalline graphitic layers, indicated by the G-peak. Where the temperature of the substrates is higher the D-band line-width is smaller but the ratio of intensities of D and G peaks is still high. The Raman spectra confirm that when the substrate temperature increases the CNT density distribution decreases. The CVD method of growth is totally selective. It is possible to obtain the isolated arrays of CNTs and then to realize the gas sensing (NO_2) devices.

Coffee break

Tuesday afternoon, 16 September, 15:30
Main Hall

Wednesday, 17 September

Session 4

Wednesday morning, 17 September, 9:00
Room 231
Chair: Mahdavi, Siavash

9:00 Invited oral

Coupling of magnetism and structure in Heusler shape-memory alloys

Antoni Planes, Xavier Moya, Lluís Mañosa

Universitat de Barcelona, Departament d'Estructura i Constituents de la Materia, Barcelona 08028, Spain

e-mail: toni@ecm.ub.es

Magnetic shape-memory properties are a consequence of the coupling between magnetic and structural degrees of freedom in systems undergoing a martensitic transition. The application of a moderate magnetic field in this class of functional materials gives rise to large strains by either inducing the transition or rearranging twin-related variants in the martensitic phase. Related to this martensitic transition, these systems also show other interesting functional properties such as giant magnetocaloric and magnetoresistance effects. Ni-Mn-Ga in a range of compositions close to the Heusler composition (Ni_2MnGa) was the first to be discovered and it is considered to be the prototypical material which displays these properties. In recent years, research has been extended to other magnetic alloys and most particularly to alloys of the Ni-Mn-X family where X is a group IIIA-VA element.

In the present talk, after briefly summarizing the general properties of this class of materials, we will present recent results of relevance for the understanding of the effect of magnetism on the martensitic transformation. Finally, the requirements for the occurrence of multifunctional properties will be discussed.

9:30 Invited oral

Field induced structural modifications and magnetocaloric effects in martensitic Heusler alloys

Mehmet Acet[1], Seda Aksoy[1], Pascale Deen[3], Eberhard F. Wassermann[1], Xavier Moya[2], Lluís Mañosa[2], Antoni Planes[2]

1. *Duisburg-Essen University, Experimental Physics, Lotharstr. 1, Duisburg D-47048, Germany* **2.** *Universitat de Barcelona, Departament d'Estructura i Constituents de la Materia, Barcelona 08028, Spain* **3.** *Institut Laue Langevin (ILL), Avenue des martyrs, Grenoble 38042, France*

e-mail: mehmet.acet@uni-due.de

Applying a magnetic field to ferromagnetic systems in the temperature vicinity of a first order structural transition can lead to magnetic field induced structural modifications and large magnetocaloric effects. Many Ni-Mn-based ferromagnetic Heusler alloys undergo first order martensitic transformations. Applying a magnetic field at temperatures close to the transition causes large field-induced strains and large magnetocaloric effects. In many of these systems, the field-induced strain is due to a field-induced reverse martensitic transformation to the austenitic state. The magnetocaloric effect around the transition is ‘inverse’, in which case the sample cools on applying a field as opposed to the ‘conventional’ case where it warms. In order to gain more insight into the mechanism of the large field-induced strains and the inverse magnetocaloric effect, we have performed diffuse polarized neutron diffraction experiments using the XYZ-polarization analysis technique. These experiments reveal the development of strong antiferromagnetic correlations just below the martensitic transition temperature. We discuss the relationship of these correlations with the inverse magnetocaloric effect and the field-induced strains.

10:00 Oral

Structure formation in annealed NiMnGa shape memory alloys

Rafał Wróblewski, Marcin Leonowicz

Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland

e-mail: rwroblewski@inmat.pw.edu.pl

Effect of annealing conditions on the structure and phase transition temperatures for polycrystalline $Ni_{50}Mn_{29}Ga_{21}$ alloy was studied. The final structure strongly depends on the annealing temperature and cooling rate. Ordering of the austenitic phase, performed by annealing at elevated temperatures, plays an important role in formation of the proper martensitic structure. For the $Ni_{50}Mn_{29}Ga_{21}$ alloy annealing below the ordering temperature (1033 K) forms 5M modulated martensitic structure, irrespective of the cooling rate. The 7M modulated martensitic structure can be produced after annealing above the ordering temperature, followed by slow cooling.

10:15 Oral

The investigation of longitudinal acoustic waves in Heusler $Ni_{53}Mn_{25}Ga_{22}$ alloy crystal with coupled magnetostructural transition

Yuri A. Kuzavko

The Polesie Agrarian Ecological Institute of the National Academy of Science of Belarus (PAEI), Brest 224000, Belarus

e-mail: kuzavko@newmail.ru

Heusler $Ni_{53}Mn_{25}Ga_{22}$ ferromagnetic alloy crystal (sizes 4.0 x 3.8 x 10 mm) with shape memory effects (SME) has the coupled magnetostructural phase transition (the austenite starting temperature $A_s=116^oC$ and finishing one $A_f=134^oC$, the martensite starting temperature $M_s=109^oC$ and finishing one $M_f=97^oC$) below the Curie temperature $T_c=134^o$ C. This characterising temperatures were defined by acoustical measurements using the longitude uldtrasound transducers with 2.8, 3.5, 5 MHz resonance frequences. Temperature was measured with accuracy of 0.025K, the minimal heating speed was 1 K / 3 min and holding one was 1 K / 10 min. The sample is placed at 2 Oe constant magnet at necessity. Sample was temperature-controlledm heated with a low-ohm warmer from a power supply. Temperature was measured by termo-couple and microvolmeter.

This alloy has reversible thermoelastic martensite transitions. The process of a return to parent shape is coupled with a reveversible transition of a deformed martensite (D_{4h}) phase into a high-temperature austenitic (O_h) one. For our crystall the lattice parameters are a=b=0.7753 nm, c=0.6598 nm, as for Ni_2MnGa a=b=0.5920 nm, c=0.5566 nm at D_{4h} phase, a=0.5825 nm at O_h.

We have studied experimentally the temperature dependences of the ultrasound speed and amplitude of pulse signals my means of digital measuring equipments.

The presence of a soft transverse mode TA_2 takes place for the alloy [2]. It propagates along directions [110] and related with accession to zero of the elasticity constant $c`=(c_{11}-c_{12})/2$. The theory was designed for investigated effects consisting the linear and nonlinear magnetoacoustical ones.

Coffee break

Wednesday morning, 17 September, 10:30
Main Hall

Session 5

Wednesday morning, 17 September, 11:00
Room 231
Chair: Planes, Antoni

11:00 Invited oral

Electron microscopy studies of Ni-based shape memory materials revealing (un)expected microstructural features

Dominique Schryvers

University of Antwerp, EMAT, Groenenborgerlaan 171, Antwerp B-2020, Belgium

e-mail: nick.schryvers@ua.ac.be

Many of today's shape memory systems are based on the Ni-Ti alloy used near to its equiatomic composition. However, regular Ni-Ti-based systems operate with a substantial hysteresis which can for some applications be a hinderance. In the present lecture we will present results on different ternary system $Ni_{50-x}Ti_{50}X_x$ (X = Pd, Pt, Au) in which different amounts of ternary compound substitution on Ni positions lead to special ratios between the austenite and martensite lattice parameters. The applied alloying elements and conditions for the low hysteresis were obtained based on the non-linear crystallographic theory of Ball and James. As a result of the compatibility between austenite and martensite, the hysteresis of the transformation becomes very narrow and the amount of microtwinning, necessary to yield an invariant plane strain, decreases drastically. Also, when changing the amount of alloying element, the type of stable microtwinning changes from Type I & II into compound. Detwinning and rearrangement of the martensite plates lead to a radically different microstructure which can account for the decrease of hysteresis. Still, practical samples appear to be rather inhomogeneous containing large precipitates disturbing local compatibility conditions.

11:30 Oral

SMA Thin Strip for Rotary-Driving Element

Hisaaki Tobushi[1], Elzbieta A. Pieczyska[2], W. Nowacki[2], Yoshiki Sugimoto[1]

1. *Aichi Institute of Technology (AIT), 1247 Yachigusa, Takusa-cho, Toyota 470-0392, Japan* **2.** *Polish Academy of Sciences, Institute of Fundamental Technological Research (IPPT PAN), Świętokrzyska 21, Warszawa 00-049, Poland*

e-mail: tobushi@aitech.ac.jp

The shape memory effect (SME) and superelasticity (SE) appear in shape memory alloy (SMA). If an SMA thin strip is twisted, the rotary motion can be obtained easily and therefore we can develop a simple rotary-driving element by using the SMA thin strip. In the present study, the performance of the SMA thin strip for rotary-driving elements is investigated. The torsional deformation properties of the SMA thin strip are investigated. Elongation of the edge in the SMA thin strip is measured. The variation in temperature on the surface of the strip is observed by the infrared thermograph. The highest temperature rise appears at the edge of the strip due to the martensitic transformation during twisting. The cyclic deformation properties in torsion of the strip are investigated in both temperature regions of SME ans SE. The relationship between torque and angle of twist varies slightly till 50 cycles in both SME and SE. The torsional fatigue properties are investigated by both pulsating and alternating fatigue tests. The fatigue life in alternating torsion is shorter than that in pulsating torsion. The relationship between angle of twist and the number of cycles to failure in the low-cycle fatigue region is expressed by a power function for both pulsating torsion and alternating torsion. A door model composed of an SME-SMA strip and an SE-SMA strip is fabricated. The two-way motion with opening and closing of the door is demonstrated.

11:45 Oral

SME and TWSME study in Ti-Ni alloy after strain aging

Elena P. Ryklina, Sergey D. Prokoshkin, Anna A. Chernavina, Nathaly N. Perevoshchikova

Moscow State Steal & Alloys Institute, Moscow 117936, Russian Federation

e-mail: rykluna@tmo.misis.ru

This paper focuses on the optimization of shape memory effect (SME) and two-way SME (TWSME) training parameters bringing maximum two-way recovery strain. the joint effect of isothermal annealing at 430°C after Low-Temperature Thermomechanical Treatment (LTMT) and external training parameters on functional properties of Ti-50.7%Ni alloy is studied. The homogenizing annealing at 700°C, 20 min is chosen as a reference heat treatment (RHT). Under experiment procedure, the bending loading mode, strain state, loading value and loading time were varied. Increasing of strain aging time from 10min to 10hr affects characteristic temperatures A_s and A_f after aging and RHT, however, in the case of LTMT the A_s - A_f temperature range is significantly wider than after RHT. The TEM and X-ray studies testify that it is caused by two factors: heterogeneity of nano-size subgrain structure and nano-phase Ti_3Ni_4 precipitates.

The evolution of SME and two-way TWSME parameters is studied as well. The recovery strain ε_r and TWSME amplitude ε_{TW} increase with aging time. variation of loading time is effective for ε_{TW} regulation under multi-cycle training procedure. The achievement of required TWSME value is possible after minimum number of training cycles owing to exposure time increasing in a constrained condition. The loading mode and constraining strain ε_t strongly affect all studied SME and TWSME parameters.

Variation of training parameters enables additional precise regulation of final functional properties. The obtained results can be used for development elements functioning in conditions of TWSME realization.

12:00 Oral

Confining Jacket for Concrete Cylinders using Ni-Ti-Nb Shape Memory Alloy Wires

Eunsoo Choi[1], Nam Tae-hyun[2], Chung Young-Soo[3], Cho Baik-Soon[4]

1. *Department of Civil Engineering, Hongik University, Seoul 121-791, Korea, South* **2.** *Gyeoungsang National University, Department of Metal & Material Engineering, Jinjoo, Korea, South* **3.** *Chungang University, Department of Civil Engineering, Seoul 156-756, Korea, South* **4.** *Inje Uisversity, Department of Civil Engineering, Kimhae, Korea, South*

e-mail: eunsoochoi@krri.re.kr

Ni-Ti-Nb shape memory alloy wires can induce more recovery stress than Ni-Ti alloy wires. This study used the prestrained Ni-Ti-Nb SMA wires to confine concrete cylinders. At first, several tests to measure the recovery stress were conducted with varying the maximal strain of the wires. Then, the concrete cylinder of 150 mm and 300 mm (diameter and length) were wrapped by the prestrained wires. The unconfined concrete cylinders were tested and their results were compared to those of the confined cylinders with the SMA wires. Also, the performance of the Ni-Ti-Nb wires compared to that of the Ni-Ti wires from a previous study. The Ni-Ti-Nb SMA wires increased the compressive strength and the ductility of the cylinders due to the confining effect. Also, the wires were more effective to increase the ultimate strength of the cylinders than the conventional Ni-Ti wires. The study showed the potential of the proposed method to retrofit reinforced concrete columns using SMA wires to protect themselves from an earthquake.

12:15 Oral

Factors Influencing The Development of Two-Way Shape Memory Effect Induced by Bending Deformation in TiNi Alloy

Zohre Balak

Science and Technology, Tehran 0098, Iran

e-mail: homa55ir@yahoo.com

Number of training cycle, amount of pre-strain and composition influencing the development of two-way shape memory effect induced by bending deformation in TiNi alloy which trained in martensitic state, were investigated. The transformation temperatures was measurement by differential scanning calorimetry (DSC). the results showed, optimum number of training cycle and pre-strain were 30 cycles and 12.5% respectively. Also it was found that two-way shape memory alloy increases with increasing the training cycles and decreasing in Ti content.

Lunch break

Wednesday afternoon, 17 September, 12:30
Inner Courtyards

Session 6

Wednesday afternoon, 17 September, 14:00
Room 231
Chair: Schryvers, Dominique

14:00 Invited oral

Reversible strain tuning of magnetism and electrical conductivity

Kathrin Dorr

Institut fuer Metallische Werkstoffe, IFW, Dresden, Germany

e-mail: k.doerr@ifw-dresden.de

A versatile experimental method for the electrical control of quantitatively defined biaxial strain in thin films will be introduced. It relies on growing the films epitaxially onto piezoelectric substrates of pseudocubic $0.72Pb(Mg_{1/3}Nb_{2/3})O_3 - 0.28PbTiO_3(001)$ (PMN-PT). Uniform reversible piezoelectric in-plane strain of ≤ 0.4 % can be applied. In this way, the strain-dependent magnetization and electrical conductivity of strongly correlated magnetic oxide films have been explored. Giant responses to reversible strain of the magnetization and conductivity of various manganites $R_{1-x}A_xMnO_3$ (R = La, Pr; A = Sr, Ca) will be discussed. An even larger effect on electron transport has been discovered in strained $La_{1-x}Sr_xCoO_3$ films [1]. We employed x-ray diffraction methods to study quantitatively the elastic film strains.
[1] A. D. Rata et al., *Phys. Rev. Lett.* 100, 076401 (2008)

14:30 Oral

A Simulation Study of Magnetostrictive Material Terfenol-D in Automotive CNG Fuel Injection Actuation

Habibullah A. Chowdhury, Saiful A. Mazlan, Abdul G. Olabi

School of Mechanical and Manufacturing Engineering, Dublin City University, Dublin Dublin9, Ireland

e-mail: chowdhh2@mail.dcu.ie

Magnetostriction is the deformation that spontaneously occurs in ferromagnetic materials when an external magnetic field is applied. In applications broadly defined for actuation, magnetostrictive material Terfenol-D ($Tb_{0.3}D_{0.7}Fe_{1.9}$) possesses intrinsic rapid response times while providing small and accurate displacements and high-energy efficiency, which are some of the essential parameters required for fast control of fuel injector valves for decreased engine emissions and lower fuel consumption compared with the traditional solenoid fuel injection system. A prototype CNG fuel injector assembly was designed using Pro-Engineer which included magnetostrictive material Terfenol-D as the actuator material. A 2D cross-sectional geometry of the injector assembly, which incorporated the real linear or non-linear magnetic properties of corresponding materials, was modeled in both Finite Element Method Magnetics (FEMM) and ANSYS for 2D axisymmetric magnetic simulation. The coil-circuit parameters and the magnetic field strength were determined to achieve the required magnetostrictive strain, and consequently, the injector needle lift. The FEMM magnetic simulations were carried out with four different types of AWG coil wires and four different coil thicknesses. Eventually, the optimized parameters that were obtained for each coil thickness from FEMM results analysis were verified against ANSYS non-linear electromagnetic simulation, which showed identical consequences. Subsequently, a 3D replica of the CNG flow conduit was modeled in GAMBIT with the resultant injector lift. The meshed conduit was then simulated in FLUENT using the 3D time independent segregated solver with standard k-epsilon viscous model to determine the mass flow rate of CNG to be injected. Eventually, the simulated flow rate was verified against mathematically derived static flow rate required for a standard automotive fuel injector considering standard horsepower, BSFC and injector duty cycle.

14:45 Oral

Differential magntoelastic compressive force sensor utilizing two amorphous alloy ring cores

Adam Bieńkowski[1], Roman Szewczyk[1], Jacek Salach[1], Roman Kolano[2]

1. *Warsaw University of Technology, Faculty of Mechatronics, Św. Andrzeja Boboli 8, Warszawa 05-525, Poland* **2.** *Institute of Nonferrous Metals, Sowińskiego 5, Gliwice 44-100, Poland*

e-mail: a.bienkowski@mchtr.pw.edu.pl

Magnetoelastic effect can be observed as changes of permeability of soft magnetic material subjected to stresses generated by external forces. This effect can be used for development of high sensitivity stress and force sensors for industrial applications.

Paper presents results of investigation on functional characteristics of magnetoelastic compressive force sensor utilizing two $Fe_{81}Si_4B_{15}$ amorphous alloy ring-shaped cores. Uniform distribution of stresses in core was achieved due to special non-magnetic backings. Signal from sensing coils of cores was connected to differential amplifier, whereas sine wave voltage signal was applied to magnetizing circuit.

Result of investigation indicated, that differential configuration enable to reduce temperature sensitivity of magnetoelastic sensor. Moreover high stress sensitivity of developed sensor was indicated. These results confirm, that differential configuration of magnetoelastic sensor is suitable for practical application in sensors development.

This work was supported by Polish Ministry of Science and Higher Education under Grant PBZ-KBN-095/T08/2003.

15:00 Oral

Microstructure and magnetic properties of two phase b+g ferromagnetic Co-Ni-Al alloys

Wojciech Maziarz[1], Jan M. Dutkiewicz[1], Marcin Leonowicz[2], Rafał Wróblewski[2]

1. *Polish Academy of Sciences, Institute of Metallurgy and Materials Sciences (IMIM PAN), Reymonta 25, Kraków 30-059, Poland* **2.** *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland*

e-mail: nmmaziar@imim-pan.krakow.pl

The microstructure and magnetic properties of two ferromagnetic alloys with composition as: $Co_{35}Ni_{37}Al_{28}$ and $Co_{37}Ni_{35}Al_{28}$ (in at. %) were investigated by optical microscopy (OM), analytical transmission electron microscopy (TEM) and vibrating sample magnetometer (VSM). The plastically deformed alloys up to 45% were then heat treated in order to promote the martensitic transformation. Differential scanning calorimeter (DSC) was used for determination of characteristic temperatures of transformation, and it was observed a drop of M_s temperature due to the increase of Co content in alloys. The elongated twined grains of size of about 200 mm and small precipitation of g phase has been identified by OM techniques. TEM observations allowed identifying the $L1_0$ non modulated martensite within elongated grains and small amount of ordered g (g') was still observed after heat treatment. The elemental mapping technique and chemical point analyses allowed determining the composition of particulate phases. The VSM measurements performed for two directions of samples i.e. parallel and perpendicular to the rolling direction, allowed determining the phase transition temperatures, Curie temperature and basic magnetic properties of investigated alloys.

15:15 Oral

Texture analysis of hot rolled Ni-Mn-Ga alloys

Henryk Morawiec, Tomasz Goryczka, Krystian Prusik, Andrzej Drdzeń, Jozef Lelatko

University of Silesia, Institute of Materials Science, 12, Bankowa Str., Katowice 40-007, Poland

e-mail: morawiec@us.edu.pl

One of the important factor which controls the MSM effect is the magneto-crystalline anisotropy of the martensite with the c/a<1. A crystallographic texture of the polycrystalline alloy can significantly improve this effect. The preferred orientation is the <001> direction which is the easy magnetization direction.

The studies were carried out on two Ni-Mn-Ga polycrystalline alloys with the 10M martensite structure. The specimens were cut along the [001] and [110] directions of the columnar grains from the ingots of either round or flat shape. The rolling was carried out on the samples imbedded in steel channel bar and "sealed" in a flat pipe. The samples were heated up to 1000^0C and rolled in one direction in several steps. Before each step the sample was reheated. The final reduction of the samples thickness was: 28%, 36%, 57% and 69%.

The texture was studied by the EBSD and X-ray diffraction using the {001}, {110} and {111} pole figures.

The texture of the initial [001] orientation rolled with the highest deformation 60% shows the following orientation components: {111}<011>, {111}<112>, {112}<011> which are typical for deformed and recrystallized metals of the A2 structure. The presence of the {011}<100> components was not stated. The texture of the specimen with the initial [110] orientation rolled with 69% can be described as a fibre texture scattered along the <110> direction. This kind of texture for the rolled samples of the A2 structure is also known in the praxis. As a conclusion one can state that the hot rolling of the Ni-Mn-Ga alloys is not efficient to produce the texture with [001] orientation.

Coffee break

Wednesday afternoon, 17 September, 15:30
Main Hall

Joint Poster Session 2

Wednesday afternoon, 17 September, 16:00
Main Hall

Thursday, 18 September

Session 7

Thursday morning, 18 September, 9:00
Room 231
Chair: Proksch, Roger

9:00 Invited oral

Smart technologies for adaptive impact absorption.

Jan Holnicki-Szulc, Piotr Pawłowski

Polish Academy of Sciences, Institute of Fundamental Technological Research (IPPT PAN), Świętokrzyska 21, Warszawa 00-049, Poland

e-mail: holnicki@ippt.gov.pl

This presentation demonstrates progress in applications of so-called *Smart Technologies* to *Adaptive Impact Absorption*. The monograph (Ref.[1]) presents more detailed discussion of the considered problems and research results obtained recently in the Smart-Tech team at the IPPT.

Smart Technologies are understood as incorporation of imbedded systems (distributed hardware with driving electronics and software tools) into engineering structures in order to improve their safety or performance.

Motivation for the undertaken research on *Adaptive Impact Absorption* (AIA) is to respond to requirements for high impact energy dissipation. Typically, the suggested solutions focus on the design of passive energy absorbing systems, which are designed to work effectively in pre-defined impact scenarios. In contrast to the standard passive systems the proposed approach provides *active adaptation* of energy absorbing structures (equipped with sensor system detecting and identifying impact in advance and controllable semi-active dissipaters, so-called *structural fuses*) with high ability of adaptation to extreme overloading (cf. Ref.[2]).Feasible, dissipative devices (*structural fuses*) under considerations can be based on the following technologies: adaptive dissipaters based on MR fluids or adaptive dissipaters based on (hydraulic or pneumatic) piezo or magnetostrictive-valves.

The presentation will demonstrate the following AIA applications, which are currently under development: *Adaptive Landing Gears (ADLAND, Ref.[3]), Adaptive wind turbines (UPWIND, Ref.[4])* and *Adaptive Inflatable Structures.*

References

[1] Jan Holnicki-Szulc (Ed.) „Smart Technologies for Structural Safety", J.Wiley, 2008
[2] L. Knap, J. Holnicki-Szulc, "Adaptive Crashworthiness Concept", *Int. Journal of Impact Enegineering,* (2004).
[3] EU Project ADLAND IST-FP6-2002-2006, http://smart.ippt.gov.pl/adland/.
[4] EU Project UPWIND FP6-ENERGY-2006-2009, http://www.duwind.tudelft.nl/

9:30 Oral

Performance of Shape Memory Composite with SMA and SMP

Hisaaki Tobushi[1], Shunichi Hayashi[2], Yoshiki Sugimoto[1], Kousuke Date[1]

1. *Department of Mechanical Engineering, AICHI Institute of Technology (AIT), 1247, Yachigusa-cho, Toyota 470-0392, Japan*
2. *DiAPLEX Co., Ltd., Ebisu-minami 1-5-2, Shibuya-ku, Tokyo 150-0022, Japan*

e-mail: tobushi@aitech.ac.jp

The shape memory efect (SME) and superelasticity (SE) appear due to the martensitic transformation in shape memory alloy (SMA). The shape fixity and shape recovery appear due to the glass transition in shape memory polymer (SMP). Elastic modulus and yield stress in SMA are high at high temperature and low at low temperature. In SMP, they are high at low temperature and low at high temperature. The two-way deformation is hard to be obtained in SMA and SMP by themselves. If the shape memory composites (SMC) with SMA and SMP are developed, not only the above-mentioned characteristics but also new function can be obtained. In the present study, SMC with SMA and SMP is fabricated and the basic properties are investigated. In the SMC, two SMA thin strips to show SME and SE are used. The bent shape is shape-memorized in both SMA strips. Two SMA strips bent in the opposite direction are combined. They are sandwiched between two SMC sheets and are putted in the central part of the SMC. The two-way deformation in bending is demostrated by heating and cooloing. The behavior of recovery force is investigated by the three-point bending test. In the test, recovery force increases and decreases during heating and cooling, respectively. In SMCs, we can combine variopus kinds of shape on SMA and SMP. We can also combine various kinds of phase transformation temperatures in SMA and glass transition temperature in SMP. We can obtain high performance in SMCs by the combination of these various kinds of shapes and phase transformation temperatures in SMAs and SMPs.

9:45 Oral

Urethane magnetorheological elastomers – manufacturing, microstructure and properties

Anna Boczkowska, Stefan F. Awietjan

Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland

e-mail: abocz@meil.pw.edu.pl

Studies on urethane magnetorheological elastomers (MREs) microstructure in respect to their magnetic and mechanical properties are reported. MREs were obtained from a mixture of polyurethane gel and carbonyl-iron particles cured in a magnetic field of 100 and 300 mT. The amount of particles was varied from 1.5 to 33 vol. %. Samples with different particles arrangement were produced. Effect of the amount of ferromagnetic particles and their arrangement on microstructure and properties in relation to the external magnetic field was investigated. The microstructure was studied using scanning electron and light microscopes. Magnetic properties were measured using VSM. Rheological and mechanical properties under compressive loads were also examined.

It was found that the microstructure of the MRE depends on the amount of ferrous particles and manufacturing conditions. The orientation of the iron particles into aligned chains is possible for lower volume content of the ferromagnetic fillers. High carbonyl-iron volume content in the matrix leads to the formation of more complex three-dimensional lattices. Also the magnetic measurements confirmed the existence of the microstructure anisotropy for the lower volume content of the iron particles. The structural and magnetic anisotropy has not been found in the MREs with 33 vol. % of particles. To evaluate the effect of the external magnetic field on the magnetorheological properties compressive strength, storage and loss modulus as well as loss angle were measured. The experiments showed that both, the particles content and the field strength used during curing, have significant effect on the magnetorheological elastomers microstructure and consequently, on their properties.

10:00 Oral

Magnetoviscosity of novel ferrofluids synthesized by biotemplating

Zhenyu Wu[1], Chenchen Ma[1], Anna Müller[2], Emil Ruff[2], Alexander M. Bittner[3], Christina Wege[2], Carl E. Krill III[1]

1. *Ulm University, Institute of Micro and Nanomaterials, Albert-Einstein-Allee 47, Ulm 89081, Germany* **2.** *Universität Stuttgart, Dept. of Molecular Biology and Plant Virology, Pfaffenwaldring 57, Stuttgart 70550, Germany* **3.** *Max-Planck-Institut FKF, Heisenbergstr. 1, Stuttgart D70569, Germany*

e-mail: carl.krill@uni-ulm.de

As colloidal suspensions of ferromagnetic nanoparticles in a carrier liquid, ferrofluids combine the magnetic properties of solids with the flow properties of liquids. One outstanding feature of ferrofluids is the dramatic increase in viscosity that is induced by an externally applied magnetic field. However, in conventional ferrofluids this *magnetoviscosity* largely vanishes when the fluid is subjected to shear forces, because the latter disrupt the dynamic formation of the chain-like nanoparticle aggregates that are thought to be responsible for the viscosity enhancement. If these loose nanoparticle chains could somehow be replaced with stiff ferromagnetic nanowires or nanotubes, then we should expect the magnetoviscosity to manifest a significantly improved stability against shear thinning, thus making ferrofluids ideal working substances for adaptive damping systems or any other applications relying on switchable force transfer via a liquid.

We report the synthesis of nanotube ferrofluids by the metallization of a nanotube-shaped biotemplate—the Tobacco mosaic virus (TMV). The magnetoviscous properties of liquid-phase suspensions of the resulting nanotubes were studied using a squeeze-flow viscometer at magnetic fields up to 150 mT and frequencies up to 400 Hz. The measured viscosity behavior is compared to that of conventional ferrofluids and to suspensions of Fe nanorods prepared by aerosol condensation.

10:15 Oral

Elastomers containing fillers with magnetic properties

Marian Zaborski, Joanna Pietrasik, Marcin Masłowski

Technical University of Łódź, Faculty of Chemistry, Institute of Polymer and Dye Technology (PŁ), Stefanowskiego 12/16, Łódź 90-924, Poland

e-mail: m.maslowski@poczta.onet.pl

Composites of ethylene – propylene, acrylonitrile – butadiene with micro size Fe_3O_4, Fe_2O_3 and nano size Fe_3O_4 as the fillers were tested. Iron oxides were found to be active fillers which improved mechanical properties of elastomers. Additionally, they also changed their magnetic properties. Moreover, a chemical modification of the surface of micro size Fe_3O_4 was done, in order to upgrade mechanical properties of the vulcanizates. Itaconic acid, methacryloxypropyltrimethoxy silane and monododecyl maleate were used as the modifiers. To improve dispersion in polymers matrix, non-ionic (NF-PEG), anionic (calcium stearate), cationic (DTAB, DTAC, DDAB, CTAB) and ionic liquids ($HMIMBF_4$, $BMIMPF_6$, $OMIMPF_6$) as the dispersing agents were tested. It was observed that non-modified and modified micro iron oxides and non-modified nano iron oxides showed better properties of tested vulcanizates.

Coffee break

Thursday morning, 18 September, 10:30
Main Hall

Session 8

Thursday morning, 18 September, 11:00
Room 231
Chair: Holnicki-Szulc, Jan

11:00 Invited oral

Multifrequency atomic force microscopy and functional materials

Roger Proksch

Asylum Research, Santa Barbara, CA 93117, United States

e-mail: roger@rasy.com

Atomic Force Microscopy (AFM) has proven to be an effective means of accessing topographic information of many materials on the nanoscale. However, tip-sample interactions are complex and many of the measured quantities in conventional AC AFM are complicated mixtures of several tip-sample interaction parameters. Simply put, there are more unknowns than there are measurements in conventional AC AFM. This problem is particularly pressing in active materials where information beyond simple topography is routinely desired. Recently developed multifrequency methods open up new channels for information transfer and allow the unambiguous determination of model parameters. Some examples of these new multifrequency methods include bimodal AC AFM where multiple resonant modes of the cantilever probe are simultaneously excited, Dual-Frequency Resonance Tracking (DFRT) where driving with two frequencies near the resonance allow sample stiffness and dissipation as well as other properties to be unambiguously extracted and, finally, Band-Excitation (BE), where the cantilever spectral response is extracted in a band of frequencies. These new techniques have been used to extract information on a large array of samples. Some examples include extracting high spatial resolution mechanical properties on soft polymer and biological samples, piezo and ferro-electric samples properties and magnetic systems.

11:45 Oral

An attempt to improve the soft magnetic properties of iron-based bulk metallic glasses by annealing

Jarosław Ferenc, Tatiana Erenc-Sędziak, Maciej Kowalczyk, Tadeusz Kulik

Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland

e-mail: jferenc@inmat.pw.edu.pl

Bulk metallic glasses based on iron are known to possess very good soft magnetic properties due to their amorphous structure. The lack of crystallinity results in the very small magnetocrystalline anisotropy, minimising its contribution to the overall magnetic anisotropy. However, the presence of stress in the alloy, inevitable in the as-quenched state, may provoke magnetoelastic anisotropy. This factor may be reduced by either reduction of stress level by stress-relief annealing, or by modification of chemical composition in order to decrease the magnetostriction coefficient, λ. Specifically, if cobalt is added to an alloy for the improvement of its glass forming ability, magnetostriction is usually high, so the latter method may be inefficient. This work will show the efficiency of the stress relieving on the reduction of the coercive field of the studied materials, such as Fe-Co-(Ni)-Si-Nb-B and Fe-Co-Ni-Nb-Y-B glassy alloys.

12:00 Oral

Active control of landing gear shock absorber characteristic with usage of magnetoreological fluid.

Zbigniew Skorupka, Rafal Kajka, Wojciech Kowalski, Ryszard Harla, Grażyna Balcerkiewicz, Maciej Parafiniak, Magdalena Kacprzak, Wiesław Lechniak, Jerzy Pacholski

Instytut Lotnictwa (ILOT), Al. Krakowska 110/114, Warszawa 02-256, Poland

e-mail: zk.skorupka@ilot.edu.pl

Smart materials are being used in much larger scale in mechanical solutions. Aviation usage of these materials seems to be natural because of interest in new technologies use in this industry. In this article authors discuss characteristic of magnetoreological fluids as a smart materials, examples of its industrial usage, requirements on landing gear characteristics, design and lab tests of model shock absorber in which MRF was used as damping fluid.

12:15 Oral

Application of nanocrystalline alloys for force sensors

Józef L. Kwiczala[1], Bogusław Kasperczyk[1], Roman Kolano[2], Aleksandra Kolano-Burian[2]

1. *Silesian University of Technology, Gliwice 44-100, Poland* **2.** *Institute of Nonferrous Metals, Sowińskiego 5, Gliwice 44-100, Poland*

e-mail: jozef.kwiczala@polsl.pl

The nanocrystalline alloys applied to construction of the magnetoelastic force transducers have been tested. The magnetoelastic sensitivity and its dependence on the stress against the magnetic field direction is presented. The magnetoelastic properties have been investigated by means of specially constructed ring core. Transducers consisting of toroidally wound nanocrystalline ribbon with a magnetizing windings have been used.

The ribbon ring core was made of nanocrystalline alloys. The special construction of the sample makes possible to excite the magnetic flux either parallel or perpendicular to the direction of the stress.

The general idea of magnetoelastic force transducers is based on changes of the magnetic material properties caused by the stress following the force applied. In order to detect the changes, appropriate windings have been wounded on the core. Two kind of tape was used to construction of cores – with transversal and longitudinal magnetic anisotropy induced in ribbon and two method of placement of measuring windings in holes was applied – horizontally and vertically.

The compressive stress decreases the permeability of the magnetic materials of the cores. The impedance of properly connection windings is also decreased as a result of external force. The change of the impedance of 10% may be reached for compressive force of about 200 N. The sensor with core made of ribbon with transversal anisotropy and horizontally windings (parallel magnetic flux to stress) has the greatest sensitivity of the all tested sensors. The properties of nanocrystalline alloys are well suited for the stress sensors application.

Lunch break

Thursday afternoon, 18 September, 12:30
Inner Courtyards

Session 9

Thursday afternoon, 18 September, 14:00
Room 231
Chair: Tobushi, Hisaaki

14:00 Invited oral

Energy conversion improvement in piezoelectric materials by switching the output voltage

Daniel Guyomar

LGEF-INSA-Lyon, 8 rue de la physique, Lyon 69621, France

e-mail: daniel.guyomar@insa-lyon.fr

This paper addresses the problem of piezoelectric conversion enhancement from mechanical to electrical energy and illustrates this improvement on specific applications. Considering a mechanical structure equipped with piezoelements bonded on its surface, it can be shown a non-linear processing of the piezoelement output voltage improves significantly the energy conversion. This non-linear processing simply corresponds to short circuit the voltage for a very brief period of time when the voltage is maximum or minimum. This processing results in the generation of a dry-friction type of mechanical dissipative force that appears to be very efficient to pump out mechanical energy or to convert it to electrical energy. Several self-powered wireless applications (vibration control, energy harvesting on vibrations, structural health monitoring) will be presented. Theoretical aspects of the processing will be developed and experimental results on the applications previously mentioned will be given for narrow-band and random vibrations.

14:30 Oral

Auto Healing of Early Aged Cracking of High Strength Concrete, damaged by Cyclic Freeze-Thaw

Taejun Cho[1], Koichi Maekawa[2], Kenichiro Nakarai[3], Seong-Soo Kim[1], Andrzej S. Nowak[4], Tae Soo Kim[5]

1. *Daejin University (TJCHO), Sundan11-1, Pocheon 487-711, Korea, South* **2.** *The University of Tokyo, Bunkyo-ku, Tokyo 113-8655, Japan* **3.** *Gunma University, Tenjin-cho, Kiryu-shi, Gunma 1-5-1, Japan* **4.** *University of Nebraska-Lincoln, W181 NH Lincoln NE 68588-0531, Lincoln 68588-0531, United States* **5.** *Hanbat National University, Deajeon 305-719, Korea, South*

e-mail: taejun@daejin.ac.kr

This paper presents an innovative solution for the auto healing concrete structures damaged by cyclic freeze-thaw. The additional hydration of high strength concrete, cured in high temperature, applied as auto curing for the damaged concrete micro-pore structures. Modeling of micro pore structure is prior to damage analysis. The micro-pore structure is composed as gel-pore and capillary pores, which grows with hydration. The amount of ice volume with temperature dependent surface tensions, freezing pressure and resulting deformations, and cycle and temperature dependent pore volume has been calculated and compared with available test results. The damaged and hydrated micro pore structures are modeled numerically. Heating the selected area of specimen in frozen chamber, the experimental results show approximately 100%of strength recovery after two weeks of freeze-thaw tests, fluctuating from 4° to -6° Celsius.

14:45 Oral

Tensile Stress-Strain Relationships of Magnetorheological Fluids under Various Factors

Saiful A. Mazlan, Ahmed Issa, Habibullah A. Chowdhury, Abdul G. Olabi

School of Mechanical and Manufacturing Engineering, Dublin City University, Dublin Dublin9, Ireland

e-mail: saiful.mazlan2@mail.dcu.ie

Magnetorheological (MR) fluids are commonly suspensions consisting of magnetic particles and carrier liquids. The materials are remarkable for their precipitous and capable of being reversed of fluid viscosity controlled by applied magnetic field. In this paper, experimental investigations of three types of MR fluids in tension mode have been carried out. MRF-241ES was a water-based MR fluid, while MRF-132DG and MRF-122-2ED were hydrocarbon-based MR fluids. Magnetic properties of the MR fluids vary significantly due to a higher particle density in MRF-241ES (3.80 to 3.92 g/cm^3) than MRF-132DG (2.98 to 3.18 g/cm^3) and MRF-122-2ED (2.32 to 2.44 g/cm^3). The results were presented starting with different electrical currents to generate magnetic fields, using different initial gap sizes and tensile speeds. The tension process, in terms of stress-strain relationship of MR fluids, can be separated into three regions. The tensile stress curves in the first region increased dramatically to the peak point as the tensile strain increased. Subsequently, in the second region, the tensile stress curves declined rapidly for small values of the tensile strain. Lastly, in the third region, the tensile stress curves further decreased slowly with further elongation. The results revealed that high values of stress occurred where the strain was high, and that even higher values were obtained when the electrical current was high. Furthermore, the magnitude of the stress, for a given strain, depended on the initial gap size. Curves showing the relationships between the stress and the strain were constructed for two different initial gap sizes. It was seen that, for larger initial gap sizes, there were larger stress values. The sizes of the three regions depended on the initial gap sizes. However, contradicting with the effects of the applied current and the initial gap size, the tensile speed had a small effect on the stress-strain relationship which was considered as being neglected.

15:00 Oral

Suppressed field emission screening effect with a triode structure of CNT-based electron sources

Nima Davoudzadeh[1,2], Javad Koohsorkhi[1,2], Shamsoddin Mohajerzadeh[1], Hasan Ghafouri Fard[2]

1. *University of Tehran (UT), North-Kargar, Tehran 14395-731, Iran* **2.** *Amirkabir University of Technology (AUT), Hafez, Tehran 15914, Iran*

e-mail: nidavidson@gmail.com

Carbon nanotubes have drawn significant attention due to their exceptional electronic and mechanical properties. Field emission devices have been investigated by several researchers due to their potential application for CNT-logic realization. In this paper an attempt has been made to investigate the field performance of emitters including a novel self-defined structure for the realization of field emission devices which were reported. These devices can find application in flat-panel displays, nanolithography systems and new sensor technologies. Comparing with other field emitters, CNT-based electron sources revealed an efficient performance at normal vacuum. The proposed structure consists of vertical CNT's grown on a silicon substrate which are encapsulated by a metal and oxide bi-layer. The presence of small holes in the metal-oxide bi-layer at the place of a cluster of carbon nanotube resembles a metallic surface on top of the silicon substrate acting as a gate-plate. The formation of field-emission requires a second substrate which is located 100 μm away from the bottom one. To investigate the field properties of this configuration, arrays of nanotubes were studied with different spatial distances. Simulation has been performed using CST package. The simulation results show that the filed amplification factor (β) relates to the distance between two cluster arrays and also increases with the length of nanotubes. For distances less than the CNT length, the screening effect will occur. It was observed that the presence of the metal-oxide gate has a favorable effect to minimize the screening effect and allows one to increase the density of CNTs in each array spot and to increase the cluster array density on the substrate, hence to increase the density of emission current. In this structure the screening effect occurs in the distance about the less than half of the CNT's length. The distance between metal gate and the CNT's tip is a parameter which will be studied.

15:15 Oral

Studies on graphite based anti static electromagnetic/radio frequency interference (EMI/RFI) shelding coating

Roohollah Reza soltani, Ali asqar Sarabi

Amirkabir University of Technology (AUT), Hafez, Tehran 15914, Iran

e-mail: r_r_soltani@yahoo.com

Electrically conductive coatings are mainly required for static charge dissipation and electromagnetic/radio frequency interference (EMI/RFI) shielding. Electrically conductive coatings are prepared by the incorporation of the metallic pigments/graphite or carbon black onto the binder.

In the present investigation a study on the correlation between electrical percolation ,filler volume concentration and some other physical and mechanical properties for graphite (GP) filled epoxy coating was carried out through an examination of the filler concentration dependence of the volume resistivity and other mechanical properties.

It is found that there are two critical threshold, in plot of electrical resistivity v.s. filler volume concentration.

The impact strength of epoxy resin filled with graphite was also investigated. A decrease in impact strength with an increase in filler content was observed

The adhesion of the filled resin to substrate was also determined by pull-off test. A decrease in the adhesion to substrate with an increase in filler content was observed in

Then to find out the correlation between filler concentration and viscoelastic behavior of the system Tensile test carried out.

Then for expand a theory that can explain the transfer between insulator-semi conductor and semi conductor-conductor behavior of graphite filled system images was gived by SEM and optical microscopy and also oil absorption (for determine CPVC)test carried out. All data show that formation of e internal network by graphite particles and particle by particle contact of them is the reason of formation a conductive network in epoxy system.

Coffee break

Thursday afternoon, 18 September, 15:30
Main Hall

Friday, 19 September

E-MRS & EPDIC Joint Plenary Session

Friday morning, 19 September, 9:00
Small Hall (237)

Coffee break

Friday morning, 19 September, 10:30
Main Hall

Posters

Monday, 15 September

Joint Poster Session 1

Monday & Wednesday
Monday afternoon, 15 September, 16:00
Main Hall

16:00	Poster	C01

The Role of Ordering in Martensite Microstructures in Copper Based Shape Memory Alloys

Osman Adiguzel

Firat University, Department of Physics, Elazig 23169, Turkey

e-mail: oadiguzel@firat.edu.tr

Copper based alloys are widely used as shape memory element in devices. These alloys are metastable in beta phase field and possess simple bcc- structures, austenite structure, at high temperatures. These alloys undergoe the martensitic transition, following two ordering reactions on cooling. This transition, which is the source of shape memory, occurs with shears and shear mechanism on {110}-type planes of parent phase, basal plane for product phase. The product martensite has unusual layered structures with complicated stacking sequences called as 3R, 9R or 18R martensites depending on the periodicity of layers on the basal plane. Martensitic transitions are displacive and the product structures inherit the order in the parent phase. The basal plane is subjected to the hexagonal distortion with martensite formation on which atom sizes have important effect. In the disordered case, the lattice sites are occupied randomly, and this distribution makes the basal plane nearly close packed taking the atomic sizes approximately equal. In the ordered case, lattice sites are occupied regularly by certain atoms which have different atomic sizes, and basal plane deviates from the regular hexagonal arrangement of the atoms due to the atom size differences. Due to this distortion, the knowledge on the interplane distances of the particularly selected diffraction plane pairs reveals the ordering degree of martensite. In the present contribution, x-ray diffraction and transmission electron microscopy (TEM) studies were carried out on two copper based ternary alloys given different heat treatments. **Key Words**: Shape memory effect, martensite, atom sizes, and layered structures.

16:00	Poster	C02

Image analysis of magnetorheological elastomers microstructure

Stefan F. Awietjan, Anna Boczkowska

Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland

e-mail: stefan_a@wp.pl

Magnetorheological elastomers (MREs) are solid analogues of magnetorheological fluids. These both consist of micrometer-sized magnetically permeable particles in a non-magnetic matrix material. As in the case of MR fluids, the particles try to arrange themselves in the direction of the magnetic field. The advantage of MREs over MR fluids is that ferrous particles do not undergo sedimentation. Due to the characteristic MRE microstructure, the response time and strain magnitude versus magnetic field intensity can be shortened. Interest in such intelligent materials has increased recently as they hold promise in enabling variable-stiffness devices and adaptive structures in aerospace, automotive, civil and electrical engineering applications.

The presented results are a part of the studies on development of MREs based on ferromagnetic particles in a polyurethane matrix. The influence of the amount of the ferromagnetic particles and their arrangement in relation to the external magnetic field was investigated. The amount of ferrous particles varied from 1.5 to 33 vol. %. Three types of particles were used; carbonyl iron in average sizes of 1-2 mm and 6-9 mm as well as 70 mm porous iron. Scanning electron and light microscopy were used to observe MREs microstructure. Obtained microstructures were analysed with image analysis using software *Micrometer v.9.2*. Images were analysed in two perpendicular directions to measure the microstructure anisotropy level. The largest microstructure anisotropy has been observed for samples with lower amounts of Fe particles. For samples with larger volume percentage of Fe the anisotropy has not been confirmed.

16:00 Poster C03

Properties investigations of $Bi_2O_3 \cdot GeO_2$ glass systems

Ciceron A. Berbecaru[1], Silviu Polosan[2], Horia V. Alexandru[1]

1. *University of Bucharest, Faculty of Physics, Bucharest-Magurele p.o.box mg-11, Bucharest 76900, Romania* **2.** *National Institute for Materials Physics, Bucharest- Magurele 010555, Romania*

e-mail: berbecaru2ciceron@yahoo.com

The oxides family of the PbO-Bi_2O_3-Ga_2O_3 (BGO) system is widely used in electronics, optoelectronics, fiber-optic amplifiers and lasers in the mid-IR, as scintillators, etc [1, 2]. Theirs low technological requirements and consequently low costs, make them subjects of intensive studies. Some new aspects in producing and characterizing BGO glasses will be presented. A 30 % Bi_2O_3 and 70 % GeO_2 mixtures were prepared by wet-mixage in acetone. The mixtures, were dried at 100 ^oC, were melted at 1050 ^oC and than poured on a preheated graphite plate at different temperatures, below and over the glass transition temperature. Samples of ~1 mm thick and ~0.5 cm^2 surface were structurally and optically analyzed at room temperature and compared to [3]. The permittivity and losses were also investigated on 45Hz-5MHz frequency range and continuously from -100 ^oC to +200 ^oC temperature interval, using a Quatro Cryosystem and HIOKI 035-22 RLC bridge. The relative permittivity continuously increases at a rate of 3.5 10^{-3}/ ^oC on this temperature range. Important changes could be noticed with frequencies and temperatures in subsequent measurements till 400 ^oC, were the samples properties are affected by crystallization processes. At temperatures higher than 250 ^oC, the higher mobility of building units in the lattice increases the permittivity values. The cluster mobility may be responsible for the permittivity increase in the range temperature, 275-300 ^oC at low frequencies. At high temperatures (≥ 300 ^oC) individual atomic/ionic components appear to have much higher mobility. The losses behavior shows the contribution of different activated mechanism with temperatures and frequency.

References: [1] S. Polosan, E. Apostol, M. Secu, G. Aldica, Phys. Stat. Sol. (c) **2** (**1**) 93 (2005). [2] Sharaf El-Deen et al, Coplex. Internat., vol.09, (2002), p1-17. [3] Y.G. Choi and J. Heo, J. Non-Cryst. Solids **217**, 199 (1997).

16:00 Poster C04

The applicative phenothiazine and carbazole chromophores

Joanna Cabaj, Jadwiga, Maria Sołoducho, Anna Nowakowska

Wrocław University of Technology, Department of Chemistry, Wybrzeże Wyspiańskiego 27, Wrocław 50-370, Poland

e-mail: joanna.cabaj@pwr.wroc.pl

The novel, functional light emitting materials have to meet many requirements, most notably good π-electron delocalization along the chain and a high degree of intramolecular order, good intramolecular π-stacking and ordered supermolecular morphology and the most important low ionization potential [1]. Phenothiazine and carbazole used in this study are electron donating groups which can facilitate the charge transport of the carrier. On the other hand, carbazole derivatives have attracted much attention in LED fabrication due to fine hole transporting capability, high photochemical stability [2].Some compounds containing both, electron donor and acceptor moieties exhibit the intermolecular charge transfer absorbance and fluorescence behavior. In such a donor – acceptor molecules (D-A), very large changes in charge distribution can be induced in the excited state upon absorption of light photons. Therefore, recently these organic D-A compounds have been increasing interest and usually been used as the fluorescent probe to study microenvironments [3]. A series of substituted chalcones show strongly intermolecular charge transfer behaviors in various aprotic solvents. The absorption spectrum of chalcone phenothiazine derivative in different solvents undergoes a red – shift with increasing polarity. This absorption band should attribute to the charge transfer between keto – fragments and phenothiazine N-alkyl units in structure. Furthermore, charge transfer direction comes from the observed blue-shift of the absorption maximum in strongly hydrogen bonding solvents. Such behaviour is consistent with the restriction of charge transfer process from phenothiazine For these compounds were also widely adopted approach to prepare structurally ordered thin films by LB technique. [1]. Y. Zhu, A. Babel, S.A. Jenekhe, Macromolecules, 148, 7983 (2005) [2]. Z. V. Vardeny, A. J. Heeger, A. Dodabalapur, Synth. Met. 148, 1 (2005) [3]. H. Hayen, U. Karst, Anal. Chem. 75, 4833 (2003)

16:00 Poster C05

One-way Shape Memory Effect in a Cryogenic Treated Cu-base Alloy

Iulian Ciupitu[1], Dana Daisa[1], Elvira Alexandrescu[1], Doina Raducanu[2]

1. *METAV-CD SA, CA Rosetti Nr 31 Sect. 2, Bucharest 70000, Romania* **2.** *University Politehnica of Bucharest, Polizu 1-7, Bucharest, Romania*

e-mail: ciupitu@metav-cd.ro

As it is known, in a binary system Cu-Zn case the Ms temperature is to down placed so that (therefore) thermo elastic martensitic transformation it is effective non-utile. The additions of Al, Sn, Si, Ge, Be can sensible adjuste the place of Ms point towards moderate temperatures, even positive values. The our experiments was utilised a 21 % zinc and a 5,4 % aluminium amounts. For comparison, the experimental material was hot (at 650^{0}C), cold (at 20^0 C) and cryogenic processed (at -70^{0}C). Martensitic structures with various proportion of martensite were obtained. The literature indicates the getting of SME-termoresponsive martensitic transformation as a result of heat treatments, after plastic deformation. In the usually quenching treatment, the rapidly cooling of metals most commonly accomplished by immersing the material in oil or water. Within our work, the total thermo elastic martensite transformation was realized by a particular final heat treatment, which includes an annealing at 700^{0}C followed by cryogenic quenching in a carbonic snow (at -70^{0}C) for few minutes. This procedure, which was inspired by cooling stage of DSC, induces one-way shape memory effect in the experimental alloy.

Keywords:*brass with aluminium, shape memory, rolling, thermo elastic martensitic transformation, cryogenic quenching*

16:00 Poster C06

Deformation simulation during martensite transformation in shape memory materials

Jacinto Cortés-Pérez[1], Jorge C. Bolaños[2], José Gonzalo G. Reyes[3], Horacio F. Zúñiga[4], Alberto R. Solis[1]

1. *Universidad Nacional Autónoma de México, Facultad de Estudios Superiores Aragón, CTA (UNAM), Av. Rancho Seco S/N, col. impulsora, Cd. Nezahualcoyotl, Edo. de México, México 57130, Mexico* **2.** *Universidad Nacional Autónoma de México, Circuito exterior s/n, México 04510, Mexico* **3.** *Universidad Nacional Autónoma de México, Instituto de Investigaciones en Materiales (UNAM), Circuito Exterior S/N Cd. Universitaria Coyoacan Mexico D.F. Mexico, México 70-360, Mexico* **4.** *Centro de Investigaciones en Materiales Avanzados, SEP-Conacyt (CIMAV), Miguel de Cervantes No. 120, complejo industrial Chihuahua, Chiuahua 31109, Mexico*

e-mail: jacop@correo.unam.mx

The deformation paths during grown of a single martensite variant in a shape memory material are treated in the present work. For get the last it is employed a non-homogenous and evolutionary displacement field which is defined in a single reference system named: transformational' basis and then it is related to a second reference system called: observation basis.

The displacement field defined before is after used for deducting a tensorial strain field and a constitutive stress-strain-temperature-orientation relationship for monocristalline shape memory materials and were simulated the next patterns:

a) Distortion of the observation surface,

b) Distortion of a mark placed on the observation surface and

c) The displacement field related to the martensite transformation on the observation surface.

Then the model is employed for to simulate the typical uniaxil strain-temperature curves a hypothetical serial grains pilycristalline sample.

The results obtained are important to the interpretation information comes to experiments in shape memory materials during stress induced martensite transformation.

16:00 Poster C07

Structural properties and electrical behaviour in the polycrystalline lanthanum-deficient manganites $La_{1-x}\square_xMnO_3$

Radhia Dhahri[1], Moez Bejar[1], Amel Alaya[2], Kamel Khirouni[2], Luís C. Costa[3], Essebti Dhahri[1]

1. *Faculty of Sciences of Sfax, Route Soukra Km 3.5, Sfax 3018, Tunisia* **2.** *Faculté des Sciences de Gabès, Cité Erriadh 6072 Zrig Gabès Tunisie, Gabes 6072, Tunisia* **3.** *Physics Department (UA), Campus Universitario, Aveiro 3810-193, Portugal*

e-mail: kady@ua.pt

Electrical conductance and X-ray diffraction (XRD) measurements of lanthanum-deficient $La_{1-x}\square_xMnO_3$ ($x = 0.05$, 0.10 and 0.20) polycrystalline samples were performed to examine the effect of the internal pressure at B-site on the conduction mechanism. The structural study reveals that all samples crystallize in the rhombohedral system. The electronic conduction appears to be thermally activated at high temperature, which indicates the presence of semiconductor behaviour. The increase of the x content converts $3x$ Mn^{3+} to Mn^{4+} ions with smaller ionic radius, which reduces the internal pressure and leads to the increase of the one-electron bandwidth W. This increase causes the appearance of metallic behaviour at low temperature for $x = 0.10$ and 0.20 content.

16:00 Poster C08

Effect of the substitution of calcium by potassium on the structure and dielectric properties in $La_{0.7}Ca_{0.3-x}K_xMnO_3$ compounds.

Radhia Dhahri[1], Sdiri Nasr[1], Moez Bejar[1], Luís C. Costa[3], Manuel Almeida Valente[2], Essebti Dhahri[1]

1. *Faculty of Sciences of Sfax, Route Soukra Km 3.5, Sfax 3018, Tunisia* **2.** *Departamento de Física, Universidade de Aveiro, Campus de Santiago, Aveiro 3810-193, Portugal* **3.** *Physics Department (UA), Campus Universitario, Aveiro 3810-193, Portugal*

e-mail: sdirinasr@yahoo.fr

X-ray diffraction and impedance spectroscopy measurements were performed to examine the effect of the substitution of calcium by potassium on the structure and dielectric properties in $La_{0.7}Ca_{0.3-x}K_xMnO_3$ compounds. Polycrystalline samples of $La_{0.7}Ca_{0.3-x}K_xMnO_3$ were prepared using solid state method. X-ray diffraction patterns show that these compounds exist at a single phase having a perovskite-like structure at room temperature. The X-ray data were analysed by the Rietveld method. For 0 £ x £ 0.075 the structure is orthorhombic. It becomes rhombohedral for x=0.1 and x=0.15. The impedance plane plots show semicircle arcs at different temperature and an electrical equivalent circuit has been proposed to explain the impedance results. A high frequency dielectric relaxation was also observed.

16:00 Poster C09

Shape Memory Assemblies using Ultrasonic Welding

Corneliu M. Craciunescu[1], Octavian Oanca[2], Dorin Dehelean[2]

1. *Politehnica University of Timisoara (UPT), Bd. Mihai Viteazul 1, Timisoara 300222, Romania* **2.** *National RD Institute for Welding and Material Testing (ISIM), BD Mihai Viteazul, Timisoara 300222, Romania*

e-mail: craciunescucm@yahoo.com

The paper describes the research done in order to assemble shape memory alloys using welding technologies with the aim to reduce the heat affected zone. Ultrasonic and hybrid welding can be solutions that could be considered for this purpose. Experiments on welding shape memory and ferromagnetic shape memory alloys have been performed on bulk and thin films and the interface has been characterized using microscopic observations. Our observations show the difficulties in assembling shape memory ribbons with conventional sonotrode/anvil solutions due to the low thickness of the ribbons and the need to develop microstriations on the surface of the ultrasonic welding tools.

16:00 Poster C10

Nano-Silicon Sol-Gel Film Refraction Index Modulation with Femtosecond Laser

Antonela Dima[1], Massimo Gagliardi[2], Dun Liu[1], Walter Perrie[1], Craig J. Williams[1], Ivo Rendina[2], Geoff Dearden[2], Ken G. Watkins[2]

1. *The University of Liverpool (UOL), Oxford Street, Liverpool L697ZD, United Kingdom* **2.** *Istituto per la Microelettronica e Microsistemi (IMM-CNR), via P. Castellino 111, Napoli 80131, Italy*

e-mail: antonela.dima@liv.ac.uk

Patterned structures were created by exposing a SiO_2 sol-gel film containing nano-silicon particles to a Clark MXR CPA-2010 fs laser (387 nm wavelength). The refractive index variation of 0.2 is similar to that of polymer films, however belonging to an entirely superior stability class (structural, chemical, thermal, radiation, etc). The useful optical range of refractive index modulation is beyond 800 nm, respectively near-IR. Of course, the films can be used below 800 nm as absorbers, then the un-cured ones are transparent in visible, while the laser-cured ones opaque. Applications therefore can be holographic plates, optical isolators, etc.

More attractive application is phase matching Mach-Zehnder interferometers in ultra-fast light pulse modulation applications. The active modulating elements may cause static unbalance of the interferometer setup. Balancing this via a bias on the said active elements reduces the available dynamic range of the modulator, hence a precise phase matching element in the optical circuit is very useful – especially when this can be produced without further material deposition, just through irradiation.

The optical transparency of the laser-cured material decreases drastically in visible (up to 600 nm) due to the 1.5 eV bandgap. This onset is correlated with the formation of a cured glassy phase (revealed by Raman spectroscopy) unaxial optically (determined ellipsometrically). The refractive index value of pristine films is 1.47, while that of laser-cured ones 1.20 - 1.32. AFM images revealed a homogeneous film with nano-silicon particles under 200 nm.

The synthesis of laser-modified structures with a strong periodic modulation of refractive indices of the alternating structures was been developed with success. It is interesting to note that the pristine films display a moderately wide bandgap (3.87 eV), contrasting with that of the laser-cured ones – which can be useful in holographic and perhaps photovoltaic applications.

16:00 Poster C11

Sensor of current or magnetic field based on magnetoresistance effect in $(La_{0.7}Ca_{0.3})_{0.8}Mn_{1.2}O_3$ manganite

Vladimir P. Dyakonov[1], Andrzej Szewczyk[1], Stanislaw Piechota[1], Kazimierz Piotrowski[1], Henryk Szymczak[1], Aleksandr A. Shemiakov[2], Valentin P. Pashchenko[2], Aleksey V. Pashchenko[2], Vladimir I. Mikhaylov[2]

1. *Polish Academy of Sciences, Institute of Physics, al. Lotników 32/46, Warszawa 02-668, Poland* **2.** *National Academy of Sciences of Ukraine, Donetsk Technical-Physical Institute, R. Luxemburg 72, Donetsk 83114, Ukraine*

e-mail: dyakon@ifpan.edu.pl

The basis for work of the majority magnetoresistors serving as the sensors of current is the dependence of resistance on magnetic field, so-called magnetoresistance effect (MRE).

The main objective of the proposed investigations was to enhance the sensitivity of the sensor of current. New design of the sensor of current based on MRE was developed and studied. The sensor was produced in the form of annular magnet with gap from material characterized by high magnetic induction in small magnetic field (ferrites or permalloy). To improve the sensitivity of the sensor, the $(La_{0.7}Sr_{0.3})_{0.8}Mn_{1.2}O_3$ film as the magnetosensitive element was used. This element possesses both the high metal-insulator transition temperature (above room temperature) and large negative MRE. It was inserted into the gap of magnet. At the current in the conduction line of about 1 A, the magnetic field in the gap of 1 mm reaches the value of about 1 T, and the magnetoresistance effect of several tens of percentage is obtained. The limit of the change of current depends on the size of the gap in the annular magnet and can be changed from tenth parts to a hundred of amperes. At the same time the temperature dependence of magnetic permeability changes insignificantly.

Due to high sensitivity, the large limits of the measured current values, lack of moving electric contacts and high reliability the proposed sensors of current based on MRE can be applied in many electrical arrangements and devices.

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16:00 Poster C12

Structure and shape memory effect in annealed Ni-Ti-Co strip produced by twin roll casting technique

Tomasz Goryczka

University of Silesia, Institute of Materials Science, 12, Bankowa Str., Katowice 40-007, Poland

e-mail: goryczka@us.edu.pl

Ternary Ni-Ti-Co alloy belongs to a large family, which reveals shape memory effect (SME). Addition of cobalt causes changes in thermal behavior as well as sequence of the martensitic transformation. Applying twin rolls casting, rapid solidification, technique for shape memory alloy (SMA) production significantly influences microstructure and grains formation. Additional thermal treatment opens wide possibility in steering of transformation behavior.

In reported results the ternary $Ni_{47}Ti_{50}Co_3$ alloy was produced using twin rolls casting technique. Optimized processing parameters allowed to obtain polycrystalline strips 25 cm long, 45mm wide and 300um thick. The samples were cut from the central part of the strip and subjected to annealing at 300^0C, 400^0C, 500^0C for 1 hour. Annealing was carried out in real condition without protection atmosphere. The as-cast strip reveals two stages in the range of the martensitic transformation. It is a consequence of increase in dislocation density introduced during cold-rolling, which is realized during twin rolls casting. Annealing causes reduction of dislocation density and one stage of the martensitic transformation was observed. Also, shape recovery of the annealed strip is discussed. The effect was measured as elongation versus change of temperature under constant load.

16:00 Poster C13

Red-emitting Ba(Eu,Gd)B_9O_{16} phosphors for LED

Mohammad M. Haque[1], Hong Kyu Lee[1], Ji Eun Lee[1], Weekyung Kang[2], Dong-Kuk Kim[1]

1. *Kyungpook National University, Department of Chemistry, Daegu 702-701, Korea, South* **2.** *Dept. of Chemistry, Soongsil University, 511, Sangdo-dong, Dongjak-ku, Seoul 156-743, Korea, South*

e-mail: masuqul2003@yahoo.com

Recently, considerable efforts have been devoted to research on new materials to be used for Solid-State Lighting (SSL). In the past few years, several new rare-earth (Ln) and alkaline earth borates such as $LnCa_4O(BO_3)_3$, $Ln_2CaO(BO_3)_2$ and $LnBaB_9O_{16}$ have been synthesized. Among these compounds, the structure and luminescence properties of $LnBaB_9O_{16}$ have attracted considerable interest as universal hosts of the luminescent materials for tri-color lamps. Rare earth doped borates with high B_2O_3 contents are especially attractive, because of their excellent chemical and thermal stability, which is due to the small alkaline earth content and the rigid covalent boron-oxygen network. Motivated by the need for new efficient red phosphors for solid-state lighting applications, we have attempted to synthesis a borate base red phosphor which can emit efficiently under the UV and blue light excitation. Eu-doped red-emitting $BaGdB_9O_{16}$ phosphors were synthesized via a sol-gel process and the conventional solid state method. They were characterized by XRD, PL and SEM, respectively. No concentration quenching of Eu^{3+} was observed in this research work. The excitation and emission spectra indicate that these phosphors can be effectively excited by UV (395nm) and blue (466nm) light, and exhibit a satisfactory red performance (613nm), nicely fitting in with the widely applied UV or blue LED chips. The luminescent intensity of sol-gel derived is comparable with the solid state product. In comparison with the commercial red phosphor, CaS:Eu^{2+}, our synthesized $BaEuB_9O_{16}$ shows higher PL intensity when excited with 466 nm light. The intense red emission of $BaEuB_9O_{16}$ under 395 nm and 466 nm excitation suggests that this phosphor is promising candidate as red-emitting phosphor for near-UV/ blue-GaN based light-emitting diodes for white light generation.

16:00 Poster C14

Advances in metallic biomaterials surface finishing

Tadeusz Hryniewicz

Technical University of Koszalin (PK), Śniadeckich 2, Koszalin 75-343, Poland

e-mail: Tadeusz.Hryniewicz@tu.koszalin.pl

Electropolishing (EP) is one of the most important surface treatment processes used for surface finishing of metallic biomaterials. A modified surface technology, including electropolishing with the use of an externally applied magnetic field (MEP), has been proposed to improve several surface characteristics of metallic biomaterials after treatment.

Metallic implants, stents, filters, and sutures have many surface features that must be corrosion resistant, as well as haemo- and biocompatible. Chloride ions have been proven to be aggressive and responsive for the pitting and crevice corrosion of various metals in aqueous environments. Degradation follows immediately after these reactions. In attempt to refine and improve these critical features, a new process has been developed which is the magnetoelectropolishing (MEP).

In our investigations, the following metallic biomaterials used in medicine for implants and stents have been studied: (1) metals such as tantalum and titanium (Grade 2), (2) alloys such as stainless steels AISI 316L and 304L, Co-Cr-W alloy, and (3) intermetallic compounds, such as Nitinol™. Both electrochemical investigation methods (OCP, PC, and EIS determination) and surface analysis methods (static CAM, surface roughness measurements, AFM, SEM, Auger electron spectroscopy AES, and XPS studies) were carried out to present new achievements in biomaterials surface treatment.

The main findings are improvement of the biomaterials surface properties concerning chemical composition, morphology and thickness of the oxide film obtained, hydrophilicity, decreased surface microroughness, and improved corrosion resistance, minimization of external surface soiling and improved cleanability. By means of an external magnetic field, with the MEP process we could e.g. decrease the content of iron in the surface film of 316L SS below the level of chromium content and reveal quite new, more advantageous stainless steel surface properties.

16:00 Poster C15

Microelectromechanical actuators based on polymeric membranes

Mircea Ignat

National Research Institute for Electrical Engineering, Splaiul Unirii 313, 030138, Bucuresti, Romania, Bucharest 030138, Romania

e-mail: mignat@icpe-ca.ro

The paper presents some microelectromechanical structure of piezo and electrostrictive actuators based on polymeric membranes.

The microstructure are the planar and multilayers microactuators

with the thin disc element .

A composite film based on a poly(ether imide) with pyrite powder and Magnetic powders were mechanically incorporated in a polymeric matrix consisting in interconnected polydimethylsiloxane/silica networks has been prepared and its nanoactuation has been investigated.

In Fig.1 is presented a specific electrostrictive linear actuation for a polymeric membrane.

The authors propose some methods for experimental investigations of the specific nano and microelectromechanical parameters of the electrostrictive or piezoelectric polymeric membrane which are utilized in structure of microactuators or artificial muscle.

There are presented the investigations of the nano and microdisplacement , the microforce, the behaviour of the membrane to different electric signal or differents micromechanical stress. The resolution of the experimental nano and microdisplacements is 2 nm.

This method are based on the AGILENT interferometric System and VEECO optical interferometric microscope NT 1100 which are endowed the MEMS and NEMS laboratory of the INCDIE CA.

Fig. 1. Nanometric displacement of the composite polymer film containing 20% pyrite,

at 10 V dc with flexible thin electrodes, at 3.5 seconds commutation time.

16:00 Poster C16

Optical properties of GaAs-based 2D hexagonal photonic crystal with p6mm symmetry

Đorđe M. Jovanović[1], Rados Gajic[1], Dejan Djokić[1], Kurt Hingerl[2]

1. *Institute of Physics (IF), Pregrevica 118, Belgrade 11080, Serbia* **2.** *Institut für Halbleiter und Feskörperphysik, Johannes Kepler Universität (FKP-JKU), Altenbergerstr. 69, Linz 4040, Austria*

e-mail: djordje@phy.bg.ac.yu

In this paper we theoretically study (with plane wave expansion and finite-difference time- domain models) optical properties of 2D hexagonal dielectric photonic crystal of the p6mm plane symmetry group. The structure is made of GaAs dielectric rods in air. We perform the calculations of the band structures, equi-frequency contours and electromagnetic propagation through the basic structure and waveguide.

16:00 Poster C17

BST-based multilayer structures with low temperature coefficient of capacitance

Anatoli A. Khodorov[1], Sebastian Czardybon[2], Agata Lisinska-Czekaj[2], Dionizy Czekaj[2], Maria J. Gomes[1]

1. *University of Minho (UM), Campus de Gualtar, Braga 4710057, Portugal* **2.** *Silesian University, Department of Materials Science, Śnieżna 2, Sosnowiec 41-200, Poland*

e-mail: anatoli@fisica.uminho.pt

Recently, strong interest have been paid to the development of tunable dielectric materials for microwave devices, such as tunable filters, voltage controlled oscillators, varactors, delay lines and phase shifters. $Ba_{1-x}Sr_xTiO_3$ (BST) thin films are considered as one of the forerunner material systems for realization of such tunable components due to their high dielectric constant and dielectric tunability, reasonably low dielectric loss, and controllable Curie temperature by adjusting the barium-to-strontium ratio. A practical concern in a tunable microwave resonator is that its resonant frequency changes with the temperature because it strongly depends upon the dielectric constant of material, which, for example, is highly temperature dependent for BST films of fixed composition. To improve the temperature stability of the dielectric constant, and simultaneously enhance the dielectric tunability and lower the dielectric loss, a promising approach is to prepare BST-based multilayer structures with different Ba/Sr ratios.

In this work a set of BST60/40 and 40/60 BST multilayers separated by nano-size layer of TiO_2 were produced by pulsed laser (KrF) deposition technique on a *(111)*$Pt/TiO_2/SiO_2/Si$ substrate. The study of dielectric properties and the impedance spectroscopy analysis have been performed in the frequency window $10\text{-}10^6$ Hz and temperature range 10-150 °C. The study of processing – structure – property relationships has been performed and the results are presented.

Acknowledgement.*The Authors (D.C. and A.L-C) acknowledge the support of Polish Ministry of Education and Science within a research project N507 098 31/2319 funded from the funds for science in 2006-2009.*

16:00 Poster C18

Preparation and study of BST thin films and graded structures

Anatoli A. Khodorov[1], Tomasz Pokrywka, Dionizy Czekaj[2], Agata Lisinska-Czekaj[2], Maria J. Gomes[1]

1. *University of Minho (UM), Campus de Gualtar, Braga 4710057, Portugal* **2.** *Silesian University, Department of Materials Science, Śnieżna 2, Sosnowiec 41-200, Poland*

e-mail: anatoli@fisica.uminho.pt

Ferroelectric thin films have been studied extensively due to their various applications in a number of microelectronic and optoelectronic devices such as ferroelectric memories, infrared pyroelectric sensors, micro-electro-mechanical systems, optical waveguides. Ferroelectric multilayers and thin films with composition gradient across the film through thickness are recently well known for their striking properties that were not observed in conventional ferroelectric layers. The compositionally graded structures were reported to have a higher tunability, polarization and flatter temperature characteristics because of their enhanced chemical heterogeneity. The Curie temperature of compositionally graded $Ba_{1-x}Sr_xTiO3$ (BST) thin films can be tailored by the composition gradients to meet the requirements of enhanced ferroelectric properties near room temperature, which is very interest from application point of view.

In this work a set of BST thin films and graded structures of composition 100/0, 80/20 and 60/40 were produced by pulsed laser deposition technique on a *(111)*$Pt/TiO_2/SiO_2/Si$ substrate. A KrF excimer laser with a wavelength of 248 nm and pulse duration of 10 ns was used. The deposition was performed with an oxygen pressure of 0.20 mbar at the substrate temperature of 650 °C. After deposition the films were annealed at 700 °C for 30 min in ambient air that resulted in formation of pure perovskite phase and good crystallinity. The films are characterized with XRD, SEM and Raman spectroscopy. The dielectric and ferroelectric properties were studied in the frequency window $10\text{-}10^6$ Hz and temperature range 10-200 °C. The comparable analysis of physical properties of homogenous BST films and graded structures has been carried out and the results are presented.

Acknowledgement.*The Authors (D.C. and A.L-C) acknowledge the support of Polish Ministry of Education and Science within a research project N507 098 31/2319 funded from the funds for science in 2006-2009.*

16:00 Poster C19

Shutoff valve with a shape memory active element

Mikhail A. Khusainov[1], Vladimir A. Andreev[2], Andrey B. Bondarev[2], Dmitriy A. Maslenkov[1]

1. *Yaroslav the Wise Novgorod State University, Bolshaya St-Petersburgskaya 41, Novgorod the Great 173003, Russian Federation* **2.** *Industrial Centre MATEKS (MATEKS), 13/2 Tolbuchina str., Moscow 121596, Russian Federation*

e-mail: mikhail.khusainov@novsu.ru

Shutoff valves are intended for rapid shutting of input hole when the fluid temperature reaches a definite value. Thermosensitive element in this valve design is a TiNi shape memory spherical segment which used at the same time as an actuator. Mirror-like bended spherical segment loses stability and turns into the initial form with a snap at the temperature near A_f. The active element is as a trigger in this valve design and the hermeticity of closed input hole of valve is provided with a hardness of the force spring. Increasing a hardness of the force spring we can apply the valve under sufficiently high pressure of the operating fluid (water, gas and petroleum products).

This paper represents the design of shutoff valve, diagrams of the active elements deforming and their mechanical behavior during continuous operation.

16:00 Poster C20

Martensitic transformation and magnetic properties in Fe-Co-based ferromagnetic shape memory alloys.

Larisa E. Kozlova, Volodymyr V. Kokorin

Institute of Magnetism, NAS of Ukraine, 36-B Vernadsky str., Kiev 03142, Ukraine

e-mail: kozlova@imag.kiev.ua

Ferromagnetic shape memory alloys has became the popular objects of researches from the moment of finding out a plastic deformation caused by magnetic field in the alloys of Ni-Mn-Ga. The study of deformations induced by field was conducted also and in Fe based alloys, such as Fe-Pd, Fe-Pt and Fe-Ni-Co-Ti.Such factors as fragility of high temperature phase, comparatively low saturated magnetization and low Curie temperature hinder to the wide practical application of Ni-Mn-Ga alloys capable of to generate considerable deformations induced by magnetic field. The alloys of the system of Fe-Co-Ni-Ti excel Ni-Mn-Ga in the parameters indicated higher and in principle can be examined as an alternative material to be used as the actuators.An addition of Cu is a way to lower the elastic module of an austenite phase to decrease an elastic energy of the growing coherent martensite crystals that gives rise as a result the hysteresis narrowing.Measured temperature dependences of magnetizations of Fe-Co-Ni-Ti ferromagnetic alloys doped by Cu have shown that martensite magnetizations of the considered alloys are more than three times larger in comparison with Ni-Mn-Ga alloy at the field of 10 kOe.

16:00 Poster C21

Stainless steel processing using additive technology

Tomasz Kurzynowski, Edward Chlebus

Politechnika Wrocławska (PWR), Wybrzeże Wyspiańskiego, Wrocław 50-370, Poland

e-mail: tomasz.kurzynowski@pwr.wroc.pl

Rapid Prototyping Techniques (Layer Based Manufacturing Methods - LBMMs) give a possibility of producing highly complex geometrical parts directly from 3D-CAD data. At the beginning, LBMMs were used only for building prototypes from plastic materials for model visualizations and investigations of construction validity in early product development stages. Nowadays, LBMMs have transformed into additive technologies, capable of manufacturing objects from selected plastics and almost any metal (stainless steel, tool steel, titanium and its alloys, Co-Cr, aluminium alloys). For the metal technologies the objective is the capability to manufacture fully functional products (e.g. medical implants, inserts with conformal cooling channels for moulds) with customized mechanical properties. The paper will present results of research on one such technology – selective laser melting (SLM), in the Centre for Advanced Manufacturing Technologies at the Wroclaw University of Technology.

16:00 Poster C22

The acoustical spectral investigations of a ferromagnet Heusler $Ni_{53}Mn_{25}Ga_{22}$ alloy crystal

Yuri A. Kuzavko[1], Vasiliy D. Buchelnikov[2], V V. Koledov[3], Dmitriy A. Kostiuk[4], Vladimir V. Khovailo[3], Vladimir G. Shavrov[3]

1. *The Polesie Agrarian Ecological Institute of the National Academy of Science of Belarus (PAEI), Brest 224000, Belarus* **2.** *Chelyabinsk State University (ChelSU), Br. Kashirinykh Str, 129, Chelyabinsk 454021, Russian Federation* **3.** *Institute of Radio Engineering and Electronics RAS (IRE RAS), Mokhovaya, 11, Moscow 125009, Russian Federation* **4.** *Brest State Technical University, Brest 224017, Belarus*

e-mail: kuzavko@newmail.ru

Big attention is paid to materials with reversible form and size control by means of magnetic field, especially to Heusler Ni-Mn-Ga alloys (HA) with nonstechiometric composition, which are the highest achievement in this area allowing 6% of crystal size change.

That stimulated the undertaken research of longitudinal (LA) & transverse (TA) acoustic waves at their inclined fall in the (100) plane and reflection from the free border of a crystal (110), as far as from its border with liquid and dielectric. The ability of the temperature and magnetic field to effectively control the angles of reflection and transformation of wave types is shown.

There are investigated effects of a strong acoustic anisotropy and nonlinearity in $Ni_{53}Mn_{25}Ga_{22}$ HA at region of martensitic, premartensitic and spin-orientational phase transitions (PT). The reflection & transition were numericaly examined for HA bondary with dielectric (liquid). The effect of full LA to TA transformation was registered as far as the appearance of accompanying surface oscillations and displacement up to cleavage of acoustical beams at the mediums bondary.

The existence of high harmonics (HG) at spread of LA & TA in solids is well-known, but their amplitudes are usually larger due to negligible elastic unharmonicity. HG measured in some crystalls were great acoustic nonlinearities. It takes place in Ni-Mn-Ga HA with giant magnetodeformation (up to 10%), coexisting with strong nonlinearity supplied martensitic and premartensitic PT.

Theoretical calculations were supported experimentally in polycrystalline $Ni_{1.95}Mn_{1.05}Ga_{0.05}$ with 40^oC PT temperature and $Ni_{53}Mn_{25}Ga_{22}$ crystal with a coupled magnetostructural PT. Sound speeds at this crystal along [110], [1T0], [001] directions are subsequently v_L=6.47 km/s, v_L=6.91 km/s, and v_L=5.71 km/s. The influence of reconstruction of structural variants & magnet domains may be caused by HG generation.

Authors are grateful to BRFFI and RFFI for support.

16:00 Poster C23

The surface waves acoustoelectronic sensors based on films of Heusler alloy

Yuri A. Kuzavko

The Polesie Agrarian Ecological Institute of the National Academy of Science of Belarus (PAEI), Brest 224000, Belarus

e-mail: kuzavko@newmail.ru

The surface acoustic waves (SAW) are founded to be curiously at mass loading (~1 ng/sm^2) of surface of solid waveguide. We have been used in our investigations the acoustoelectronic filters of 35 MHz on SAW consisted of a planar transducers for SAW generation and receiving at monocrystal high-Q-factor piezoelectric plates of $LiNbO_3$ (X-cut) with sizes of 10x2 mm. It is rendered on sensor substance of ferromagnetic Heysler $Ni_{2+x+y}Mn_{1-x}Ga_{1-y}$ films with shape memory, thus allowing to realize the so-called 'electronic nose' and 'electronic clapper' at known sensors. The elastic deformation can be achieved at this alloys with the magnitude of several percent by changing temperature, pressure or magnetic field. Ferromagnetic films of Heusler alloys are showing phase transitions at lower temperature, pressure and magnetic field in comparison with volumetric specimen. The passing of electric current through metallic field restores the function of a sensor. That arrangement presents the frequency etalon where it would be inserted at inverted positive relation of apmplifier supplied the generation of narrow line of frequencies. The external loading of active sensor surface would cause the shift of its resonance frequency thus allowing to perform the analysis of air and liquids for containing toxic and inflammable components. There are many types of SAW and its modes (such as Reyleigh, Love, Lemb, Gulyaev-Bleustein waves, SH-modes, etc.), and some of them are sensitive to mas loading independently. The active smart material increases the sensitivity and reversibility of a sensor. The theoretical calculations are for spreading the Rayleigh and Love waves in Ni_2MnGa-$LiNbO_3$(AsGa) structures. It was investigated experimentally on processes of evaporation of liquid drops and the registration of percent concentration of methane in air, the dynamics of bacterium colony in feeding medium with simultaneous digital photographic registration.

16:00 Poster C24

Structure and properties of high temperature nitrided/oxided surface of Ni-Ti alloy

Jozef Lelatko[1], Tomasz Goryczka[1], Tadeusz Wierzchoń[2], Henryk Morawiec[1]

1. *University of Silesia, Institute of Material Science, Bankowa 12, Katowice 40-007, Poland* **2.** *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland*

e-mail: jlelatko@us.edu.pl

Structure and properties of high temperature nitIn order to find new applications and enhance the performance of NiTi alloy, surface modifications is necessary condition for improving its biocompatibility. Nitride and oxide coatings, which are known from their low chemical reactivity, high hardness and good wear and corrosion resistance, were adopted for protecting the NiTi surface. The nitriding and oxidation processes reduce the nickel migration to the surface and improves the biocompatibility of the NiTi alloy. In the present work nearly-equiatomic NiTi (50,6 at.%Ni, Af =10°C) alloy was nitrided at 800^{o}C using glow discharge technique. Additionally, at the end of the nitriding some amount of oxygen was added. Combination of nitriding and oxidiation of the NiTi surface produces nitride/oxide complex layer of a nanocrystalline structure. The average thickness of the obtained layer was about 0,55 μm. The nitrided layer contains nanocrystalline TiN phase. Adding the oxygen at the end of the nitriding process creates TiO_2 phase on the top of the TiN layer. The layer of Ti_2Ni phase creates the interface between nitrided/oxidized NiTi surface and β-NiTi matrix. Small amount of an amorphous phase, between the nano-grains of nitride and oxide phase, was identified. The potentiodynamical studies in Tyrod's solution show good corrosion resistance of the nitrided/oxidized NiTi surface proving its high quality.

16:00 Poster C25

Magnetomechanical properties of Terfenol-D powder composites.

Daniel Lewandowski, Jerzy Kaleta, Rafał Mech

Wroclaw University of Technology, Institute of Materials Science and Applied Mechanics (PWr - IMMT), Smoluchowskiego 25, Wrocław 50-370, Poland

e-mail: daniel.lewandowski@pwr.wroc.pl

Main accepted purpose of the work was an identification of the magnetomechanical and mechanical properties of the magnetostrictive composites. An epoxy resin constituted the matrix of composite, and powder was a filler of material so-called giant magnetostrictive (Terfenol-D).

Working out the technology including productions of composite was a main task, procedures including: selection of composition, combining parameters, the elimination of oxidizing of powder, deaerate methods and getting the desired shape specimens. As a result, specimens were produced with different content of Terfenol-D powder in resin. Appropriate experiments were carried out to the purpose of getting mechanical and magnetomechanical characteristics. Value of the Young module has been determined for all produced composites and for clean resin but also solid Terfenol-D.

Next a magnetostriction of composites was examined and compared with solid Terfenol-D. The scope of changes of the magnetic field strength was included within the range 0 - 180 kA/m. Results of measurements of the magnetostriction were discussed. They showed that in produced composites the magnetostriction was lower as in solid Terfenol-D, but still several dozen times bigger than e.g. in nickel. They stated moreover, in the case of composites leak of saturation effect under the influence of applied value of the intensity of magnetic field and linear character of the magnetostriction in the function of the intensity of the magnetic field H.

Produced composite is characterized by a small value of magnetomechanical damping, what is correlated with hysteresis loop. They showed moreover that the magnetostriction in produced composites largely depended on volume contents of Terfenol-D. Get results at the work create bases for taking the next problem which is the modelling of magnetostriction in composite. Moreover suggestions were formulated in the scope of the application of manufactured composites.

16:00 Poster C26

Hydrogel formulatin for swelling response in alkaline pH ranges.

Stephanie San Juan, Jose-Manuel Lloris, Mariajose López-Tendero, Manuel Cruz-Yusta, Celia Silvestre

Asociación Investigación Industrias de Construcción (AIDICO), Parque Tecnológico Valencia, Valencia 46980, Spain

e-mail: mlopezt@aidico.es

In the last years, a lot of optic fiber sensors have been developed for structural health monitoring systems. There are several physical, chemical and environmental factors that contribute to concrete structures deterioration. There is a need to monitor all these factors to explain the produced damages after extended periods. In this paper we present the results concerning the development of a hydrogel material with a swelling response in the pH range from 13 to 10. This pH decrease indicate a possible point in the concrete structure where corrosion problems can initiate.

16:00 Poster C27

Investigation of a PTCR Effect in The $(Bi_{0.5}K_{0.5})TiO_3$-$BaTiO_3$ Solid Solution Semiconducting Ceramics

Jonghoo Paik, Young Hun Jeong, Young-Jin Lee, Yong-Jun Park

Korea Institute of Ceramic Engineering and Technology (KICET), , Gasang-Dong, Geumcheon-Gu, Seoul 153023, Korea, South

e-mail: jhpaik@kicet.re.kr

An anomalous positive temperature coefficient of electrical resistivity(PTCR) was investigated in a ferroelectric lead-free perovskite-type compound $(Bi_{0.5}K_{0.5})TiO_3$ within $BaTiO_3$-based solid solution ceramics. The effect of Nb_2O_5 content on the electrical properties and the microstructure of (1-x) $(Bi_{0.5}K_{0.5})TiO_3$- x $BaTiO_3$ (BKBT) ceramics made using a conventional mixed oxide process also has been studied. The Curie Temperature was obviously increased with the increasing of $(Bi_{0.5}K_{0.5})TiO_3$ content. The addition of Nb_2O_5 to BKBT has significantly improved its PTCR properties. For the sample containing 0.025 mol% Nb_2O_5, it showed good PTCR properties; low resistivity at room temperature (ρr) of 30 Ω•cm, a high PTCR intensity of approximately 3.3×10^3 with high Curie temperature (TC) of 155°C.

16:00 Poster C28

Magnetic field analysis for magnetron sputtering apparatus for accurate composition control

Yutaka Sakurai[1], Hiroko Nakamura[2], Ryo Nakajima[3]

1. *Toyama National College of Technology, 13 Hongo, Toyama 939-8630, Japan* **2.** *YKK Corporation, 200 Yoshida, Toyama 938-8601, Japan* **3.** *Hokuriku Electric Power Company, 15-1 Ushijima, Toyama 939-8686, Japan*

e-mail: ysakurai@toyama-nct.ac.jp

Authors use magnetron sputtering technique for controlling the film composition by modifying the magnetic field with an external solenoid in addition to the magnetic field with a permanent magnet on the back of the composite target[1]. It is necessary to understand the contribution of the solenoid quantitatively for the effective application of this technique. The magnetic field on the target was calculated by the finite element method (FEM), and correspondence with the erosion region was discussed.

Composition controllable DC magnetron sputtering apparatus from outside by controlling the solenoid current was used, and the forming of the TiNi films for the shape-memory alloy was examined[2]. Ti base composite target with Ni ring was employed there, and the composition of films formed by the apparatus was analyzed by using EDX. Axisymmetrical 3D-FEM was applied to the sputtering target, the magnet, the iron yoke and the solenoid current conductor.

Figure 1 shows the calculated vertical components of B (By) on the Ni/Ti composite target at various solenoid current values. As the solenoid current increases, the tunnel region of flux on the target (correspond with the well sputtered region by the confined plasma) moves to the center of the target. The behavior corresponds to the film content. The analyzed results also give the correction value for using the already eroded target.

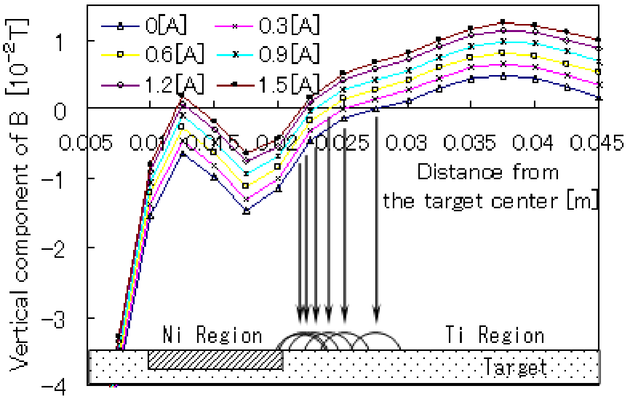

Fig. 1 Calculated vertical components of B (By) on the Ni/Ti composite target at various solenoid current values. By=0 points corresponding with the well sputtered region are schematically drawn.

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16:00 Poster C29

Local observation of stress-induced martensitic transformation in a CuAlBe shape memory alloy using digital speckle correlation technique

Francisco M. Sánchez[1], Tupak García[1], Guillermo Pulos[2], Mayo Villagrán[1]

1. *Universidad Nacional Autonoma de Mexico-Centro de Ciencias Aplicadas Desarrollo Tecnologico (CCADET), Circuito Ext. S/N Ciudad Universitaria Coyoacan, México 70-186, Mexico* **2.** *Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico (UNAM), A.P. 70-360, México 04510, Mexico*

e-mail: fsanchez@iim.unam.mx

In recent years, a combination of experimental techniques, from different fields, has been used to measure physical phenomena with more accuracy. In particular, such combination has become a powerful tool to study the behavior at different scales. Digital image correlation and speckle metrology have shown to be a robust methodology to measure the mechanical behavior of conventional materials; nevertheless, the stress-induced martensitic transformation in a CuAlBe shape memory alloy has not been studied to date using digital speckle correlation technique.

In this work a Cu-Al 11.2 wt%-Be 0.6 wt% shape memory alloy, was subjected to simple tension test using a MTS load frame equipped with an optical microscope. Displacement, force, strain data and digital images of the sample's, polished and chemically etched, surface were acquired. He-Ne laser was used to observe the speckle pattern on the sample surface at different stress levels. The speckle pattern depends on the roughness of the sample's surface, the state of the stress-strain and the laser stability was observed in the calibration results. When the stress-strain level is changed the speckle patterns change too. These changes were determined using a digital speckle correlation technique. From the images, displacement vectors fields were obtained in specific grains where plates of martensite grew during the tension test. The displacement vector fields present a hyperbolic shape but also non-homogeneous local deformations which were associated to the stress-induced martensite plates. The displacement vector fields were related to the stress-strain curve. Hence, it was possible to observe the mechanical behavior of the material at micro and macro scales.

16:00 Poster C30

Monte Carlo study of magnetostructural phase transition in $Ni_{50}Mn_{25+x}Sb_{25-x}$ Heusler alloys

Vladimir V. Sokolovskiy, Vasiliy D. Buchelnikov, Sergey V. Taskaev

Chelyabinsk State University (ChelSU), Br. Kashirinykh Str, 129, Chelyabinsk 454021, Russian Federation

e-mail: vsokolovsky84@mail.ru

Heusler Ni-Mn-X (X = In, Sn, Sb) alloys have unique properties, such as the shape memory effect, the giant magnetocaloric effect and the large magnetoresistance. These properties are associated with the martensitic transition. In our work we present the modeling of thermomagnetization curves in relatively a low magnetic field for non-stoichiometric Heusler $Ni_{50}Mn_{25+x}Sb_{25-x}$ compounds by the help of the Monte Carlo method.

In the proposed model we use the three-dimensional cubic lattice with periodic boundary conditions. The sites of lattice only occupy the magnetic Mn atoms due to that the magnetic moment of Ni atoms is much more less then magnetic momentum of Mn atoms and Sb atoms have not the magnetic momentum. The whole system can be representing as two interacting parts – magnetic and structural subsystems. The magnetic part is described by the "*q*-state" Potts model for the magnetic phase transition from ferromagnetic to paramagnetic one [1]. The structural part is described by the degenerated three state BEG model for the structural transformation from the austenitic phase to the martensitic phase [2]. In the martensitic state we consider two types of the magnetic interaction between nearest sites of the lattice. One of part of Mn atoms interact with each other ferromagnetically and another part of Mn atom interact with other Mn atoms antiferromagnetically. In the austenitic phase we consider that each atom of Mn interact with each other ferromagnetically. The initial configuration of Mn atoms with antiferromagnetic interaction on the cubic lattice was set random and was determined from experimental data of $Ni_{50}Mn_{25+x}Sb_{25-x}$ alloys. By the help model the temperature dependences of the magnetization for different concentrations are obtained. It is shown that theory are in good agreement with experimental data.

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16:00 Poster C31

Measurements of strain in ceramic components using magnetostrictive delay line

Roman Szewczyk[1], Jacek Salach[1], Adam Bieńkowski[1], Marek Kostecki[2], A. Olszyna[2], Aleksandra Kolano-Burian[3]

1. *Warsaw University of Technology, Faculty of Mechatronics, Św. Andrzeja Boboli 8, Warszawa 05-525, Poland* **2.** *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland* **3.** *Institute of Non-ferrous Metals, Sowińskiego 5, Gliwice 44-100, Poland*

e-mail: szewczyk@mchtr.pw.edu.pl

The real time measurements of strain of ceramic components is required in many machine industry applications. This paper presents novel application of magnetostrictive delay lines, which gives possibility of real time monitoring of strain in ceramic components.

Magnetostrictive delay line was made of Fe-Si-B amorphous alloy in as-quenched state. Such alloy exhibit high saturation magnetostriction (which exceeds 30 μm/m) together with high stress strength. As a result such amorphous alloy exactly meets requirements of material for magnetostrictive delay line.

Amorphous alloy based magnetostrictive delay line was mounted outside of ceramic bar to improve wave propagation conditions. Manuscript presents the results of measurements of influence of external force applied to ceramic bar on the shape of signal generated by wave in magnetoelastic delay line.

Moreover specialized electronic converter utilizing sample-and-hold integrated circuit was developed. Paper presents transfer characteristics of developed sensor based on magnetostrictive delay line. These characteristics connect value of force applied to ceramic bar with output voltage. It was verified, that changes of output signal exceed 3 volts, which confirm possibility of technical application of developed sensor.

This work was supported by Polish Ministry of Science and Higher Education under Grant PBZ-KBN-095/T08/2003.

16:00 Poster C32

Experimental validation of numerical methods of MRE simulations

Wiesław Szymczyk[1], Anna Boczkowska[2], Tadeusz Niezgoda[1], Konrad Zubko[1]

1. *Military University of Technology (WAT), Kaliskiego 2, Warszawa 00-908, Poland* **2.** *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland*

e-mail: w.szymczyk@wme.wat.edu.pl

This paper deals with the development of magnetoactive elastomers based on carbonyl iron particles-filled polyurethane resin. Their stiffness can be changed easily by magnetic field. Such a property can be useful in construction of active vibration damping structural elements.

For the needs of numerical modelling methods validation the elementary case of the two magnetic dipoles was investigated experimentally.

Special "macro samples" were prepared with pairs of "dipoles" of cylindrical as well as apherical shape of diameter of 20 mm. The gap distance was established on the level of 1/4 of the diameter. Thanks to this all the observations were easy while the magnetic field intensity was changed in the range 50-400 mT. The change in the gap distance between the dipoles was registered in function of the magnetic field intensity. The deformation field was also obtained from the digital image processing.

Then the experiment was simulated with the use of 2D as well as 3D FEM models. The computations were conducted in the two ways:

1- the magnetic force was calculated with the use of appropriate formulas and then applicated to the model dipoles;

2- the dipoles were loaded by the displacements measured experimentally.

Calculations were performed on the MSC Nastran platform.

The results of calculations were compared with the experimental ones. The validaton of the base concept of MRE modelling was completed successfully.

16:00 Poster C33

FEM simulations of a magnetorheological elastomer with consideration of magneto mechanical coupling

Wiesław Szymczyk[1], Anna Boczkowska[2], Tadeusz Niezgoda[1], Konrad Zubko[1]

1. *Military University of Technology (WAT), Kaliskiego 2, Warszawa 00-908, Poland* **2.** *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland*

e-mail: w.szymczyk@wme.wat.edu.pl

There were investigated magnetorheological elastomers (MRE) based on carbonyl iron particles-filled polyurethane resin. Their stiffness can be changed easily by magnetic field. Such a property can be useful in construction of active vibration damping structural elements.

Numerical simulations were performed on the MSC Nastran platform. The NeoHookean material model was used to describe properties of the resin matrix. Magneto-mechanical coupling was taken in consideration with the use of the 2 different iterative methods. The compliance of results confirms the correctness of applied numerical simulation methods of MRE behaviour under applied magnetic field.

16:00 Poster C34

New oxide layer formed by oxygen molecular beam on vanadium and its alloys as observed by photoemission spectroscopy with synchrotron radiation

Yuden Teraoka, Akitaka Yoshigoe

Japan Atomic Energy Agency (JAEA), 1-1-1 Kouto, Sayo-cho,Sayo-gun, Hyogo 679-5148, Japan

e-mail: yteraoka@spring8.or.jp

We have been studying correlation between thermal desorption of hydrogen and chemical bonding states of overlayer on the surface of hydrogen storage metals because desorption and absorption of hydrogen take place through the overlayer. Poly-crystalline Vanadium and VCrTa alloy are important as candidates for fuel cells of automobiles. In this study, native oxides, their thermal instability and artificial oxides formation via supersonic oxygen molecular beams (SSOMB) have been investigated using photoemission spectroscopy with synchrotron radiation (SR-PES). Various photon energies ranging from 600 eV to 1800 eV were used to investigate depth distributions in the native overlayer. All experiments have been performed at the surface chemistry end-station (SUREAC2000) of BL23SU in the SPring-8. Although carbon contamination was observed in the overlayer of both metals, nitrogen was negligible. C1s and O1s photoemission peaks decreased with increasing surface temperature. Especially, a new C1s peak appeared in the low binding energy side in the poly-Vanadium case. The peak strength moved from the original peak to the new peak. The native overlayer could be removed by heating up to 1273 K. The bare Vanadium surface was irradiated by SSOMB with the translational energy of 0.4 eV until saturation. This pure oxide overlayer could be removed by the same heating procedure. We verified again the oxidation of the surface using SSOMB with 2.3 eV. The saturated oxygen was larger than that of 0.4 eV case and an oxidation rate in the early stage was also large compared to the 0.4 eV case. Translational-energy–induced oxidation was found in the poly-Vanadium oxidation. In other words, we can control artificially the surface oxide thickness at room temperature using kinetic energy of oxygen as a parameter.

16:00 Poster C35

Coordinate transformation based design of confined metamaterial structures

Borislav Vasic[1], Goran Isic[1,2], Rados Gajic[1], Kurt Hingerl[3]

1. *Institute of Physics (IF), Pregrevica 118, Belgrade 11080, Serbia* **2.** *School of Electronic and Electrical Engineering, University of Leeds, Leeds LS29JT, United Kingdom* **3.** *Institut für Halbleiter und Feskörperphysik, Johannes Kepler Universität (FKP-JKU), Altenbergerstr. 69, Linz 4040, Austria*

e-mail: bvasic@phy.bg.ac.yu

We study metamaterial structures coated with highly conductive layers in order to manipulate the propagation of electromagnetic beams. These structures are described and analyzed by coordinate transformations applied to domains bounded by perfectly conducting surfaces. The perfectly conducting boundary conditions are shown to remain invariant under the transformations. Our approach is a generalization of the previously reported coordinate transformation method facilitating the design of novel metamaterial devices and offering an alternative approach to existing ones. These represent various metamaterial structures for reflectionless beam rotation, spatial displacement and metamaterial layers which can be inserted into waveguides to obtain a reflectionless shape change and waveguide miniaturization. Several two-dimensional versions of the proposed devices, including the beam shifter and rotator are numerically simulated fully confirming our predictions. It is shown that devices offering extraordinary control over the electromagnetic fields can be devised if anisotropic metamaterials with spatially varying parameters are available. The properties of metamaterials required for the fabrication of these devices are determined by the type of local change of the beam's shape. In parts of the structure in which the original beam is stretched, the phase velocity exceeds *c*, so material dispersion is expected meaning that the conditions for the reflectionless field manipulation can be met only in a limited range of frequencies. We expect that the proposed devices will be interesting for single frequency applications such as various waveguiding structures or electromagnetic cavities.

16:00 Poster C36

Kinetics of swelling and drug release from PNIPAAm/alginate stimuli responsive hydrogels for controlled drug release

Cornelia A. Vasile, Raluca P. Dumitriu, Ana Maria Oprea

Petru Poni Institute of Macromolecular Chemistry of the Romanian Academy, Aleea Grigore Ghica Voda 41A, Iasi, Romania

e-mail: cvasile@icmpp.ro

Environmentally responsive hydrogels are very attractive for applications in sustained and /or targeted drug delivery systems. As the release of drugs is related to the swelling behavior of hydrogels, the swelling kinetic studies become of great importance to appreciate the release kinetic from hydrogels matrices.

Hydrogels with high performance properties have been prepared from N-isopropyl amide (NIPAAm) and sodium alginate, crosslinked with N, N`-methylene- bis-(acrylamide) (MBAAm).

This study is focused on the investigation of swelling and drug release kinetics, completed by morphological studies.

The kinetic parameters of the swelling performed at different temperatures and pHs for hydrogels samples with different mixing ratios of the components and various crosslinking degrees have been evaluated and showed their dual responsive behavior (under temperature and pH changes). The results obtained by swelling kinetics investigation showed the decrease of the swelling rate constant with increasing temperature and increase with the alginate content in the samples.

The drug release kinetic study from the prepared hydrogel matrices was performed in twice-distilled water and ethanol for bioactive agents as vanillin and ketoprofen, respectively. An increase of alginate content results in a slower rate and smaller percentage of vanillin and ketoprofen released. The ketoprofen release behavior fitted with case II of transport and vanillin release behavior fitted with an anomalous transport of drugs. The values of *k* decreased by increasing ethanol quantity in case of 75/25 NIPAAm/alginate hydrogels and decreased also by increasing content of alginate in hydrogels with various compositions.
Morphological studies performed by environmental scanning electron microscopy (ESEM) allowed us to observe the behavior of the hydrogel samples according to water content changes (relative humidity RH %) and to explain the behaviour both at swelling and release profiles.

16:00 Poster C37

Localization of rare-earth dopants in the lattice of nanocrystalline ZrO_2 - EXAFS study

Roman Pielaszek[1], Anna Wolska[2], Agnieszka Opalińska[1,3], Witold Łojkowski[1], Stefan Mangold[4], Stephen Doyle[4]

1. *Polish Academy of Sciences, Institute of High Pressure Physics (UNIPRESS), Sokolowska 29/37, Warszawa 01-142, Poland* **2.** *Polish Academy of Sciences, Institute of Physics, al. Lotników 32/46, Warszawa 02-668, Poland* **3.** *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland* **4.** *Forschungszentrum Karlsruhe GmbH, Institut für Synchrotronstrahlung, ANKA (ANKA), Hermann-von-Helmholtz-Platz 1, Karlsruhe 76344, Germany*

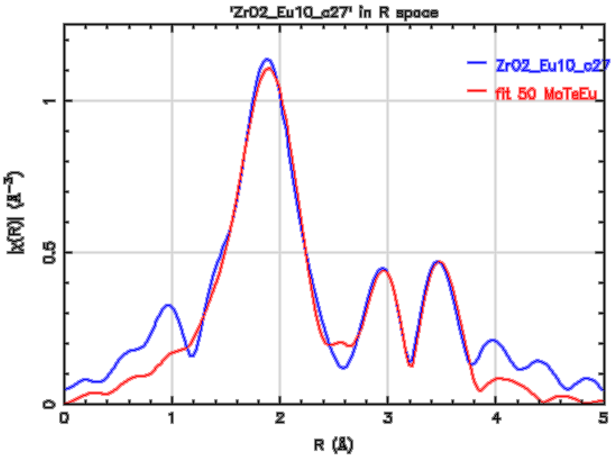
e-mail: roman@pielaszek.net

Selected crystalline lattices, such as YAG or ZrO_2, doped with rare earth atoms become effective light sources used for manufacturing of LEDs, lasers and scintillators. Emission efficiency raises with concentration of the rare-earth with the limit posed by solubility of the dopant on the one hand and concentration quenching phenomena on another.

Nanocrystalline host lattice inherits desired optical features of model infinite lattice but allows for much higher solubility of rare earth dopants. Simultaneously, in case of nanocrystalline lattice, the long-distance crystal order is cut on the grain boundary which relaxes quenching.

In the present work we show preliminary EXAFS study of rare-earth atoms buried in zirconia nanocrystals, 10-40nm in diameter. The experiments show that dopants are evenly distributed in nanocrystals and do not segregate even at very high concentrations. Surprisingly, most of dopants are located in monoclinic phase of ZrO_2 (zriconia, as synthesized, is usually a mixture of tetragonal and monoclinic phases). This knowledge strongly influences synthesis procedures used to obtain high-intensity luminescent zirconia powders.

Figure below shows average electron density (blue) around Eu dopant in the ZrO_2 being mixture of tetragonal and monoclinic phase. Red curve is theoretical density asumming: even distribution of Eu within ZrO_2, lack of Eu segregation (e.g. as oxide), non-surface position, most of Eu in monoclinic nanocrystals only (a trace in tetragonal, however) and very high concentration of Eu.



16:00 Poster C38

Field dependence of the refrigerant capacity for La-based manganites

Ritta Szymczak[1], Roman Kolano[2], Aleksandra Kolano-Burian[2], Roman Puzniak[1], Henryk Szymczak[1]

1. *Polish Academy of Sciences, Institute of Physics, Warszawa 02-668, Poland* **2.** *Institute of Nonferrous Metals, Sowińskiego 5, Gliwice 44-100, Poland*

e-mail: szymh@ifpan.edu.pl

In recent years, there has been increasing interest in using manganities not only as material having colossal magnetoresistivity but also as material having promising magnetocaloric properties. A large magnetocaloric effect makes manganities excellent candidate for working materials in magnetic refrigeration units especially because these are less costly than any other materials, particularly materials based on gadolinium. Moreover, we have shown that the magnetic entropy change $|\Delta S_M|$ in La-based manganites is larger than that exhibited by gadolinium. In order to compare existing magnetic refrigerant materials, either the peak of magnetic entropy change $|\Delta S_M|$ or the refrigerant capacity (RC) is used. The refrigerant capacity is defined as RC $= \Delta S_M \Delta T$, where ΔT is the operating temperature range of the cycle. The optimal refrigeration cycle is that which maximizes of RC. We present the results of RC measurements on $La_{1-x}Ca_x MnO_3$ (x = 0.5-0.7) polycrystalline manganites in magnetic fields up to 9T.The maximum of RC is larger than that of gadolinium measured under the same experimental conditions It was shown that the refrigerant capacity for manganites can be expressed as RC $\sim H^{\alpha}$. The field dependence of the refrigerant capacity was analyzed in frames of scaling model, showing a power dependence related directly to critical exponents in agreement with experiment..

This work is party supported by the Ministry of Science and Higher Education of Poland Project PBZ-KBN-115/T08/2004

16:00	Poster	C39

Giant magnetoimpedance effect in soft magnetic alloys for magnetic sensors

Marek Kuźmiński[1], Jacek Gierałtowski[2], Saida Nabily[2], Vladimir P. Dyakonov[1,3]

1. *Polish Academy of Sciences, Institute of Physics, al. Lotników 32/46, Warszawa 02-668, Poland* **2.** *Université de Bretagne Occidentale, Laboratoire de Magnétisme de Bretagne CNRS, 6 Av. Victor le Gorgeu, Brest 29238, France* **3.** *National Academy of Sciences of Ukraine, Donetsk Technical-Physical Institute, R. Luxemburg 72, Donetsk 83114, Ukraine*

e-mail: kuzmi@ifpan.edu.pl

The giant magnetoimpedance effect (GMI) attracts much attention mainly due to possible applications (e.g. miniaturized magnetometers) [1-4]. In the present work, the GMI-effect was studied in Co-based low magnetostrictive metallic glass ribbons of different widths. As-quenched, stress-relaxed and partially crystallized samples, with the properties modified by thermal treatment, were studied. The purpose of these processes was to optimize the GMI-effect in the ribbon in respect to its application as a magnetic sensing element. Isothermal annealing process (200 - 550°C) leads to changes in magnetic and magneto-impedance characteristics of the ribbon because of the structural relaxation or precipitation of new crystalline phases in the amorphous matrix. The magnetization characteristics and dependences of the impedance (two components: R and X) on a DC-magnetic field at various frequencies of an AC-current (0.1 - 500 MHz) have been measured. A possibility of tailoring of magnetoimpedance effect has been demonstrated, e.g. high temperature annealing can lead to partial recrystallization and very high value of (dZ/dH) near the maxima of impedance. This work was in part financed by the Polish Ministry of Education and Science as a Targeted Research Project, over the period 2005–2008 (Project PBZ-KBN-115/T08/01).

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Novel syntheis processes and design of nanomaterials for catalytic applications

Symposium D

Welcome

This symposium is focused of novel synthesis processes and design of nanomaterials with finely tuned morphological, structural, compositional and surface characteristics made to measure for particular catalytic applications.

The discovery of new catalysts and new processes with continuously enhanced performances and controlable behaviors is nowadays one of the driving forces for modern catalysis, often involving a necessary multidisciplinary approach covering the chemistry, physics, surface analysis, microstructure or chemical engineering fields. Research has therefore to be focussed on the simultaneous development of both new active phases and new catalyst supports, and more generally new catalytic materials and new processes, and, in parallel, on the necessary understanding of mechanisms and reaction steps at the molecular level involved in both material synthesis procedures and catalytic reactions. Nowadays, the macroscoping shaping of tailor-made catalytic (nano)materials has gained an increased interest in the last decades, and finely tuning and controlling the catalytic material characteristics from the nano- to the macro-scale is a great challenge.

Six wide scope keynote lectures are devoted to nanoparticle toxicity, the today- and tomorrow-use of catalyst technologies towards cleaner vehicle emissions,the preparation of nanostructured oxide thin films by plasma and related methods, the use of surface sciences for resolving catalytic phenomena at the atomic scale and anchoring metal nanoparticles on single crystal titania, the design of nanostructured carbons seen as a Janus material for catalysis and hydrogen storage, and the building of heterogeneous biocatalysts by enzymes encapsulation in silica. Beside keynotes, five extended talks will allow the authors to enlarge their contribution scope and to extensively detail their topics and results in-depth. Amongst other, thematic sessions are devoted to the nanoparticle aspects and problematics, as well as to the carbon, silica, titania and mesoporous catalyst fields, without any exclusive, whereas the targeted catalytic reactions cover the whole spectra of catalysis, with emphasis on environmental, energy and more generally sustainable development applications.

The symposium aims to provide a plateform for the report of a state-of-the-art and recent progresses in the elaboration of the major kinds of tailor-made nanomaterials (metal oxides, carbon-based and related solids, metals, mesoporous and zeolites, ...) made to measure and correlated with their catalytic properties.

Special attention is given to multi-functional composite materials associating at least two classes of nanomaterials with specific properties. The impact of the nanostructuration, the particle assembly at the nanoscale, the active particles/support interfaces or within the composite materials is discussed and correlated to catalytic properties through several contributions. The processing of these tailored nanostructured materials, their hierachisation and upscaling to enable industrial purposes at medium or large scale is also highly challenging. Focus is also performed on how both material designs at the nano- and the macro-scale levels can influence the catalytic behavior.

Through worldwide contributions from both academic and industrial worlds, we hope to be successful in illustrating promising material aspects of catalysis as an improving and exciting research field, whatever its complementary fundamental or applied approach.

Organisers

Valérie Keller-Spitzer, Nicolas Keller, Cuong Pham-Huu. Laboratoire des Matériaux, Surfaces et Procédés pour la Catalyse - European Laboratory for Catalysis and Surface Sciences, CNRS - Louis Pasteur University, 25, rue Becquerel, 67087 Strasbourg, FRANCE
E-mail : vkeller@chimie.u-strasbg.fr - nkeller@chimie.u-strasbg.fr - cuong.lcmc@ecpm.u-strasbg.fr

Gabriele Centi. Departement of Industrial Chemistry and Materials Engineering, University of Messina, Messina, ITALY
E-mail : centi@unime.it

SCIENTIFIC COMMITTEE

Marc J. Ledoux, CNRS, Paris, France - **Avelino Corma**, Consejo Superior de Investigaciones Científicas, Instituto de Tecnologias Quimicas, Valencia, Spain - **Kazunari Domen**, The University of Tokyo, Department of Chemical System Engineering, School of Engineering, Tokyo, Japan - **Jose Miguel Yacaman**, Department of Chemical Engineering and Texas Materials Institute, University of Texas, Austin, USA - **André Ayral**, IEM (Institut Européen des Membranes), Montpellier , France - **Daniel Lincot**, Laboratoire d'Électrochimie et de Chimie Analytique, ENSCP, France - **Yasuhiro Iwasawa**, Department of Chemistry, Graduate School of Science, The University of Tokyo, Tokyo, Japan

Proceedings

Selected oral and poster contributions will be published in an Issue of **Solid State Science** (Elsevier) entitled **Novel synthesis processes and design of nanomaterials for catalytic applications**, following an usual peer reviewing process.

Sponsors

The symposium **Novel synthesis processes and design of nanomaterials for catalytic applications,** is organized under the auspices and through the sponsorship of the IDECAT european Network of Excellence (Integrated Design of Catalytic Nanomaterials for a Sustainable Development - www.idecat.org).

Acknowledgements

The organisers acknowledge the European Materials Research Society, and its polish staff for the logistic of the symposium. All the participants are greatly thanked for contributing to a fruitful and friendly scientific symposium.

Programme

Monday, 15 September

Opening & Plenary Session

Czochralski Award Ceremony
Monday morning, 15 September, 10:00
Small Hall (237)

Lunch break

Monday afternoon, 15 September, 12:30
Inner Courtyards

Joint Poster Session I

Monday & Wednesday
Monday afternoon, 15 September, 16:00
Main Hall

Tuesday, 16 September

Parallel Session

Tuesday morning, 16 September, 9:00
Room 134

9:00 Invited oral

Toxicity of nanoparticles

Armelle Baeza

Paris Diderot University, Laboratoire de Cytophysiologie et Toxicologie cellulaire, case 70 73, 2 Place Jussieu, Paris cedex 05, Paris 75251, France

e-mail: baeza@univ-paris-diderot.fr

Increasing utilizations of nanomaterials in the industrial as well as consumer products increase the possibilities of environmental and occupational human exposures. Due to this fact nanoparticles (NPs) have become candidates for the risk assessment. Among the possible exposure routes, inhalation represents the most important route of non intentional exposure to NPs. There are increasing evidences that NPs exhibit ability to cross biological barriers getting access to the bloodstream and secondary target organs where they could accumulate. The knowledge of the behaviour and fate of NPs especially insoluble NPs is of prime interest to assess the pathological consequences linked to long term exposure. The surface area and reactivity of particles increase many fold relative to particle mass as particle size is reduced. Together with chemical composition, they constitute important determinants of NPs toxicity. They also contribute in the production of reactive oxygen species leading to the toxicological outcomes induced by NPs. According to the level of oxidative stress, cellular responses differ from effective antioxidant defence at low level to cell death at high levels going through inflammatory response, specific signalling pathways and gene expression being involved at each step. The potentially deleterious effects of NPs require further studies in order to build on our mechanistic understanding of the toxicological events in which they can be implicated and the development of methodological tools to face the huge variety of NPs to be evaluated.

9:45 Oral

Metal nanoparticles: from synthesis to catalytic properties

Karine Philippot

Laboratoire de Chimie de Coordination (LCC), 205 route de Narbonne, Toulouse 31077, France

e-mail: karine.philippot@lcc-toulouse.fr

The use of well-defined metal nanoparticles for catalysis is an exciting and rapidly growing area. Nanocatalysts have yet been reported as efficient and selective catalysts,[1] the most known ones being Pt(Pd)/cinchonidine ones for ethyl pyruvate hydrogenation.[2] However, other systems are now emerging.

In our group, the synthesis of metal nanoparticles is performed through an organometallic approach, giving rise to well-dispersed and small nanoparticles with a narrow size distribution.[3] In addition they display a controlled surface composition that can be tuned by addition of ligands. This confers them surface coordination chemistry properties[4] that can lead to applications in the field of catalysis. Depending on their nature, the ligands may have a high influence on nanoparticles catalytic properties and can induce particular properties.

The synthesis and the characterization of organic ligand stabilized metal nanoparticles will be described as well as interesting catalytic properties in aromatic compounds hydrogenation[5] or enantioselective allylic alkylation.[6]

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10:00 Oral

Early Transition Metal Carbides and Nitrides Nanoparticles as Promoters for the Use of Alcohols as Alkylation agents.

Philippe Makowski[1], Frédéric Goettmann[2], Cristina Giordano[1], Markus Antonietti[1]

1. *Max Planck Institute of Colloids and Interfaces (MPIKGF), Research Campus Golm, Potsdam 14424, Germany* **2.** *Laboratory of Self-healing Nanomaterials (ICSM), UMR 5257 centre de Marcoule, Bagnols sur Ceze 30207, France*

e-mail: philippe.makowski@mpikg.mpg.de

It was early recognised, that early transition metal carbides and nitrides featured catalytic activities similar to the ones of platinum group metals (PGMs). Such ceramics thus attracted a lot of attention, especially from people interested in oil refining and petrochemistry. The use of urea as either a carbon or a nitrogen source enabled the synthesis of various early transition metal nitrides and carbides nanoparticles (TiN, Mo_3N_2, WN, NbC, Mo_2C and W_2C). The ability of these particles to promote the alkylation of ketones with alcohols was tested on benzyl alcohol and acetophenone at 150°C for 20h. All the tested ceramics proved able to catalyse the formation of 1,3-diphenyl propenone. TiN featured the highest activity and was further tested for more difficult alkylations. Interestingly, group VI ceramics promoted Friedel-Crafts reactions. This ability was also studied.

10:15 Oral

Thermal Stability of TiO_2 Nanoparticles with Controlled Size and Shape: Toward Use of a New Catalyst Supports

Celine Perego[1], Renaud Revel[1], Olivier Durupthy[2], Sophie Cassaignon[2], Jean-Pierre Jolivet[2]

1. *IFP-Lyon, Rond-point de l'echangeur de Solaize, BP 3, Solaize 69360, France* **2.** *Chimie de la Matiere Condensee de Paris UPMC (CMCP-UPMC), 4 place jussieu, Paris 75252, France*

e-mail: celine.perego@ifp.fr

Transition alumina are largely used as catalyst supports in refining and petrochemicals. However, titanium dioxide TiO_2, was shown to display higher catalytic activity as a support of MoS_2 in desulphurization process. The low surface area generally obtained for these materials and the relatively poor thermal stability observed restrain their use. Therefore, the synthesis of smaller particles (10-100 nm) and the preservation of their size during thermal treatment should enhance catalytic performances. Indeed, these properties strongly depend on the surface properties of the support, which are closely related to the structure, the size and the shape of particles.

Previous studies have shown that it was possible to synthesize nanoparticles of TiO_2 (anatase, brookite and rutile) with controlled size and morphology. In the present work, the synthesis parameters have been tuned in order to mainly obtained pure phases and to increase the synthesis volume (for a possible industrial application). For each pure polymorph, several morphologies in nanometric scale have been synthesized. The thermal stability of these particles, depending of their structure, size and shape, and specific adsorption of ions was studied. We show that the evolution of nanoparticles size and the temperature of phase transition depend not only on the initial structure, but also on the morphology and the nature of adsorbed species. Crystal growth mechanisms were investigated through TDA/TGA, XRD, and HRTEM. Finally, we expect that this study will provide a promising titanium oxide catalyst supports.

Coffee break

Tuesday morning, 16 September, 10:30
Main Hall

Parallel Session

Tuesday morning, 16 September, 11:00
Room 134

11:00 Oral

Formation, functionalisation and formulation via continuous hydrothermal synthesis

Ed Lester, Helen Hobbs, Sandy Gordon

University of Nottingham, Nottingham, United Kingdom

e-mail: edward.lester@nottingham.ac.uk

At present there are few commercially viable methods for producing sufficient quantities of *high quality* dispersed and formulated nanoparticles to supply the mass market demands of applied nanotechnology.

Continuous hydrothermal synthesis (cHS) sidesteps some of the problems associated with nanomaterial manufacture; it is a relatively simple route that is inherently scalable as it is a continuous process, not batch, and a chemically much more benign method of producing high quality nanoparticles. cHS produces nanoparticulate materials by mixing sub-, near or supercritical water with a solution of a metal salt. The drawback for the technology has been in controlling the mixing of the two fluids.

The authors have developed and patented a nozzle reactor (reactor d) which uses a pipe in pipe counter current mixing arrangement. This reactor does not block and has been used to make over 35 different nanomaterials from nano silver (at 12nm), zirconia (4nm) to YAG:Eu (50nm), Fe2O3 (4nm). Control over particle shape, morphology and phase has also been demonstrated e.g rods, spheres, plates for different materials. Recent work has been focussed on the addition of capping agents during particle production and the scaling up of the reactor with a view to producing tons/per annum. A scale up reactor, capable of producing kg's/day quantities has been commissioned which uses the same reactor design.

Promethean Particles is a new spin out company from The University of Nottingham, and is using the IP developed in nanomanufacturing at Nottingham to service the needs of customers interested in controlled, formulated nanomaterials for products and applications, both industrial and academic.

11:30 Oral

Onion-type vesicular microreactors for a new bio-inspired route to metal nanoparticle-based heterogeneous catalysts

Damien P. Debecker[1], Chrystel Faure[2], Marie-Edith Meyre[2], Alain Derré[2], Eric M. Gaigneaux[1]

1. *Université catholique de Louvain, unité de catalyse et chimie des matériaux divisés (UCL), Croix du Sud, 2/17, Louvain-la-Neuve 1348, Belgium* **2.** *Centre de Recherche Paul Pascal (CRPP), niversité de Bordeaux 1, Avenue du Dr. Albert Schweitzer, Bordeaux 33600, France*

e-mail: damien.debecker@uclouvain.be

Chemical reactions often require metal-based catalysts which usually demand small and stable metal particles. However, classical preparation methods often imply a thermal treatment during which sintering phenomena are hardly controlled. Onion-type multilamellar vesicles (MLVs), mainly known for their potential applications in biotechnology, can be used for the spontaneous and controlled production of metal nanoparticles. This process has the advantage of not requiring any thermal treatment.

The possibility to use preformed and tailored nanoparticles formed through this bio-inspired route for the preparation of metal nanoparticle-based catalysts is presented here. This innovative concept[1] takes advantage of the expertise in nanobiotechnology to answer issues encountered in the field of inorganic catalysis.

The synthesis of silver nanoparticles inside MLVs was performed spontaneously at room temperature using the surfactant itself (Genamin T020) as the reductant. No thermal, chemical or electrochemical treatment was applied. Silver nanoparticle-loaded MLVs were quantitatively transferred onto a TiO_2 support and a V_2O_5/TiO_2 catalyst, as attested by TEM images, XPS and ICP-AES analysis. The method (impregnation of a colloidal suspension, evaporation under vacuum, drying) did not involve any separation of the organic matter, which only accounts for ~5% of the final mass of the fresh catalyst.

In order to validate this new preparation method, the materials were tested in the total oxidation of benzene, chosen as a model for industrial and domestic air pollutants. We evidence the activity of the Ag nanoparticles on TiO_2. A synergetic effect between the V-based catalyst and the added silver nanoparticles is also described. We finally show that small nanoparticles (~5 nm) survive relatively high temperature. A protection mechanism (vs. sintering) involving the surfactant is proposed.

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11:45 Oral

Fabrication of Metal-Shelled Coaxial Nanowires and Annealing-Induced Formation of Metal Nanoparticles for Catalytic Applications

Hyo Sung Kim[1], Hyoun Woo Kim[1], Sang Eon Park[2]

1. *Inha University, School of Materials science and engineering, 253 Yong Hyun Dong, Nam Ku, Incheon 402-751, Korea, South* **2.** *Inha University, Dept of Chem, 253 Yonghyundong, Incheon 402-751, Korea, South*

e-mail: hyosunglove@hanmail.net

In recent years, there have been great interests in the fabrication of coaxial nanocable-like one-dimensional (1D) structures, which combine the different types of nanotubes and nanowires in axial or radial directions [1,2]. Furthermore, as the demand for fabricating special nanowire structures increases, to develop the method not only for synthesizing a wide variety of nanowires but also for modifying or improving the properties of as-synthesized nanowires becomes very important. In the present study, we have fabricated the core-metal shell heteronanowires by using the sputtering technique. Metal nanostructures have attracted considerable attention from materials scientists on account of their application to many areas of fundamental and technical importance [3]. In addition, we have carried out the thermal annealing, generating metal nanoparticles on the surface of core nanowires. We have carried out experimenst for evaluating the catalytic effect of metal nanoparticles. We believe that the fabrication of metal nanoparticles on core nanowires will encourage their use in various areas including heterogeneous catalysis.

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12:00 Oral

Synthesis of vanadium doped TiO_2 nanowires: thermal stability and photoactivity for hydrogen production by water splitting.

Daniela D'Elia[1,2], Yoshikazu Suzuki[3], Marie-Hélène Berger[4], Jean-Christophe Valmalette[5], Jean-Francois Hochepied[1], Christian Beauger[2], Arnaud Rigacci[2], Patrick Achard[2]

1. *Laboratoire de Systemes Colloidaux dans le Processus Industriels (SCPI), Ecole des Mines de Paris, Paris F - 75272, France* **2.** *Ecole des Mines de Paris, Center for Energy and Processes, Sophia Antipolis 06904, France* **3.** *Institute of Advanced Energy, Kyoto University, Kyoto 611-0011, Japan* **4.** *Ecole des Mines de Paris Center of Materials EVRY, Paris 91003, France* **5.** *Universite du Sud Toulon-Var (UTV), Av. de l'université Bat.R., La Garde, Toulon 83957, France*

e-mail: daniela.delia@ensmp.fr

The most important energy challenge of the near future is to produce clean energy from renewable sources. The using of solar energy to split water in order to produce hydrogen can represent a good solution. In addition this process uses TiO_2 as catalyst, cheap, abundant and chemical stable material.

In the recent years titania nanotubes, nanowires, nanofibers, nanorods, have been investigated to create pathways, potentially enhancing electron percolation, light conversion, as well as to improve ion diffusion at the semiconductor–electrolyte interface [1].

From the pioneers works of Kasuga [2] many studies have been carried out in order to improve the performances of the 1 D titania structures. Ion doping is one of the most classical and efficient technique to avoid the fast recombination of the photo-generated electron/hole pairs and to shift the photo-response of TiO_2 into visible spectrum [3]. Particularly interesting is the effect of the introduction of vanadium in the TiO_2 lattice [4].

In this work anatase nanowires have been doped with vanadium by wet impregnation technique using $VO(acac)_2$. After calcination treatment the samples have been characterized by Xray diffraction, nitrogen adsorption/desorption isotherms applying BET model, Transmission

Electron Microscopy, HT-XRD, Infra-red and Raman spectroscopy. Photocatalytic H_2 production reaction, carried out on TiO_2 suspensions in a closed gas-circulation system using a high-pressure Hg lamp as the light source, has been also discussed.

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Lunch break

Tuesday afternoon, 16 September, 12:30
Inner Courtyards

Parallel Session

Tuesday afternoon, 16 September, 14:00
Room 134

14:00 Oral

ZnO-based thin films and membranes for applications coupled with photocatalysis

Lívia Naszályi Nagy[1,2], André Ayral[2], Zoltán Hórvölgyi[1]

1. *Budapest University of Technology and Economics, Department of Physical Chemistry and Materials (BME), Budafoki út 6-8., Budapest 1111, Hungary* **2.** *Institut Européen des Membranes, Montpellier 34095, France*

e-mail: lnaszalyi@mail.bme.hu

The concept of multifunctional materials has arisen in the scope of energy-saving strategies. Zinc oxide is an ideal candidate for the preparation of multifunctional materials due to its various intrinsic properties (unspecific sorption capacity, photoactivity under near UV light, etc). For instance, a recent article revealed a higher photocatalytic activity of ZnO under solar light in comparison that of titania. In this study, multifunctional thin films were designed and built up using ZnO-based nanoparticles prepared by different colloidal chemistry synthesis routes.

Self-cleaning and antireflective coatings were obtained with Langmuir-Blodgett (LB) technique using monodisperse sols of nearly spherical ZnO particles with 3 nm (Meulenkamp EA, J. Phys Chem. B 102 (1998) 5566) and 110-410 nm (Seelig EW et al., Mater. Chem. Phys. 80 (2003) 257) mean diameter. Mono- and multilayered LB films were prepared from identical ZnO particles. Mixed and complex LB films were also obtained from ZnO and silica particles. Optical model fitting confirmed the establishment of complex layered structures. The transmittance of glass substrate was increased (antireflective effect) in a broad range of wavelengths (visible-near infrared) depending on the size of particles, number and sequence of layers. The photocatalytic activity of the samples was interpreted as a function of availability of ZnO surface in the films.

Porous ceramic membranes were considered for coupling separation and photocatalysis. A concentrated (350 mg.L^{-1} solid content) hydrosol of core/shell silica/ZnO particles was first prepared for the deposition of membranes by dip coating or slip-casting techniques. The membrane properties investigated with a tangential filtration device showed adequacy for ultrafiltration applications. The photocatalytic activity of the membrane material was investigated from the photodegradation of methylene blue in aqueous solution and of adsorbed stearic acid.

14:30 Oral

The Na$^+$ ion diffusion effect on the photocatalytic and photoinduced super-hydrophilicity of TiO_2 sol-gel coating

Mohamed Nawfal Ghazzal, Nouari Chaoui, Alain Koch, Didier Robert

Laboratoire de chimie et méthodologie pour l'environnement (LCME), Rue Victor Demange, Metz 57500, France

e-mail: g_nawfel@yahoo.fr

TiO_2 coatings are still widely studied because of numerous potential industrial applications. Recently, it has been reported that the surface of TiO_2 becomes highly hydrophilic with a water contact angle close to 0° under ultraviolet (UV) illumination[1]. This phenomenon constitutes the physical principle at the origin of the development of antifogging mirrors[2]. Furthermore, TiO_2 under its anatase form is particularly known as an excellent photocatalyst. The combination of these peculiar wettability properties and photocatalytic performances of TiO_2 coatings allowed the development of self-cleaning glass[3,4]. In most cases, TiO_2 is grown on soda-lime glass containing approximately 14 at.% Na and other alkali elements. To study the effect of ions diffusion from the glass substrate on the photocatalytic and the photoinduced super-hydrophilic (PSH) properties of the TiO_2 photocatalyst (see figure), TiO_2 thin films were grown on three kinds of glass support (soda-lime glass (SGL), Pyrex and quartz). The TiO_2 films were characterized using XRD and scanning electron microscopy (SEM).

The poisoning effect of Na ion diffusion from the SGL to the photocatalytic efficiency of the TiO_2 coating was observed on our previous work[5]. In this study, the influence of the Na ion diffusion on the wettability conversion of TiO_2 films was investigated through the evolution of the contact angle on deliberately contaminated TiO_2 surface by the film of the stearic acid. We observe that the Na$^+$ diffusion decease the photocatalytic degradation rate of stearic acid and the wettability conversion of the TiO_2 surface. The rate of the photoinduced conversion of the TiO_2 films depend on the kinetic of the photocatalytic degradation of hydrocarbon adsorbed on the surface.

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14:45 Oral

Photoinduced properties of titanium dioxide thin films

Henryk Tomaszewski

Institute of Electronic Materials Technology (ITME), Wólczyńska 133, Warszawa 01-919, Poland

e-mail: tomasz_h@itme.edu.pl

Photocatalytic activity and surface water wettability conversion of TiO_2 thin films prepared by DC magnetron sputtering from ceramic target has been studied. Thin films were deposited at three deposition pressures. It resulted in obtaining different film microstructures.

Higher deposition pressures favourited creating more porous films with higher specific area than it happened in case of lower pressures. In both cases films were columnar in character with columns consisting of small nanograin-type creatures. Films recognized by X-ray as amorphous ones crystallised to anatase by annealing at 573-773K. It was found that deposition pressure influenced not only the initial film microstructure but the way of anatase crystallization during annealing as well. Strong preferential (001) orientation was found in case of films prepared at higher deposition pressures. To evaluate photocatalytic activity of TiO_2 films ethanol breakdown was measured. Water contact angle measurements showed that thin films were hydrophobic if stayed in dark. During UV light irradiation they converted to hydrophilic. Reaction rate and contact angle decrease rate occurred to be dependent in similar way on initial film microstructure, its crystallinity and the way of anatase crystallization.

15:00 Oral

Transparent mesoporous nanocomposite films for self-cleaning applications

Morgan Gohin, Isabelle Maurin, Thierry Gacoin, Jean-Pierre Boilot

Physique de la Matière Condensée, Ecole Polytechnique, CNRS, Palaiseau 91128, France

e-mail: morgan.gohin@polytechnique.edu

A versatile approach is studied for the elaboration of TiO_2 based photocatalytic coatings for self-cleaning applications on transparent substrates. The basic principle of the synthesis relies on the use of preformed TiO_2 colloidal particles that are further dispersed within a transparent silica binder with a mesoporous structure. Film porosity in the nanometer range is controlled by achieving the sol–gel silica condensation around self-organized micellar assemblies of a templating copolymer surfactant. The latter also acts as a stabilizer for the TiO_2 particles, thus preserving their high dispersion within the film so that excellent optical properties are maintained even for high TiO_2 loading (up to 50%).

The photocatalytic activity of the films was measured by monitoring the degradation of stearic acid deposited on the film under UV-A irradiation. Although the kinetics are found to follow a first order law over all the degradation curve, they exhibit a more complex behaviour, since the calculated rate constant k_1 values calculated for different experiments were found to decrease drastically when increasing the initial stearic acid concentration.

Studies show that such mesoporous films are at least 15 times more active than films synthesized with a microporous silica binder. Moreover, the measured quantum-yield efficiency (1.1%) is found to be among the highest reported up to now. Improved photoactivity of the films is discussed as resulting from the closer proximity between the organic molecules and the surface of the TiO_2 crystallites as well as the improved diffusion rate of water and oxygen through the interconnected pore network.

Coffee break

Tuesday afternoon, 16 September, 15:30
Main Hall

Parallel Session

Tuesday afternoon, 16 September, 16:00
Room 134

16:00 Invited oral

Towards Cleaner Vehicle Emissions: Catalyst Technologies for Today and Tomorrow

Andrew P. York

Johnson Matthey Technology Centre, Blount's Court, Reading RG49NH, United Kingdom

e-mail: ayork@matthey.com

Catalytic converters are essential for controlling harmful vehicle exhaust emissions, and are an integral part of most vehicles sold in Europe and America. Diesel vehicles provide a specific challenge due to the very lean nature of diesel exhaust. Ever tightening diesel emissions legislation will necessitate a blend of advances in engine design, electronic vehicle control systems, and catalytic devices.

In this lecture methods for tackling diesel (and lean burn) vehicle exhaust emissions using catalytic devices in production today will be presented, as well as some advances in the industry, and future requirements and challenges for tomorrow's catalysts.

The lecture will begin by addressing the systems level, where different catalytic devices are combined to give the required emissions control performance, e.g. the Continuously Regenerating Trap (CRT®), or a diesel oxidation catalyst (DOC) plus selective catalytic reduction (SCR) catalyst.

The next level of system design is to combine the catalyst and the filter function into one device, e.g. catalysed DPF (CDPF), resulting in a multi-functional catalyst; considerable space and cost savings are achievable, combined with excellent emissions control performance. Further recent developments in multifunctional emissions control catalyst design have looked at layering the individual catalysts; Isuzu's lean NO_x catalyst, and Honda's NO_x trap/SCR system will be shown. In the future, the exhaust emissions aftertreatment industry faces a number of challenges, e.g. wide array of new fuels, and new engines (direct injection spark ignition). Aftertreatment devices will be necessary in a host of new applications: locomotives, marine, and non-road mobile machinery. There will be potential for industry and academics to contribute to the design of multifunctional catalysts by i) designing/combining catalyst functions on the micro- or nano-scale, and ii) improving systems by zoning/layering catalysts in a single monolith substrate.

16:45 Oral

Molecular-Level Characterization of Ni-Mo Catalysts Supported on α-Al_2O_3 Single Crystals by Grazing-incidence EXAFS

Asma Tougerti, Xavier Carrier, Michel Che

Laboratoire de Réactivité de Surface (UPMC-CNRS), 4 place Jussieu, case 178, Paris 75252, France

e-mail: xavier.carrier@upmc.fr

A molecular-level understanding of heterogeneous catalyst preparation (deposition of a dissolved metallic salt on a metal oxide support) is a prerequisite for precise control of the final properties of these catalysts. Nevertheless, most studies of adsorption reactions are performed on high surface area oxides with a number of crystallographically different surfaces with ill-defined sorption sites. A fundamental description of sorption mechanisms is thus not possible in most cases. One way to mitigate this problem is to simplify the sorption system by using oriented single crystals that have a limited number of well-defined surface sites.

α-Al_2O_3 single crystals wafers with two crystallographic orientations (0001) et (1-102) have been used as model supports for the characterization of hydrotreating Ni promoted Mo/Al_2O_3 catalysts. Deposition of Mo^{VI} and Ni^{II} is carried out by immersing the wafers in the impregnation solution before washing and drying with a flow of N_2. Ni adsorption is carried out in the presence of a chelating ligand (ethylenediamine) with variable en/Ni ratio (1 to 3).

The samples are characterized by XPS, AFM and Grazing-Incidence EXAFS (GI-EXAFS). The latter technique is well suited for the study of surface systems due to an enhance surface sensitivity allowing to work at the low surface coverages imposed by low surface area single crystals.

Macroscopic (XPS, AFM) and molecular-scale characterization techniques (GI-EXAFS) show that the adsorption of Mo^{VI} is site-specific with no adsorption on the (0001) face since this orientation exposes only neutral surface hydroxyls. Conversely, Mo^{VI} is grafted on the most basic sites of the (1-102) face. Ni^{II} adsorption leads to the precipitation of a nickel hydroxide phase despite the presence of chelating ligands. These experiments reveal that ethylenediamine has no influence on the adsorption mode of Ni^{II} while it is claimed that the addition of this ligand improves the HDS performance of NiMo catalysts.

17:00 Oral

In operando XAS study of porous based catalysts for the selective catalytic reduction of NO with low N_2O emissions

Enrique Rodriguez Castellon[1], Mona Lisa Oliveira[2], Antonio Jimenez-Lopez[1], Ramon Moreno-Tost[1], Jose Jimenez Jimenez[1], Tiago L. Farias[2], Carla Silva[2], Alfonso Caballero[3], Juan P. Holgado[3]

1. *Universidad de Malaga (UMA), Campus Teatinos, Malaga E29071, Spain* **2.** *Instituto Superior Técnico, Lisboa 1049-001, Portugal* **3.** *Instituto de Ciencia de Materiales de Sevilla (ICMSE), Avda. Americo Vespucio, 49, Sevilla 41092, Spain*

e-mail: castellon@uma.es

One of the main disadvantages of vehicles powered with diesel engines are the emissions of nitrogen oxides and soot particles. In this context, the urea-selective catalytic reduction (SCR) process is considered to be the most promising way to decrease NOx emissions produced by the diesel heavy duty vehicles. When urea is used as reducing agent, it is hydrolised into ammonia and carbon dioxide. The ammonia so produced reacts with NO to form the non contaminating byproducts water and nitrogen. The commercial catalyst based on vanadium (a toxic element) tends to form N_2O, a noxious greenhouse gas, at high reaction tempertaures. We have recently found the natural mordenites based catalysts and porous phosphate heterostructures (PPH), with copper or iron species as active phases, are execllent for the SCR -NO using ammonia or methane as reducing agent, and the very low formation of N_2O was observed. In this communciation, this catalytic reaction was study by means of X-ray Absorption Spectroscopy (XAS) using synchrotron radiation, where the chemical environment of Cu and Fe under real operation conditions is checked, since the oxidation state of both elements during the catalytic process is a subject of many controversies. Moreover, the evolution of the chemical state duting the SCR of NO give us some answers to explain why N_2O is not formed with these catalysts, in comparison with some other systems.

17:15 Oral

Mutual Influences of Metallic and Acidic Functions in Pt Catalysts Supported on Siliceous, Silicoaluminic and Aluminic Mesoporous Oxides

Soraya Handjani[1], Eric Marceau[1], Juliette Blanchard[1], Stanislaw Dzwigaj[1], Michel Che[1], Päivi Mäki-Arvela[2], Dmitry Murzin[2], Narendra Kumar[2]

1. *Laboratoire de réactivité de Surface, CNRS UPMC (LRS), 4 place Jussieu, casier 178, Paris 75252, France* **2.** *Abo Akademi, Laboratory of Industrial Chemistry and Reaction Engineering (AA), Biskopsgatan 8, Turku 20500, Finland*

e-mail: eric.marceau@upmc.fr

This paper aims at investigating the influences that metallic and acidic functions exert on each other in mesoporous oxide-supported catalysts, and their consequences on catalysis. Three parameters are kept constant in the systems studied: Pt particles size (smaller than 2 nm), particles surface density over the support and pore size distribution centered on the same diameter (6 nm). Siliceous SBA-15 served as a reference support. Al-SBA-15 exhibiting Brønsted acidity was prepared by post-synthesis grafting of $Al(OiPr)_3$ in cyclohexane. Mesoporous alumina was synthesized using glucose as an organic additive; the Pt content was 0.5 wt% instead of 1% on SBA-15 systems, due to a twice lower specific surface area.

^{27}Al NMR, FTIR of adsorbed CO and probe catalytic tests (isopropanol dehydration, cumene cracking) showed that Pt/Al-SBA-15 is less acidic than parent Al-SBA-15. Comparison with a blank system prepared without Pt suggests a redistribution of Al atoms during Pt introduction. Upon hydration of Al-SBA-15 and thermal treatment, 25% of strong and mild Brønsted sites (Si-O(H)-Al) transform into strong Lewis sites (isolated tetracoordinated Al atoms). The introduction of Pt may thus significantly influence the acidic properties of a mesoporous support.

Liquid phase hydrogenation of cinnamaldehyde to cinnamyl alcohol was used as a test reaction. Selectivities are similar on Pt/SBA-15 and Pt/Al-SBA-15 (13% at a conversion of 70%), but the presence of acidic sites on the latter leads to higher reaction rates, possibly because desorption of reactants is facilitated on particles whose electron population is depleted (blue-shift of the CO/Pt IR band on the acidic catalyst compared with Pt/SBA-15). In contrast, Pt/Al_2O_3 exhibits both high reaction rates and the highest selectivity toward cinnamyl alcohol (44% at total conversion). A direct action of Lewis acidic sites neighbouring the particles, which may favour the adsorption of the molecules by the C=O bond, is suggested.

Wednesday, 17 September

Parallel Session

Wednesday morning, 17 September, 9:00
Room 134

9:00 Invited oral

Nanostructured oxide thin films prepared by plasma and related Methods

Agustin R. González-Elipe, Angel Barranco, Ana Borras, Juan Pedro Espinos

Instituto de Ciencia de Materiales de Sevilla (ICMSE), Avda. Americo Vespucio, 49, Sevilla 41092, Spain

e-mail: arge@icmse.csic.es

Oxide thin films prepared by plasma and other related “dry” methods are typically used for a large variety of functional applications because of their optical, electrical and/or magnetic properties. Modifications of these classical methodologies may lead to an efficient control of the nanostructure, porosity and composition of the synthesized films, thus opening new areas of applications as membranes, photo-catalysts, sensors , etc. This presentation discusses recent developments in nanostructuring processes of oxide thin films prepared by plasma or evaporation at glancing angles and about the characterization of porosity these thin films.

Different examples of SiO_2 and TiO_2 thin films illustrate the possibilities of these methods for an efficient control of the nanostructure and the use of these materials as diffusion membranes, optical sensors and/or photo-catalytic plates. The synthesis at low temperatures of nanofiber oxide films by plasma techniques is another recent development that permits the preparation of advanced materials with controlled hydrophilicity and photovoltaic device applications.

A critical issue with these nanostructured thin films is the assessment of their porosity. Total pore volume and type of pores can be determined with a quartz crystal monitor to measure the adsorption isotherms of water in the pores. Preliminary results about the surface functionalization of the internal pores of the films and their use for the tailored synthesis of new nanostructured composite materials are also presented.

9:45 Oral

Design of new hybrid titanias as efficient supports for gold catalysts

Violaine Mendez, Marlène Daniel, Stephane Daniele, Valérie Caps

Institut de recherches sur la Catalyse et l'Environnement de Lyon (IRCELYON), 2, avenue Albert Einstein, Villeurbanne 69626, France

e-mail: valerie.caps@ircelyon.univ-lyon1.fr

Supported gold nanoparticles have been shown to catalyze alkene epoxidations in the liquid phase in the presence of catalytic amounts of *tert*-butylhydroperoxide (TBHP). The Au/TiO_2 reference catalyst from the World Gold Council in particular exhibits high selectivity for the aerobic epoxidation of stilbene.[1] However, the reference catalyst is poorly dispersed within the apolar reaction medium. Improvement in the overall efficiency of the reaction is thus expected by optimizing mass transfer of the catalytic system. Here, we present the design of a new family of nanosized hybrid titanias that allows to stabilize small gold particles and enhance dispersion of the resulting catalytic powder in the reaction mixture.

First, we have synthesized new well-defined citrate-modified titanium precursors and characterized them by molecular spectroscopies. We have then used them to prepare crystalline surface-modified titania nanoparticles in an original one step, efficient, low temperature (100°C) and aqueous sol-gel synthetic methodology.[2] It leads to high and precise control of the organic loadings and a very good chemical stability of the hybrid titania powders, as shown by TG-DTA-MS, BET, XRD, FTIR characterization. These materials are then reacted with aqueous solutions of $HAuCl_4.3H_2O$ or home-made $Au(en)_2Cl_3$ at 100°C for 3 h, in the presence of tannic acid, PVA / $NaBH_4$, or NaOH / NH_4OH. Catalytic evaluation is carried out with *trans*-stilbene (1 mmol), solvent (methylcyclohexane, 20 mL), TBHP (0.05 mmol) and gold catalyst (2 mmol Au) in air (atmospheric pressure) at 80°C for 24 h.

The role of citrate content in gold deposition, particle growth (TEM), catalytic conversions and selectivities (HPLC) will be discussed. We will also show how the resulting catalytic powders get dispersed within the apolar liquid reaction medium and increase turnover numbers.

References

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10:00 Oral

1D nanostructures of hydrated TiO_2 for CO oxidation

Anastasia V. Grigorieva[1], Eugene A. Goodilin[1], Lyudmila E. Derlyukova[2], Tatyana A. Anufrieva[2], Yuri A. Dobrovolskii[2], Yuri D. Tretyakov[1]

1. *M.V. Lomonosov Moscow State University, Vorobyevy gory, Moscow 119992, Russian Federation* **2.** *Russian Academy of Sciences, Institute of Problems of Chemical Physics (IPCP RAS), Institutskii pr., 18, Chernogolovka 142432, Russian Federation*

e-mail: anastasia@inorg.chem.msu.ru

One dimensional (1D) nanostructures are of interest because of their extraordinary functional properties originated from their structural peculiarities. Nowadays an application of individual nanoparticles in micro- and nano-electronics is not a routine procedure yet, a detailed study of individual particles behaviour is limited by instrumental facilities.

Titanium dioxide nanotubes and nanorods were obtained in a form of bundles. Both the materials could serve as a porous matrix, for instance, for drinking water filtration, water refinement in industry etc. These materials demonstrate high efficiency in photochemical processes, in catalysis, in electrochemical current sources, in solar cells. Nanotubes and also nanorods are the materials possessing high deficiency, this fact results in oxygen transport improvement and should improve the catalytic activities of nanomaterials in comparison with bulk anatase and rutile.

We studied titanium dioxide nanotubes and nanorods as semiconductor catalysts in the CO oxidation process. The CO/O_2 ratio was varied from 0.75 to 4, the CO concentration we varied in a range of 1 – 25 %. We found an increase of initial conversion temperature with increasing the CO/O_2 ratio. At high total concentration of reactants the 100% conversion level was not achieved on heating up to 300°C. The investigating catalytic process could be described due to the Mars-van Krevelen mechanism.

The degradation of 1D nanostructures in the studied process is a result of dehydratation. The structures of nanotubes and nanorods changes above 500^oC resulting in O-H group concentration decrease and growth of Ti^{3+} concentration due to XPS spectra, recrystallization. The specific surface area of nanorods increases in this process with the advent of cavities appearance. The diameter of cavities was about 5 – 10 nm.

10:15 Oral

Well-Defined Single-Site Heterogeneous Ir-NHC Catalysts for H/D Exchange Reaction via Surface OrganoMetallic Chemistry on Hybrid Organic-Inorganic Materials

Tarun Maishal[1], Johan Alauzun[2], Jean-Marie Basset[1], Christophe Coperet[1], Robert J. Corriu[2], Erwan Jeanneau[3], Ahmad Mehdi[2], Catherine Reyé[2], Laurent Veyre[1], Chloe M. Thieuleux[1]

1. *Chimie, Catalyse, Polymère, Procédé, UMR CNRS CPE UCBL (CCPP), 43 bd du 11 Nov. 1918, Villeurbanne 69616, France* **2.** *Institut Charles Gerhardt, CC15, Place eugène Bataillon, Montpellier 34095, France* **3.** *UCBL, Centre de Diffractometrie Henri Longchambon, 43, Bd du 11 Novembre 1918, Villeurbanne 69616, France*

e-mail: thieuleux@cpe.fr

A well-defined Ir-NHC-based heterogeneous catalyst was synthesized by Surface Organometallic Chemistry on mesostructured hybrid organic inorganic silica. This Ir-NHC catalyst was obtained in three key steps: i) synthesis of a mesostructured material with regularly distributed imidazolium units, ii) formation of Ag-NHC moieties and iii) transmetallation with $[Cp^*IrCl_2]_2$, each step being fully controlled and supported by several analytical techniques (XRD, BET, elemental analysis and solid state NMR). This Ir-NHC material is highly active in H/D-exchange reaction of acetophenone with methanol-d_4. Noteworthy, this catalytic material has catalytic performances similar to homogeneous homologues with the advantage of being easily recyclable.

Coffee break

Wednesday morning, 17 September, 10:30
Main Hall

Parallel Session

Wednesday morning, 17 September, 11:00
Room 134

11:00 Oral

Controlled Pore Structure Synthetic Carbons for Use as Catalyst Supports

Steve Tennison

MAST Carbon Technology Ltd (MAST), Henley Park, Guildford Surrey GU32AF, United Kingdom

e-mail: steve.tennison@mastcarbon.co.uk

Powdered activated carbons are widely used as liquid phase catalyst supports in batch stirred reactors. The small size of ~30microns is required to achieve acceptable mass transfer properties. However the small size tends lead to problems in the recovery of the catalyst from the product. They also have poor attrintion resistance leading to further problems in catalyst recovery. The carbons to be described in this paper were developed in two EU sponsored projects specifically to overcome the problems of mass transfer and mechanical stablity.

These novel carbons are produced from a phenolic resin precursor via a patented dispersion process that allows the production of bead materials with a mean particle size between around 20 microns and 2mm diameter. The beads have high crush strength, even at very high porosities, and very high attrition resistance. The beads also have a precisely controlled micropore structure with a mean pore size of ~1nm with surface areas that can exceed 2500m2/g allowing the production of highly dispersed metal cataysts. These carbons also have a unique surface structure that allows the surface chemistry to be varied between acidic and basic and across a wide range of different types of surface oxide compositions. This permits a unique degree of control of the metal dispersion via different preparative routes.

The most important characteristic of these carbons is their mesopore structure which can be tailored to give mean pore sizes between 2 and 200 nm. Studies have shown that due to this "transport" pore structure catalyst particle sizes of of several hundred microns can now be used with no loss in performance. This allows much easier catalyst recovery whilst the improved mechanical properties prevent losses due to attrition. The use of these larger beads can also now allow the use of novel reactor geomtries.

The prodution, properties and catalyst performance of these novel carbon supports will be discussed.

11:30 Oral

Synthesis and Acid Catalysis of Cellulose-Derived Carbon-Based Solid Acid

Satoshi Suganuma[1], Keiko Ichikawa[1], Masaaki Kitano[2], Kiyotaka Nakajima[1], Hideki Kato[1], Shigenobu Hayashi[3], Michikazu Hara[1,2]

1. *Materials and Structures Laboratory, Tokyo Institute of Technology, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan* **2.** *Kanagawa Academy of Science and Technology (KAST), 3-2-1 Sakado, Takatsu-ku, Kawasaki 213-0012, Japan* **3.** *National Institute of Advanced Industrial Science and Technology (AIST), Central 5, 1-1-1 Higashi, Tsukuba, Ibaraki 305-8565, Japan*

e-mail: suganuma.s.aa@m.titech.ac.jp

Carbon-based solid acid, amorphous carbon consisting of graphene sheets with sulfonic acid groups, functions as an efficient catalyst for liquid-phase acid catalyzed reactions. In the present work, the catalysis-related structure has been studied. Structural analyses by solid-state NMR and Raman spectroscopy revealed that the carbon material consists of nanosize-graphene sheets (~ 1.2 nm) with high densities of $–SO_3H$ (1.5 mmol g^{-1}) and phenolic OH groups (5.4 mmol g^{-1}) in addition to -COOH. The acid catalysis of the carbon material was demonstrated through the esterification of acetic acid with ethanol and the hydrolysis of cellobiose. The catalytic activity of carbon-based solid acid was comparable to those of conventional SO_3H-containing solid acid (Nafion and Amberlyst-15). Carbon-based solid acid could be readily recovered by decantation or filtration, and reused after simple water-washing treatment without decrease in activity. In the case of the hydrolysis of β-1,4-glucan of cellobiose, the carbon material exhibited much higher catalytic performance than the tested conventional solid acid catalysts: the yield of D-glucose by using the carbon material exceeded five times those of Nafion and Amberlyst-15. Such high catalytic activity of the carbon material can be attributed to the effect of graphene sheets in the carbon material, which bear OH and COOH in addition to SO_3H.

11:45 Oral

Reversed particle size effect for Pt on carbon nanofibers in the cinnamaldehyde hydrogenation

Arie J. Plomp[1], Heli Vuori[2], Outi Krause[2], Krijn P. De Jong[1], Johannes H. Bitter[1]

1. *Inorganic Chemistry and Catalysis, Utrecht University, Sorbonnelaan 16, Utrecht 3584CA, Netherlands* **2.** *Helsinki University of Technology (TKK), Helsinki 02015-TKK, Finland*

e-mail: a.j.plomp@uu.nl

Pt on carbon nanofibers (CNF) is one of the most active catalysts for the selective hydrogenation of cinnamaldehyde (CALD), however the selectivity towards the desired cinnamyl alcohol (CALC) is low [1]. Several studies showed that catalysts with increasing Pt particle size result in a higher selectivity to CALC [2-6]. This was also found for Pt on carbon, however Pt particle sizes were varied by applying heat treatments [3, 4]. For these catalysts, heat-treatments also decreased the amount of oxygen surface groups, which can significantly affect the catalytic behavior [1]. Therefore we studied the hydrogenation of CALD over Pt on CNF which differed independently in their metal particle sizes and amount of oxygen surface groups. Pt was deposited on CNF containing oxygen surface groups, resulting in particle sizes of either 2-3 nm (synthesized using homogeneous deposition precipitation) or 3-5 nm (synthesized using atomic layer deposition). The oxygen surface groups were removed largely via heat-treatments in inert conditions, while Pt particle sizes remained unaltered. Pt on CNF with oxygen surface groups showed an expected particle size effect, i.e. larger particles resulted in the highest selectivity to CALC. After removal of the oxygen surface groups the order of selectivity changed, i.e. the highest selectivity to CALC was found for the smallest particles. A model explaining this effect will be discussed. On a non-polar, i.e. no oxygen containing support, the adsorption of the phenyl ring is favored resulting in the direction of the C=O double bond to the metal for small particles giving rise to high selectivities.

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12:00 Oral

Catalytic activity studies on copper oxide nanoparticles decorated MWNTs

Praveen Martis, Antonio Fonseca, Narasimhaiah Nagaraju, Zineb Mekhalif, Joseph Delhalle

Laboratory of Chemistry and Electrchemistry of Surfaces, Univesity of Namur (FUNDP), Rue de Bruxelles, 61, Namur 5000, Belgium

e-mail: praveen.martis@fundp.ac.be

Carbon nanotubes (CNTs) have become one of the most important materials in the field of nanoscience and nanotechnology because of their exceptional properties that make them suitable for many potential applications as breakthrough materials for energy storage, electronics and catalysis. CNTs have been extensively used as supports for various nanoparticles such as TiO_2, SiO_2, Fe_3O_4, CdS, Au, Pd, Pt, and Ag.

Among various metal oxide particles, increasing attention has been focused on copper and copper oxide nanoparticles due to the redox chemistry, extraordinary electrical, thermal, catalytic properties. Our interest in this work is the deposition of copper oxide nanoparticles on oxygen-functionalized multiwalled carbon nanotubes (MWNTs) for catalysis. Deposition was performed using two salts of copper, namely: copper (I) phenyl acetylide and copper (II) acetate monohydrate. MWNTs are oxygen-functionalized by different oxidizing agents such as $KMnO_4$, HNO_3, and 3:1 H_2SO_4 and HNO_3. The oxidized CNTs have been characterized by XPS and TEM to know the extent of oxidation and the structural stability of the CNTs after the treatment.

Different methods have been followed to deposit copper oxide nanoparticles on oxidized MWNTs such as impregnation, mechano-chemical and polyol process. They have been characterized by TEM, XPS, FE-SEM and XRD. Our studies have shown that copper oxide nanoparticles are homogeneously decorated on the MWNTs. We have succeeded in decorating copper oxide nanoparticles on MWNTs in the range of 20 to 80nm. In some cases even smaller copper oxide nanoparticles are seen, moreover the deposition has been observed to be homogeneous.

Preliminary experiments on the prepared catalysts have indicated catalytic activity in N-formylation reactions.

Acknowledgments. FUNDP and the FNRS for the financial support

12:15 Oral

Synthesis of carbon nanostructures on foils

Estelle Vanhaecke, De Chen, Magnus Rønning

Norwegian University of Science and Technology (NTNU), Trondheim N-7491, Norway

e-mail: estelle.vanhaecke@chemeng.ntnu.no

Carbon nanotubes are studied for their potential applications in energy storage, particularly electrochemical supercapacitors with high power and high energy density applications. The explanation for this behaviour is due to their extremely high surface area to volume ratio as well as their chemical and mechanical stability. They also present a great interest as electrodes for many applications including fuel cells, electrocatalysis and chemical/biological sensing since the carbon nanotube surface easily can be modified either by physisorption or by covalent functionalization. CNTs are synthesized by the CCVD process, where you can have a selective growth on various substrates due to the cost-effectiveness stability and the repeatability of the process.

When manufacturing the carbon nanotube as the electron source, two methods are currently used. Either it is possible to print the material made into a paste or to allow the material to grow directly on the substrate.The former method is easy in processing but it is limited to making high-resolution panels. Moreover there are some problems; a) it is difficult to form the nanotubes perpendicular to the substrate, b) it is necessary to remove the residual material like binder, and c) it is difficult to keep the good uniformity and high density of the emission sites. On the other hand, the latter can easily be achieved by the selective growth, by patterning a catalyst metal layer. However there still remain several challenges; a) a limited choice of substrate materials due to the high growth temperature and, b) is it difficult to keep uniformity over the large area (1).

The aim of this work is to grow CNTs directly on electrodes, such as foils of graphite, stainless steel and titanium foils in order to minimize the contact between the active material and the current collector and also to simplify a possible electrode fabrication process.

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Lunch break

Wednesday afternoon, 17 September, 12:30
Inner Courtyards

Parallel session

Wednesday afternoon, 17 September, 14:00
Room 134

14:00 Oral

Electron-beam induced deposition of metal catalyst arrays

Heinz D. Wanzenboeck, Gottfried Hochleitner, Peter Roediger, Emmerich Bertagnolli

Vienna University of Technology Institute for Solid State Electronics (FKE), Floragasse 7/1 E362, Wien 1040, Austria

e-mail: Heinz.Wanzenboeck@tuwien.ac.at

A focused electron beam of a scanning electron microscope has been utilized to directly deposit metal structures acting as catalyst for Si-nanowire growth. Synthesis of silicon nanowires is perfomed by vapor-liquid-solid growth catalysed by gold nanoparticles. Conventional approaches rely on blanket layers of metal island films or colloid suspensions for introducing the catalytic sites to the surface. With electron-beam induced deposition for the first time the synthesis of catalytic areas was accomplished by locally confined deposition of the catalytic metal. Direct deposition of material was performed by local decomposition of a metalorganic gold precursor utilizing a focused electron beam. This maskless, resistless technique allows to custom-tailor the density and geometry of catalytic sites simply by scanning the focused electron beam. The optimum process parameters (scan parameters, precursor pressure) were investigated. The catalytic sites were designed utilizing a pattern generator for scanning the beam. Images of the resulting features will be shown and the resulting Si nanowire growth will be discussed. The potential of electron-beam induced deposition of catalyst arrays for other nanostructure synthesis will be discussed.

14:30 Oral

Nanochannels Fabrication Using Kirkendall Effect

Aurelian Marcu[1], Takeshi Yanagida[2], Tomoji Kawai[2]

1. *National Institute for Lasers Plasma and Radiation Physics (INFLPR), Atomistilor 111, Bucharest -, Romania* **2.** *Osaka University. ISIR., 8-1, Mihogaoka, Ibaraki,, Osaka 567-0047, Japan*

e-mail: marcu@ifin.nipne.ro

Nanochannels fabrication is a present aim in many nanotechnology applications. There are many approaches concerning both Top-Down and Bottom-Up techniques. However, for diameters less than 10 nm the Bottom-Up approach seems the only reliable approach. The Kirkendall effect is one of the most successful methods for nanochannels fabrication using spinel material synthesis process.

We report here investigations on nanochannels fabrication by Kirkendall effect using iron oxide (hematite) layer on MgO and ZnO nanowires. Pulsed Laser Deposition (PLD) technique and Vapor-Liquid-Solid (VLS) method have been used for nanowires growth. Iron oxide shell layer deposition has been also made by PLD with various ambient deposition conditions. Traces of nanochannels/nanopores formation have been mainly recorded for amorphous shell layers deposited at room temperatures. Some particularities for diffusion process could be noticed for each nanowire material. Some properties analysis toghether with a comparisons with the alumina shell layer case are also presented.

14:45 Oral

New basic catalysts obtained from layered double hydroxides nanocomposites

Redouane Chebout[1,2,3], Géraldine Layrac[1], Didier Tichit[1], Akila Barama[2], Bernard Coq[1]

1. *Institut Charles Gerhardt, CC15, Place eugène Bataillon, Montpellier 34095, France* **2.** *Université des sciences Houari Boumedienne (U.S.T.H.B), Bp N°9 El AliA Bab Ezzouar, Alger 16141, Algeria* **3.** *Centre de Recherche Scientifique et Technique en Analyse Physico-Chimique (CRAPC), BP248, Alger RP. Alger 16004,Algerie, Alger 16004, Algeria*

e-mail: didier.tichit@enscm.fr

Mixed oxides obtained from Layered Double Hydroxides (LDH) precursors exhibit basic properties giving rise to very efficient catalysts for syntheses of fine chemicals. Until now their properties have been mainly tailored through the activation temperature and the composition of the LDH. Alkaline, alkaline-earth or La^{3+} cations, particularly interesting to reach high basic levels, cannot be introduced in the brucite-like layers of LDHs. This work presents an original approach to avoid this drawback going through the nanocomposite route. Nanocomposites precursors have been prepared by intercalation of host Mg/Al LDH with negatively charged guest colloids. These latter are obtained by complexation of La^{3+} with strong complexing agents (citrate, edta). The intercalation degree, the composition of the colloids and the activation temperature allow to finely tune the basic properties of the mixed oxides catalysts. This has been put into evidence by physico-chemical characterizations and the reaction test of methylbutynol (MBOH) conversion. A correlation is found between the strength of the basic sites measured by microcalorimetric adsorption of CO_2 and the average charge on the oxygens calculated from Sanderson's theory of electronegativity. The basic character of the catalysts is confirmed by the catalytic conversion of MBOH, leading to acetone and acetylene. The performances of the catalysts obtained from the nanocomposite precursors, higher than those obtained with the mixture of Mg(Al)O and lanthanum oxide, resulting from the decomposition of coprecipitated Mg/Al/La LDHs, show that a synergy between the different cations is achieved using the new nanocomposite precursors.

15:00 Oral

Catalytic degradation of polyethylene: catalytic behaviour of parent restructured and pillared clays towards metal-exchanged derivatives.

Elisabetta Borsella, Giorgio Perez, Anthony A. Tomlinson, Patrizia Cafarelli, Adriana De Stefanis

Istituto per lo Studio dei Materiali Nanostrutturati (ISMN-CNR), Monterotondo, Roma I-00016, Italy

e-mail: elisabetta.borsella@ismn.cnr.it

The catalytic cracking of medium density polyethylene was carried out on modified (restructured, pillared, and/or metal exchanged) clays. It has been oserved that the spectra of the products depend on the clay used (montmorillonite and beidellite, pure montmorillonite, or saponite), on the pillars (alumina and iron-aluminium-oxides) and on metal exchange, if any.The pyrolysis of PE is known to follow the random chain scission route, resulting in mainly oligomers and dimers leading, depending on the catalyst used, to higher aliphatics and/or aromatics. The extensive screening on PE cracking has evidenced a major difference between montmorilonite and saponite based materials. Either pillared or restructured montmorillonite ones show production of aliphatics, meanwhile the saponite-based that of aromatics. These latter have the same behaviour of the H-ZSM-5. Zn-exchanged zeolites are known to promote propene cyclisation and in general to favour aromatisation routes. The active zinc species has been identified with $Zn(OH)^+$ bond to Brönsted acid sites and displaying Lewis acidity. ZnO crystallite are inert and present outside the catalyst framework. The formation of the active species can be correlated to the acidic sites present on the different catalysts frameworks. Considering the temperature (300°C) utilised, the presence of dominant Brönsted acidity of different force can be claimed for the results on montmorillonites. In confirmation of this the Zn-exchange (which gives Lewis acidity) gives an inversion of products on FAMO and HMO and to a lesser extent on K10®, known to contain both acidities. On the contrary the aromatics production on saponites should be ascribed to the presence of Lewis acidity, in which case the Zn-exchange leads to inactive ZnO crystallite presence hindering the access and decreasing aromatics production. AZA, produced from a bentonite (mixed montmorillonite beidellite) shows an intermediate behaviour.

Coffee break

Wednesday afternoon, 17 September, 15:30
Main Hall

Joint Poster Session 2

Wednesday afternoon, 17 September, 16:00
Main Hall

Thursday, 18 September

Parallel symposia

Thursday morning, 18 September, 9:00
Room 134

9:00 Invited oral

Resolving Catalytic Phenomena at the Atomic Scale: anchoring metal nanoparticles on single crystal titania.

Michael Bowker

Cardiff University, School of Chemistry, Park Place, Cardiff CF103AT, United Kingdom

e-mail: bowkerm@Cardiff.ac.uk

Heterogeneous catalysis is usually accomplished with materials in nanoparticulate form, and in this paper I will briefly review recent approaches to understanding catalytic processes and materials using surface science methods. This approach involves the fabrication of ultra-nanoparticulate model catalysts using MVD (metal vapour deposition) and MOCVD (metal-organic chemical vapour deposition) to form particles in the size range 1-10 nm. which can be imaged at very high spatial resolution (and in some cases at atomic resolution) using STM (scanning tunnelling microscopy). I will mainly focus on a system which we have used for anaerobic photocatalytic hydrogen production, namely Pd/TiO_2 powdered catalysts, and will describe a surprisingly strong dependence of the rate upon loading of the metal. Using well-defined materials fabricated in UHV, we have resolved a number of important catalytic phenomena using STM and other techniques, including:-

The Mechanism of Oxidation and Reduction of Titania. We will show that the main species involved in these processes is interstitial Ti^{3+} , which diffuses into the bulk after oxygen loss during high temperature thermal treatment, and which returns to the surface in an oxidising environment.

Spillover and Oxygen Storage. We have identified oxygen spillover from Pd nanoparticles supported on single crystal TiO_2 as a ring of material extending about 3nm. from the edge of the nanoparticles onto the support surface. Growth of TiO_2 layers around the Pd nanoparticles occurs due to the conversion of Ti^{3+} on the support to Ti^{4+}, by transport of interstitial Ti^{3+} from the bulk to the surface at temperatures > 300ºC. This is determined by *high temperature STM*.

SMSI. The strong metal-support interaction is resolved at atomic resolution as an ‘alloyed’ surface layer of Pd:Ti. The Ti is oxidised , but is probably only in the +2 state (by XPS).

9:45 Oral

New three-dimension structured photocatalytic foam media for use in traversing-flow structured-bed photoreactors

Shabnam Hajiesmaili, Sébastien Josset, Dominique Bégin, David Edouard, Cuong Pham-Huu, Nicolas Keller, Valérie Keller

CNRS, ULP, Laboratoire des Matériaux, Surfaces et Procédés pour la Catalyse (LMSPC), 25 rue Becquerel, Strasbourg 67087, France

e-mail: shabnam.hajesmaili@gmail.com

It is thought that an important obstacle in the development of highly efficient photocatalytic reactors is related to the establishment of effective reactor design as demanded by industrial and commercial applications.

The seep flow annular reactor with an uniform photocatalytic coating on the internal surface of the external tube, is actually a widely used lab-scale reference photoreactor, which benefits from a very good direct illumination by an inner lighting. However, this photoreactor suffers strongly from a low contact surface between the reactant flow and the exposed photocatalytic coating, which limits its use to low lab-scale air flow rates. Therefore new photocatalytic media and/or their associated photoreactor designs have to emerged, especially to be used in high flow rate real conditions.

This talk reports on the design of a new 3D-structured photocatalytic media, consisting in 3D alveolar foams supporting a TiO2 photocatalyst, and leading to design a new 3D-structured photocatalytic bed reactor working in a traversing mode. This photocatalyst benefits from a good illumination, and its 3D-designed alveolar structure allows the reactor working in a traversing mode with a highly improved contact surface, whereas it avoids detrimental pressure drops when working at high flow rates.

The target reaction for evidencing the interest of using this 3D-structured traversing-flow reactor compared to a conventional annular seep flow one is the gas-phase photocatalytic oxidation of methanol in dry condition.

Characterizations of foam-based supports, notably performed by light transmission evaluation through the foam, SEM and pressure drop measurements, allowed the impact of both chemical nature and alveolar size of the 3D foams to be shown, for highlighting the interest of using 3D-structured alveolar foam-based photocatalytic materials and of designing derived traversing-flow photocatalytic bed reactors.

The SICAT company is greatly thanked for supporting the study.

10:00 Oral

Optimization of the decolorisation parameters of wastewaters resulting from the process of dyeing flowers

Edison H. Gil-Pavas, Miguel A. Gómez-Garcia

UNIVERSIDAD EAFIT (EAFIT), CARRERA 49 N. 7 SUR 50, Medellín 3-300, Colombia

e-mail: egil@eafit.edu.co

This study investigates the treatment of the wastewaters resulting from the process of dyeing flowers. In some local cases for growing flowers near to Medellín, Colombia, wastewater color was found to be one of the main problems in meeting local effluent standards. Wastewaters were treated by photodegradation process (which includes photocatalysis) to obtain the degradation of the mixture of dyes and organic matter in the wastewater. A multifactorial experimental design was proposed, including as experimental factors three variables: pH, catalyst concentration (TiO_2) and hydrogen peroxide concentration (H_2O_2). Results reveal that, at optimised variables values, it is possible to reach a 99% reduction of dyes, a 76,9% of mineralization (TOC) of and a final biodegradability of 0,834. Kinetics analysis allows proposing a pseudo first order reaction for reduction, mineralization of biodegradability process.

10:15 Oral

Photocatalytic One-pot N-alkylation of Nitroaromatic Compounds Using Pt/TiO_2

Amer Hakki, Ralf Dillert, Detlef Bahnemann

Leibniz University Hannover, Institute of Technical Chemistry, Callinstrasse 3, Hannover 30167, Germany

e-mail: amerhakki@iftc.uni-hannover.de

N-alkylarylamines are important intermediates in the production of many compounds. However, traditional methods for secondary amine formation are often problematic because of harsh reaction conditions, generally poor yields, and/or low chemical selectivity.

We have employed photo-platinized TiO_2 nano-sized particles as a photocatalyst for the one-pot synthesis of N-alkylarylamines from five nitro aromatic compounds (*o*, *m*-, *p*-nitrotoluene, 5-nitro-*m*-xylene, and *p*-nitrostyrene) and ethanol through the illumination of Ar-purged suspensions of this catalyst in ethanolic solutions containing the nitro aromatic compounds.

GC/MS analysis of the UV(A)-irradiated mixtures showed a gradual conversion of the nitro aromatic compounds to N-alkylarylamines during illumination time. The produced N-alkylarylamines can be further transferred by prolonged irradiation time into N,N-dialkylarylamines. The products were identified by comparing the molecular ion and mass fragmentation pattern with those reported in the GC/MS library and/or with those of the original compounds that have been synthesized by independent methods. The N-alkylarylamines have also been obtained when *p*-nitrotoluene react with other alcohols (n-propanol, n-butanol).

The reaction mechanism has been proposed, depending on the detected intermediates, as follows: (1) the nitro aromatic compound is reduced by the photogenerated electrons in the conduction band or with those which were trapped by the Pt deposits on the semiconductor´s surface to an aromatic amine; (2) in the meantime the alcohol is dehydrogenated to an aldehyde consuming the photogenerated holes in the valance band of the illuminated TiO_2; (3) the aromatic amine reacts with aldehyde to form a Schiff base; (4) the Schiff base is hydrogenated on the Pt nanoparticles loaded at the surface of TiO_2 yielding N-alkylarylamine; (5) the latter react with the produced aldehyde forming N,N-dialkylarylamine.

Coffee break

Thursday morning, 18 September, 10:30
Main Hall

Parallel Session

Thursday morning, 18 September, 11:00
Room 134

11:00 Oral

Electrocatalytic Water Splitting Biomimicking Molecular Catalyst on Electrode Surface

Khurram Saleem Joya

Leiden Univ., Leiden, Netherlands

e-mail: khurramjoya@yahoo.com

In recent years, renewable energy resources and global environmental problems have become an increasingly vital and burning subject both in political and scientific sectors. Fossil fuels are the principle source of energy for transportation. On the other hand, chief source of CO_2 emission is the burning of fossil fuels. Fuel cell powered electricity and transportation will most probably be the future to solve addressed problems but there is a big difficulty to generate cheap and pure clean fuels like hydrogen for such systems. Best possibility is to utilize solar energy for the production of hydrogen from water. At present, there is no efficient system available that makes use of solar energy effectively to produce hydrogen from water. Photosynthesis is an excellent model for an artificial solar energy conversion system to clean fuel and oxygen evolving complex (OEC). Getting inspiration from nature, there is a continuous effort to design an artificial photosynthetic system based upon harnessing the solar energy and capable of utilizing it efficiently for water splitting to generate oxygen and hydrogen. Efficient catalytic water splitting using solar energy is a challenging research topic. Upheaval task is to establish an efficient and stable oxygen-evolving catalyst. There are many water splitting systems based on noble metal complexes and metal oxide catalysts but none of these systems have proven effective overall efficiency for water splitting. Present report describes a system based on oxo-bridged ruthenium catalyst for water splitting. Future perspective of this work is to design a model system of an active multielectron transfer site based on new robust catalytic materials for water splitting in artificial PS-II to generate clean fuel.

11:30 Oral

ZnS/carbon nanocomposites for electrocatalytic application

Michael Bredol, Michal Kaczmarek, Hubert Schulze-Dieckhoff

Fachhochschule Münster, Stegerwaldstraße 39, Steinfurt 48565, Germany

e-mail: bredol@fh-muenster.de

Electrocatalytic materials for applications in batteries, fuel cells or chemical synthesis are often composites of (conducting) carbon and nanostructured metal particles. Metals used for this purpose are typically from the family of platinum metals or nickel and therefore share

similar problems with poisoning (e.g. by CO) or deactiviation by agglomeration processes, thus often limiting the usefulness for instance of direct methanol fuel cells. In
order to overcome the inherent limitations of this class of materials, this work explores the electrocatalytic activity of semiconducting zinc chalcogenide nanoparticles, especially of those with a large band gap, in order to take advantage of their inherent chemical stability. From the literature, the photocatalytic activity of e.g. ZnS nanoparticles is well known, and thus the principal set of redox reactions that may be accelerated. Since ZnS nanoparticles are bad conductors, they have to be integrated into a carbon-based host before electrodes can be fabricated.
This work will present first data on the electrocatalytic activity of Zn(S,Se)/carbon nanocomposites in the presence of various organic materials in aqueous solution, especially alcohols. Suitable approaches to prepare the necessary semiconductor nanoparticles will be presented as well. Carbon hosts employed are varied from powder-based pastes to microporous materials, in order to acommodate the Zn(S,Se) nanoparticles in a conductive matrix. The experimental electrochemical stability window for the electrodes fabricated this way will be compared to the potential windows at which various potentially useful redox reactions are taking place. First results on ethanol oxidation on such electrodes will be presented, as derived from voltammetric analysis of the electrodes.

11:45 Oral

Fabrication and characterisation of palladium-coated porous anodic alumina membranes for gas reforming processes

Jeremy P. Wu, Ian W. Brown, Mark E. Bowden, Tim Kemmitt

Industrial Research Limited (IRL), 69 Gracefield Road, Wellington 5040, New Zealand

e-mail: j.wu@irl.cri.nz

Electrochemical and electroless deposition techniques were investigated as ways to deposit ultra-thin films of palladium on porous anodic alumina (PAA) membranes. PAA films with specific thermal and structural properties were fabricated by anodizing (~99.99%) pure aluminium in various acidic electrolytes (phosphoric, oxalic, sulfuric) under mild and/or hard anodizing conditions. Under constant voltage conditions, self-organization into a regular hexagonal pore array can be achieved. Previous work has demonstrated the thermal stability of the PAA architecture and its potential as ceramic support for thin palladium films deposited by vacuum evaporation. We have followed this up by applying and developing other deposition techniques using various plating solutions to deposit palladium with sufficient control of thickness and the mode of deposition, either blocking the pores with palladium metal and/or coat of the pore channels, leaving a continuous layer of palladium inside the pore walls.

The aim for this project is to selectively coat PAA membranes with palladium for use as membrane reactors in gas reforming processes. We propose the use of nanostructured membrane reactors to carry out gas reforming: these high surface area devices can be very efficient through enabling simultaneous reaction and selection of gas species (e.g. H2). The selection of different metal catalyst to be deposited is therefore critical to the gas selectivity of the ceramic support, which means there are huge potentials for fabricating PAA membranes with other functionalities. The thermal stability and structural integrity of the coated PAA were characterised using thermogravimetry / differential scanning calorimetry, X-ray diffractometry, and field emission scanning electron microscopy, and the methodology and the results will be presented.

12:00 Oral

Hydrogen generation through $NaBH_4$ hydrolysis on a nano Co based catalyst. Formation and evolution of a Co-B active phase.

Dariusz Świerczyński, Anthony Garron, Simona Bennici, Aline Auroux

Institut de recherches sur la Catalyse et l'Environnement de Lyon (IRCELYON), 2, avenue Albert Einstein, Villeurbanne 69626, France

e-mail: darek@chimie.u-strasbg.fr

H_2 is recognized as the environmentally desirable clean fuel of the future and a primary technical challenge is its safe generation, delivery and storage. Borohydrides can be considered as the most promising H_2 storage systems. Aqueous $NaBH_4$ solutions in contact with selected catalysts hydrolyze to H_2 gas and sodium metaborate $NaBO_2$. In terms of activity/price ratio Co-based catalysts appear as one of the best solutions. However, in spite of many research works published on the subject, the mechanism of the formation and stability of the catalyticaly active phase is still not well understood.

In this work the mechanism of the active phase formation and evolution during hydrolysis of $NaBH_4$ solution has been successfully resolved using liquid phase reaction calorimetry coupled with a volumetric measurement of the hydrogen evolved, and followed by a detailed characterization of the catalyst. This work was carried out within the framework of CASTAFHYOR project, funded by the French National Research Agency (ANR), and aimed at the understanding of catalysis and stability of the phases formed during the hydrolysis of borohydrides. The active phase, composed of nanoparticles of Co_2B, was observed to be generated in situ by reaction of the stabilized $NaBH_4$ solution using either a cobalt chloride solution or formed from different Co containing solid materials. The characterisation of the remaining catalyst after test by XRD, magnetism, TEM and TGA-MS, permitted to elucidate the evolution of the phase composition during the hydrolysis reaction. It was shown that, whatever the Co precursor was, cobalt boride was formed in situ in the presence of $NaBH_4$ solution. However the Co-B nanoparticles were not stable in alkaline solution after $NaBH_4$ consumption, and were coated by a hydroxide surface layer which retransformed into cobalt boride in the presence of additional $NaBH_4$ permitting an easy regeneration of the catalyst.

Lunch break

Thursday afternoon, 18 September, 12:30
Inner Courtyards

Parallel Session

Thursday afternoon, 18 September, 14:00
Room 134

14:00 Invited oral

Nanostructured carbons for catalysis and hydrogen storage – A Janus material

Johannes H. Bitter

Inorganic Chemistry and Catalysis, Utrecht University, Sorbonnelaan 16, Utrecht 3584CA, Netherlands

e-mail: j.h.bitter@uu.nl

Nanostructured carbons, e.g. carbon nanotubes (CNT) and carbon nanofibers (CNF) have some prominent advantages as catalyst or catalyst support compared to active carbons. Nanostructured carbons are pure, are graphitic with a high surface area, can be prepared as macroscopic strong bodies, are inert and their surface chemistry can be used to tune their behavior as a catalyst or catalyst support. In this presentation I will show that as a result of this these materials are real Janus materials i.e, on one hand the materials are excellent suited to perform fundamental catalytic studies on the other hand the physical and catalytic properties of catalysts based on nanostructured carbons are such that an application might be in reach. In the presentation I will show that CNF bodies can be obtained with a high bulk density (0.9 g/ml) and a high bulk crushing strength (1.2 MPa) which is beneficial for their use as a catalyst support. Key parameters were the metal loading of the growth catalyst and the duration of growth. Nanostructured carbon can be made active for base catalyzed reactions by replacing part of the carbon atoms by nitrogen (NCNT). In the presentation it will be shown that the activity of NCNT for a Knoevenagel condensation is related to the amount of pyridinic nitrogen incorporated in the NCNT structure which could be tuned by the synthesis parameters of the catalyst. The inertness of CNF makes them eminently suitable for fundamental catalytic studies. Here we will elaborate on the effect of particle size on the hydrogen storage properties of sodium alanate nanoparticles. It will be shown that the hydrogen desorption temperatures and activation energies decreased from 186 °C and 116 kJ.mol-1 for 1-10 µm alanate particles to 70 °C and 58 kJ.mol 1 for 1-10 nm alanate particles. In addition, decreasing particle sizes lowered the onset pressures needed for reloading to 10 bar; one of the lowest values reported sofar.

14:45 Oral

Carbon Nanowhiskers With Catalytic Features Obtained by Sol-Gel Chemistry

Gabriela Hristea, Camelia Alexandru, Valentin Teodorescu

ICPE-CA-Bucharest, 313 Splaiul Unirii, Bucharest 74204, Romania

e-mail: ghristea@icpe-ca.ro

In general, well developed methods such as laser evaporation, chemical vapor deposition (CVD) and arc discharge are used to prepare nanowhiskers/nanofibers. CVD processes imply always the presence of a metallic catalyst. In the present work, apart from common nanowhiskers or nanofiber formation, carbon nanowhiskers are obtained by using neither external carbon source nor additional metal catalyst.

Thus, resorcinol-formaldehyde (RF) solutions were prepared from resorcinol ($C_6H_4(OH)_2$) (R), formaldehyde (HCHO) (F) and sodium carbonate (Na_2CO_3) which have been used as precursors for RF carbon gels formation. It is found that nanowhiskers are formed on the surface of the RF carbon gel after a pyrolysis treatment. The results suggest that the synthesis conditions (gelation time, addition of some additives on RF initial solution, drying process etc) are responsible for the formation of carbon nanoparticles (amount and thickness).

Also, has been performed synthesis of carbon nanowhiskers doped with Pt and Pd by using the same precursors. For Pt doped carbon nanowhiskers - Pt nanoparticles deposited on carbon nanowhiskers surface have been obtained by chemical impregnation with H_2PtCl_6 followed by reduction of the carbon nanowhiskers in powder state. For Pd doped carbon nanowhiskers a sol-gel method which implies using of Pd acetate followed by a pyrolysis treatment has been applied. In a first attempt, resulted compounds have been tested as catalysts in H_2O_2 decomposition reaction. The rate of decomposition reaction was measured. Both Pt and Pd doped carbon nanowhiskers exhibit catalytic features.

Scanning and tunneling electron microscopy characterization and X-ray diffraction measurements have been done on obtained carbon nanowhiskers.

15:00 Oral

CNTs -microreactor concept for chemical processes

Izabela M. Janowska[1], Yu Liu[1], Alain Carvalho[2], David Edouard[1], Valérie Keller-Spitzer[1], Nicolas Keller[1], Marc J. Ledoux[1], Cuong Pham-Huu[1]

1. *CNRS, ULP, Laboratoire des Matériaux, Surfaces et Procédés pour la Catalyse (LMSPC), 25 rue Becquerel, Strasbourg 67087, France* **2.** *Institut de Physique et Chimie des Materiaux de Strasbourg, UMR7504, CNRS - ULP, 23, rue du Loess, BP 43, Strasbourg CEDEX 2 67034, France*

e-mail: izabela.janowska@ecpm.u-strasbg.fr

Recently, a new branch in the engineering design focused on the use of microreactor has received a huge scientific and industrial interest. The idea of chemical process miniaturisation in micro-structured reactors (channel width ranged between ten to several hundred µm) is mainly focused on process intensification and safety by providing high surface-to-volume ratio, high heat and mass transfer and isothermal operation. The aim of the present work was to develop a new catalytic microstructured reactor by filling the millimetres range channel with an array of carbon nanotubes. Such reactor allows a significant increase of the S/V ratio and eases the anchorage of the catalyst active phase through deposition onto oxygen functionalized CNTs materials. The carbon nanotubes arrays were generated by CCVD method with ferrocene as an iron-catalyst precursor and toluene as a carbon source [1]. The synthesis has been effectuated on the stainless steel plate with microchannel coated with a thin layer of SiO_2. The 2 mm thick CNTs carpet were strongly anchored onto the microchannel as no matter loss was observed after sonication for several hours. The (width x length x heigth 21 mm ′ 18 mm ′ 2 mm) channel can be filled completely with pattern of CNTs or the arrangement of CNTs can be controlled by lithography (hexagons) as well. The as-grown carbon nanotubes in the microreactor channel have subsequently been used as a nanoscopic support for the active phase. The higher catalytic efficiency was observed for CNTs-microreactor compared to the one obtained in microreactor without CNTs in the channel. Such results were attributed to the presence of the nanoscopic structure which favorize the contact surface between the reactants and the active sites.

15:15 Oral

Hydrolysis of β-1, 4 glucan using carbon based solid acid catalysts

Masaaki Kitano[1], Satoshi Suganuma[2], Kiyotaka Nakajima[2], Shigenobu Hayashi[3], Michikazu Hara[1,2]

1. *Kanagawa Academy of Science and Technology (KAST), 3-2-1 Sakado, Takatsu-ku, Kawasaki 213-0012, Japan* **2.** *Materials and Structures Laboratory, Tokyo Institute of Technology, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan* **3.** *National Institute of Advanced Industrial Science and Technology (AIST), Central 5, 1-1-1 Higashi, Tsukuba, Ibaraki 305-8565, Japan*

e-mail: hp_kitano@newkast.or.jp

Recently, a carbon-based solid acid consisting of polycyclic aromatic carbon combined functional groups such as a sulfonic acid groups has been demonstrated to act as a strong solid acid catalyst for the hydrolysis of cellulose into oligosaccharide and glucose in the presence of the water. However, the details of the amorphous carbon structure and catalysis-related structure remain to be clarified. Thus, the hydrolysis of water-soluble β-1,4 glucan, saccharide polymers linked by β-1,4 glycosidic bonds, was examined on the carbon material to understand the relationship between the catalytic activity and the structure in the present study. Carbon-based solid acid catalysts were prepared by sulfonation of amorphous carbon obtained by carbonization of cellulose, and their catalytic activities were evaluated through the hydrolysis of water-soluble β-1,4 glucan such as cellobiose and cellohexaose. The carbon material catalytically hydrolyzed cellobiose into glucose without the production of the by-products such as 5-hydroxymethylfurfural, and levulinic acid, exhibiting three times higher activity for the hydrolysis of cellobiose than the conventional solid acid catalysts. Furthermore, there was no noticeable difference in the catalytic activity and the structure before and after reaction. In the case of the hydrolysis of cellohexaose, although the tested conventional solid acid catalysts could hardly hydrolyze cellohexaose, the carbon catalyst exhibited much higher catalytic performance than the conventional solid acid catalysts. The adsorption of β-1,4 glucan on each of the solid acid catalysts suggests that the high catalytic performance of the carbon catalyst is attributed to the ability of the material to adsorb β-1,4 glucan, which does not adsorb to other solid acids.

Coffee break

Thursday afternoon, 18 September, 15:30
Main Hall

Parallel Session

Thursday afternoon, 18 September, 16:00
Room 134

16:00 Oral

Mesoporous titania prepared by monolayer grafting of Ti on SBA-15: a model support for studying the surface sulfidation of TiO_2 in HDS conditions ?

Juliette Blanchard[1], Fuxiang Zhang[1], Xavier Carrier[1], Yuji Yoshimura[2]

1. *Laboratoire de Réactivité de Surface (UPMC-CNRS), 4 place Jussieu, case 178, Paris 75252, France* **2.** *Hydrotreating Catalysis, Research center for New Fuels and Vehicle Technology (AIST), Ibaraki, Tsukuba 305-8565, Japan*

e-mail: juliette.blanchard@upmc.fr

Well-ordered mesoporous TiO_2 materials were obtained by successive grafting of $Ti(OPr^i)_4$ at the surface of a SBA-15 material used as a solid template (TiO_2-SBA-15). The successive graftings led to a gradual decrease of the surface area (from 800 initially to 420 $m^2.g^{-1}$ after 4 graftings) and pore diameter (from 65 to 42 Å). These differences can be assigned to the partial plugging of the micropores (as shown by the gradual decrease of the microporous volume) together with a coating of the mesopores with titania suggesting that the titania overlayer is ca. 10 Å thick after 4 graftings. The materials obtained after 1 and 4 graftings present the diffraction patterns and TEM images characteristic of SBA-15 materials, confirming that the SBA-15 structure is not modified whatever the number of graftings. Imaging of the material composition by energy-filtered transmission electron microscopy clearly shows that TiO_2 is homogeneously dispersed at the surface of the SBA-15 mesopores. UV-visible and XAS spectroscopies indicate the formation of small titania polymers at the surface of the support.

These materials were used for the XAS (Ti K edge) study of the modification of the titania surface (reduction and/or sulfidation) in hydrodesulfurization condition (320 to 600°C, atmospheric pressure in 5% H_2S in H_2). At temperatures commonly used for the sulfidation of the active phase (320-360°C), no sulfidation and/or reduction of the TiO_2 overlayer was observed and only a small fraction of Ti was sulfided after increasing the sulfidation temperature up to 600°C while bulk sulfidation was expected at this temperature (D. Wang et al. *J. Catal.* 209, **2002**, 266). The resistance to sulfidation is assigned to the peculiar nature of the mesoporous TiO_2-SBA-15 supports prepared by grafting Ti on SBA-15, leading to surface chemical properties differing from that of bulk TiO_2 supports.

16:15 Oral

Mesoporous Titanium Dioxide: Preparation and Catalytic Properties

Irina V. Kolesnik, Marianna V. Kharlamova, Andrey A. Eliseev, Alexey V. Lukashin, Yuri D. Tretyakov

Faculty of Materials Science, Moscow State University, Lenin Hills, Moscow 119992, Russian Federation

e-mail: kolesnik@inorg.chem.msu.ru

The aim of the present study is developing of new materials with tunable microstructure based on surfactant templated mesoporous TiO_2 and understanding of correlations between structural parameters and functional properties such as catalytic and photocatalytic activity.

Mesoporous titanium dioxide was obtained using $Ti(O^iPr)$ as titanium source and non-ionic surfactant (Pluronic P123) as a template. The samples were characterized by XRD, nitrogen sorption at 77K, XRD, TEM, UV-Vis and FTIR-spectroscopy. Mesoporous titanium dioxide obtained during our work has rather high specific surface area (up to 320 m^2/g), narrow pore size distribution with average pore size 2.4 nm and nanocrystalline pore walls which consist of anatase and brookite. Photocatalytic activity was measured in test reaction of methyl orange dye oxidation. High photocatalytic activity of mesoporous titania is determined by both surface area of the catalyst and features of phase composition.

Optical properties of mesoporous TiO_2 have been modified via doping by iron, zinc, cerium and nitrogen. The doping does not influence strongly on the microstructure of the samples and leads to the red shift of the absorption band.

Also mesoporous titanium oxide was used as a support for gold nanoparticles. Nanocomposites have been studied using TEM and DRIFTS with CO probe molecules. The confinement of the nanoparticles inside the pores allows to avoid aggregation and to enhance the stability of the catalysts.

This work was supported by RFBR (grants №№ 06-03-89507, 06-08-01443) and FASI (grant № 02.523.12.3015)

16:30 Oral

Nanoporous Hybrid Chitosan/Titania as Cooperative Bifunctional Catalysts

Abdelkrim El Kadib, Françoise Quignard, Daniel Brunel, Karine Molvinger

Institut Charles Gerhardt, CC15, Place eugène Bataillon, Montpellier 34095, France

e-mail: karine.molvinger@enscm.fr

One of the most exciting research areas in materials chemistry today is to design hybrid materials with original properties [1] such as cooperative bifunctionality brought by each component. Indeed, the development of biopolymer/silica materials has become of great interest since 15 years [2,3]. In this work, our goal was to prepare highly porous chitosan-titania hybrid in order to improve the chemical stability of the materials under base catalytic conditions, taking into account the higher stability of titania compare to silica under these conditions [4]. Moreover the additional interest of such a material featuring both basic site (NH_2) and Lewis acidic site (Ti) concerns its potential for bifunctional catalytic applications. Titania/chitosan hybrid is obtained by a classical procedure[3]. The material was fully characterised (TGA, EDX, MET, SEM, adsorption/desorption of nitrogen (480 m^2/g)).These materials were tested as catalyst for the monoglyceride formation which is of great industrial interest. It has been also tested on amine grafted on silica [5] and on chitosan/silica hybrid [6].

In conclusion, comparing with the results obtained with previous catalysts, chitosan/titania catalyst reveals better activity. In these conditions, reactions occur with high selectivity. The recycling of the catalyst shows no loss of activity. These unusual activity and selectivity may be rationalized by cooperative effect between organic and inorganic moieties. Other catalytic tests are under investigation.

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16:45 Oral

TiO_2-coated mesostructured SiO_2 nanocomposite as thermally stable catalyst supports.

Magali Bonne, Stephane Pronier, Sabine Valange, Jean-Michel Tatibouët, Sebastien Royer, Patrice Marécot, Daniel Duprez

LACCO, UMR CNRS 6503,, Poitiers ESIP, France

e-mail: sebastien.royer@univ-poitiers.fr

Since the first synthesis of silica M-41S type mesostructured silica by researchers from Mobil in 1992, many attempts are made to generalize the synthesis to other oxidic solids. Thus, the mesostructuration of transition-metal oxides is the subject of much scientific and technological attention, and particularly titanium dioxide due to its numerous applications among those photocatalysis and support for catalytic reactions like gas phase depollution, hydrodesulfurization… While specific surface areas (SSA) of commercial titania samples rarely exceed 200 $m^2.g^{-1}$, some recent synthesis procedures sol-gel based mesostructuration allow to obtain largely higher SSA (up to 700 $m^2.g^{-1}$).[1] Unfortunately, thermal stability of the solids remains low, and calcination generally results in the crystallization of the solid with the collapse of the porosity (and consequently an important decrease in SSA). In this work, we report an original synthesis procedure leading to the preparation of TiO_2 supported mesostructured SiO_2 nanocomposite. The procedure used consists in a sol-gel synthesis of TiO_2 nanocrystals inside the porosity of the SBA-15 type silica host support. A series of TiO_2/SiO_2 (TiO_2 loading from 10 to 55 wt.%) is then prepared from titanium isopropoxide as titania precursor in anhydrous ethanol as solvent. A systematic study of the impregnation steps evidences the difficulty to avoid titania segregation outside the silica porosity. A careful impregnation allows to synthesize 2-3 nm crystallized TiO_2 nanoparticles dispersed inside the silica host support. TEM analysis clearly evidences the preservation of the initial hexagonal structure of the parent support and allows to observe crystallized anatase particles anchored onto the silica walls. As an example, the 55 wt.%TiO_2/SiO_2 sample display a SSA of 480 $m^2.g^{-1}$, a pore volume of 0.47 $cm^3.g^{-1}$ and a pore diameter of 4.5 nm (sample calcined at 400 °C).

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Friday, 19 September

E-MRS & EPDIC Joint Plenary Session

Friday morning, 19 September, 9:00
Small Hall (237)

Coffee break

Friday morning, 19 September, 10:30
Main Hall

Parallel Symposia

Friday morning, 19 September, 11:00
Room 134

11:00 Invited oral

Heterogeneous biocatalysts built by enzymes encapsulation in silica using lecithin as porogen

Anne Galarneau

Institut Charles Gerhardt, CC15, Place eugène Bataillon, Montpellier 34095, France

e-mail: anne.galarneau@enscm.fr

The immobilization of enzymes in inorganic support is expected to provide breakthroughs in the area of heterogeneous catalysis. Biological molecules such as enzymes are outstanding catalysts with very high catalytic power and very high specificity. However, they are barely used, because of their fragility. Appropriate immobilization helps to maintain their quaternary structure, to protect them against external environment, to recover the products and to develop process in continuous flow. There are five kinds of enzymes: very stable enzymes, enzymes with co-factor self-regenerated, enzymes with co-factor no self-regenerated, very fragile enzymes, polyenzymatic systems. Only, the immobilization of the first kind of enzymes has been widely studied in inorganic supports [1]. We proposed a new way of enzyme encapsulation in silica supports, which has allowed to encapsulated different kind of active enzymes: very stable enzymes (lipase [2,3], hemoglobin), very fragile enzyme (Alcool dehydrogenase [4]), polyenzymatic systems (GOD and HRP) in oxidation reactions, which open the route to new catalytic processes.Our encapsulation method, is a new concept of sol-gel synthesis using egg lecithin (natural phospholipids) as self-assembling templates for silica, and sugar to protect the enzymes. Two different kind of nanostructures were synthesized: a three dimentional isotropic structure with cavities of 6 nm, called Sponge Mesoporous Silicas, and 7 nm particle size porous Nanocapsules of Silicas, named (NPS). Both structures have been compared to classical immobilization technics and may constitute a new generation of very selective catalysts.

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11:45 Oral

Synthesis of nanostructured fibrous catalyst support by templated sol-gel method

Tetyana Levchenko[1], Dmytro Nasiedkin[1], Igor Babich[2], Leon Lefferts[2], Yuri Plyuto[1]

1. *Institute of Surface Chemistry NAS of Ukraine, 17 General Naumov, Kyiv 03164, Ukraine* **2.** *University of Twente, Catalytic Processes and Materials, P.O. Box 217, Enschede 7500AE, Netherlands*

e-mail: levchtat@i.com.ua

The aim of this work was in application of the templated sol-gel approach for the rational design of mesoporous silica coatings on woven fibre glass used as advanced catalyst support.

The sol-gel precursor was synthesised by acidic hydrolysis of $Si(OC_2H_5)_4$ to which cetyltrimethylammonium bromide template was added afterwards. The initial glass fibre was dip-coated with sol-gel precursor and the resulting dry fibre material with the deposited silica coating was calcined in air at 400 ºC to complete condensation of siloxane oligomers into silica framework and to remove template molecules from the template-doped coating. In this way the apparent surface area of fibrous catalyst support was increased from 0.4 to 13.0 m^2/g due to formation of pores of ~ 2.7 nm diameter. According to SEM images, the glass filaments of 6-9 µm in diameter are completely coated with mesoporous silica film and do not form the flocks.

The model Ni catalyst was synthesised by incorporation of Ni^{2+} species into mesoporous silica coating *via* ion-exchange in $Ni(NH_3)_6(NO_3)_2$ aqueous solution. A subsequent reduction in H_2 at 400 ºC resulted in the formation of Ni nanoparticles which exhibited catalytic activity in the reaction of toluene hydrogenation to methylcyclohexane.

12:00 Oral

Vanadium oxide-porous phosphate heterostructure catalysts for the selective oxidation of H_2S to sulphur.

Marta León[2], Jose Jimenez Jimenez[2], Antonio Jimenez-Lopez[2], Enrique Rodriguez Castellon[2], María Dolores Soriano[1], José Manuel Lopéz Nieto[1]

1. *Instituto de Tecnología Química UPV-CSIC (ITQ), avda. de los Naranjos s/n, Valencia 46022, Spain* **2.** *Universidad de Malaga (UMA), Campus Teatinos, Malaga E29071, Spain*

e-mail: jmlopez@itq.upv.es

Current stringent environmental regulations oblige to treat hydrogen sulphide (H_2S) emissions originated in petroleum refineries and gas plants. Claus and Super Claus processes are the most common used, but due to thermodynamic limitations a relevant percentage of H_2S is not converted to sulphur in the Claus process, and high concentration of H_2S (2% vol) cannot be treated with the Super Claus technology. Vanadium oxide catalysts supported on mesoporous materials, based on a surfactant expanded zirconium phosphate with silica galleries into the interlayer space, named porous phosphate heterostructure (PPH), were prepared by using TEOS and vanadium oxitripropoxide in *n*-propanol as sources of Si and V, respectively; with different Si/V molar ratios of 1, 2, 5 and 25; and calcining at 550 ºC for 6 hours. Using this method, vanadium is incorporated to the structure of the gallery, but the surface area strongly decreases with the increase of the vanadium content. The solids obtained were denoted V-yPPH, where y is the Si/V molar ratio added. The catalysts were characterised before and after catalysis by XRD, XPS, TEM, FT-IR and Raman, and tested in the selective catalytic reduction of H_2S using a fixed bed reactor, at atmospheric pressure, at 180-260 ºC. The catalysts with high contents of vanadium, samples V-1PPH and V-2PPH are very active at 200 ºC, showing H_2S conversions of 85-99%, with a high selectivity to elemental sulphur and with a low formation of SO_2.

12:15 Oral

Co_3O_4 particles templated inside SBA-15 silica: optical characterization, reducibility and selectivity in the hydrogenation of alpha/beta unsaturated compounds

Sabine Valange[2], Ruben Palacio[2], Joel Barrault[2], Anne M. Davidson[1], Irene Lopez[1], Nissrine El Hassan[1]

1. *Universite Pierre et Marie Curie, Place Jussieu, Bat F Boite 39, Paris 75252, France* **2.** *LACCO, UMR CNRS 6503,, Poitiers ESIP, France*

e-mail: anne.davidson@upmc.fr

Small oxide particles have unique physical and chemical properties and understanding them is virtually important for the design of new heterogeneous catalysts. Our current work concerns Co_3O_4 which is an archetype of spinel oxides, containing metallic sites in two oxidation states Co(III) and Co(II). Unique electronic properties of this oxide have been associated with different structural modifications including : i) non stoichiometry (surface oxygen excess), ii) location, oxidation state and electronic configuration of metallic sites (inversion and existence of Co(III) high spin), iii) cationic vacancies, iv) electronic transfers. In complement to sophisticated methods (laser deposition, reduction of precursors embedded inside organic micelles) which are not straightforward and uneasy to scale up and for which thermal treatments are difficult to apply without sintering, we have studied Co_3O_4 particles templated inside SBA-15 silica before to reduce them (under an Ar/H_2 flow at 450°C) and to test their activity and selectivity for the selective hydrogenation of conjugated alpha-beta unsaturated aldehyde (cinnamaldehyde). The optical properties of the precursor catalyst, identified by UV visible Diffuse Reflectance Spectroscopy, can be correlated with both its activity and selectivity for the reaction (80% selectivity in unsaturated alcohol).

Lunch break

Friday afternoon, 19 September, 12:30
Inner Courtyards

Posters

Monday, 15 September

Joint Poster Session I

Monday & Wednesday
Monday afternoon, 15 September, 16:00
Main Hall

16:00 Poster D01

CO_2 adsorption and catalytic property of a mesoporous chromium terephthalate metal organic framework MIL-101

Wha-Seung Ahn

Inha University-Dept.Chem.Eng, 253 Yonghyun-Dong, Nam-Gu, Incheon 402-751, Korea, South

e-mail: whasahn@inha.ac.kr

Metal organic frameworks (MOFs) are a class of organic-inorganic hybrid materials made of metal clusters interconnected through an organic linker. During the last decade, they have attracted wide scientific interests due to their extremely high surface area and pore volume, which can lead to potential applications in gas storage, separation, and heterogeneous catalysis. In this work, a mesoporous chromium terephthalate, MIL-101, having regular pores made of cages of free diameter 3.4 nm and Langmuir surface areas of ca. 5900 m^2/g was hydrothermally synthesized and its adsorption and catalytic properties were investigated. High pressure CO_2 adsorption properties were measured and found to be higher than those of inorganic mesoporous materials made of silica, carbon, or aluminophosphate. Catalytic performance of MIl-101 was evaluated in liquid phase oxidation of tetralin and compared with those of other Cr-containing porous materials, demonstrating high activity and selectivity to 1-tetralone.

16:00 Poster D03

Kinetics of dyes photodegradation over cadmium doped TiO_2

Luminita Andronic, Alexandru I. Enesca, Anca Duta

Transilvania University of Brasov, Centre Product Design for Sustainable Development, Eroilor 29, Brasov 500036, Romania

e-mail: andronic-luminita@unitbv.ro

Titanium oxide semiconductor photocatalytic system appears to be the most attractive for environmental purification of textile wastewater. The only drawback of TiO_2 semiconductor is that it absorbs a small portion of solar spectrum in the UV region (band gap energy of anatase TiO_2 is 3.2 eV and 3.0 eV for rutile TiO_2). Therefore, modification of TiO_2 photocatalysts for dyes degradation using visible light is a demanding area of research.

Three main aspects were studied: (1) to prepare various cadmium doped TiO_2 by doctor blade technique, the percent of doping was Cd:Ti=0.1, 0.5, 1, 3 respectively 5 at % and the cadmium precursors were acetate, nitrate respectively chloride; (2) to characterize the catalysts by surface area and porosity, X-ray diffraction (XRD) and atomic force microscopy (AFM), (3) to evaluate the kinetic studies for evolution of dyes concentration (M) under the following conditions: (a) UV irradiation without TiO_2 (photolysis), (b) in the dark with TiO_2 (adsorption) and (c) UV irradiation with Cd doped TiO_2 (photocatalysis/photodegradation). The kinetic of adsorption and degradation of Methyl orange and Methylene blue has been investigated and compared using different concentrations of dyes in range: 0.05-0.0125 mM. The kinetic of degradation of dyes fits well with the Langmuir–Hinshelwood model below a dye concentration of about 0.0125 mM. At higher dyes concentration the important absorption of light by the dyes was suggested to be at the origin of the decrease of degradation. No correlation was observed between adsorption isotherm in the dark and the degradation kinetics. However, in the textile wastewater, often a mixture of dyes and heavy metal compounds are present, so our objectives in the future will be to study the kinetics of degradation of a mixture of dyes and cadmium ions.

16:00 Poster D04

Surface properties of MCM-41 containing aluminium and titanium

Diana C. Azevedo[1], Rinaldo S. Araújo[3], Débora S. Maia[1], Célio L. Cavalcante Jr[1], Enrique Rodriguez Castellon[2], Antonio Jimenez-Lopez[2]

1. *Universidade Federal do Ceará (UFC), Campus do Pici, bl. 709, Fortaleza 60455760, Brazil* **2.** *Universidad de Malaga (UMA), Campus Teatinos, Malaga E29071, Spain* **3.** *Centro Federal de Educação Tecnológica (CEFET-CE), Fortaleza 60000, Brazil*

e-mail: diana@pq.cnpq.br

The surface acidity of mesoporous molecular sieves of aluminium and titanium was evaluated using four different techniques: n-butylamine volumetry, cyclohexylamine thermodesorption, temperature programmed desorption of ammonia and adsorption of pyridine. The nature, strength and concentration of the acid sites were determined and correlated to the results of a probe reaction of anthracene oxidation to 9,10-anthraquinone (in liquid phase). In general, the surface acidity was highly influenced by the nature, location and coordination of the metal species (Al and Ti) in the mesoporous samples. Moderate to strong Brönsted acid sites were identified for the Al-MCM-41 sample in a large temperature range. For mesoporous materials containing Ti, the acidity was represented by a combination of weak to moderate Brönsted and Lewis acid sites. Higher acidity of moderate strength, found in the Ti-HMS sample, enhanced both conversion and selectivity in the oxidation reaction of anthracene, producing higher yields of 9,10-anthraquinone.

16:00 Poster D05

Improvement of photocatalytic activity of TiO_2 films by the adsorption of TiO_2 micro-spheres

Monserrat Bizarro, Miguel A. Tapia-Rodríguez, Maria Luisa Ojeda, Armando Ortiz

Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico (UNAM), A.P. 70-360, México 04510, Mexico

e-mail: monserrat@iim.unam.mx

Titanium oxide powders are currently applied in the degradation of pollutants of air and water, due to the high photocatalytic efficiency. However, the use of powders implicate furder water treatments to separate the catalyst from the resulting water solution, which makes the process more expensive. Thin films, on the other side, represent a one step water cleaning process where the catalyst is adhered onto the substrate. In this case, there are no catalyst loses and water can be obtain ready to use. In this work we produced TiO_2 thin films using titanium IV acetylacetonate and methanol as precursors for the solution deposited by spin coating. The samples were thermally treated at 400°C for two hours to evaporate the organic compounds. This procedure was repeated three times in order to obtain thicker films. On the last layer, TiO_2 microspheres were adsorbed on the film surfaces previous to the heat treatment. The spheres were produce using titanium isopropoxide (Ti (^{i}OPr)$_4$) and anhydrous ethanol, having an average diameter of 2 microns. This work makes the comparison between plain TiO_2 films, TiO_2 films with adsorbed microspheres and TiO_2 films with commercial TiO_2 powder adsorbed to the surface. Photocatalytic activity was drastically increased when the surface is modified, either with the microspheres or with commercial powder. Films with microspheres degradate the methyl orange more than ten times faster than plain films, and can be reused with almost the same efficiency that is not conserved in the case of films with commercial powder adhered to the surface. The particle sizes are also related with the photocatalytic activity. Samples with titanium oxide microspheres represent a good option for faster water treatment processes.

16:00 Poster D06

Synthesis of New heterogeneous catalysts through the controlled growth of inorganic nanostructures around monodispersed metal nanoparticles.

Malika Boualleg[1], Jean-Marie Basset[1], Jean-Pierre Candy[1], Katrin Pelzer[2], Laurent Veyre[1], Chloe M. Thieuleux[1]

1. *Chimie, Catalyse, Polymère, Procédé, UMR CNRS CPE UCBL (CCPP), 43 bd du 11 Nov. 1918, Villeurbanne 69616, France* **2.** *Max-Planck-Gesellschaft, Fritz-Haber-Institut, Faradayweg 4-6, Berlin D-14195, Germany*

e-mail: malika.boualleg@cpe.fr

Heterogeneous catalysts containing metal particles are currently prepared by decomposition of metal salts or complexes or by impregnation of metal particles onto oxide supports such as alumina or silica. These standard procedures are easy to handle but they can lead to a broad distribution of particles size and to an heterogeneous distribution of particles within the oxide framework.

The aim of this work is to achieve a "one-pot" synthesis of mesoporous silica (silica) nanostructures around various metal nanoparticules colloidal solutions. This new methodology shoud lead to the synthesis of new heterogeneous catalysts as mesostructured materials with a three-dimensional network of nanometric monodispered pores channels (dp varying form 2 to 10 nm) and containing regularly distributed metallic nanoparticles within the framework.

To reach this goal, we developed a synthetic pathway requiring two steps :

1) The synthesis of colloidal solution of metal nanoparticles by reduction under hydrogen of a molecular metallic complex (Ru, Pt) in presence of stabilising ligands.

2) The development of synthetic pathways to obtain mesostructured material containing metal nanoparticles using the sol-gel process *via* a templating routes.

The as-synthesized solution of metal nanoparticles and the nanoparticles containing materials were fully characterized by several techniques (nitrogen adsorption/desorption, T.E.M., hydrogen or oxygen adsorption, X Ray diffraction, elemental analysis…).

The materials were also compared to classical heterogeneous catalysts in term of stability (sintering of nanoparticles under various treatments) and catalytic performances (reaction of propene hydrogenation in a continuous tubular reactor).

16:00 Poster D08

Titanium hydrate nanoparticles for catalytic degradation of organic dyes

Yu Hua Cheng, Zhong Chen

Nanyang Technological University, Singapore, Singapore

e-mail: ch0001ua@ntu.edu.sg

Recently, it is of increasing concern to find efficient solutions for the management of wastewater. In particular, much effort is channeled to the search of new materials that are capable of degrading harmful substances such as organic dyes present in wastewater. Photo-catalysts can degrade such organic dyes under suitable light irradiation. In this study, Titanium oxide hydrate was synthesized via low temperature hydrothermal route. The particles are mono-dispersed and average at 20 nm in size. The synthesized material was found to have broad absorption spectra in the visible light range as compared to the widely known commercial photo-catalyst, Degussa P25 which absorbs only in the Ultraviolet range. The catalytic activity of the synthesized powder and P25 were evaluated for degradation of organic dye; Methylene Blue under visible light. It was found that the rate of degradation using Titanium oxide hydrate was much faster than that of commercial P25. Importantly, the structure, morphology, as well as surface chemistry have also been explored to provide a comprehensive study of the photo-catalytic material.

16:00 Poster D09

Synthesis, characterization and photocatalytic properties of $CaNb_2O_6$ nanostructure

In-Sun Cho[1], Shin-Tae Bae[1], Dong Wook Kim[1], Chin Moo Cho[1], Dong Hoe Kim[1], Hyun Suk Jung[2], Kug Sun Hong[1]

1. *Seoul National University, Department of Materials Science and Engineering (MSE, SNU), San 56-1, Sillim-dong, Gwanak-gu, Seoul 151-744, Korea, South* **2.** *Kookmin University, School of Advanced Materials Engineering, Seoul 136-702, Korea, South*

e-mail: cis005@snu.ac.kr

2D ellipsoid-like nanoplates of calcium niobates ($CaNb_2O_6$) were synthesized by controlling the reaction conditions, such as the pH, reaction time and temperature, via hyrothermal route without any surfactants or templates. The prepared powders were characterized using X-ray diffractometer (XRD), scanning electron microscopy (SEM), Transmission electron microscopy (TEM), Raman spectroscopy and UV-Vis spectroscopy. It was found that the nanoplates consisted of uniaxially aligned nanorods and can absorb the UV light with wavelengths less than 350 nm. Compared with a powder of the same material prepared by a solid-state reaction method, the 2D ellipsoid-like nanoplates exhibited a much higher photocatalytic activity for degradation of Rhodamine B dye solution under UV irradiation. The enhanced photocatalytic activity of the nanoplates was assigned to both higher optical absorption ability and higher BET surface area resulted from the reduced dimensionality.

16:00 Poster D10

Non hydrolytic Sol-Gel route for the design of Mo-based metathesis catalysts

Damien P. Debecker[1], Karim Bouchmella[2], Eric M. Gaigneaux[1], Hubert P. Mutin[2]

1. *Université catholique de Louvain, unité de catalyse et chimie des matériaux divisés (UCL), Croix du Sud, 2/17, Louvain-la-Neuve 1348, Belgium* **2.** *Institut Charles Gerhardt, UMR 5253, CNRS-UM2-ENSCM-UM1, Université de Monpellier 2, cc 1701, Montpellier 34095, France*

e-mail: damien.debecker@uclouvain.be

Light olefin metathesis is one of the most attractive reactions to upgrade abundant cheap alkenes into more demanded ones and to regulate stocks. For this purpose, MoO_3-supported heterogeneous catalysts are of great interest. With classical preparation methods (impregnation of a Mo precursor on a support and subsequent calcination) fine tuning of the textural properties of the catalyst and of the nature of the Mo surface species at the molecular level are however much difficult.

Here we report the possibilities offered by a non hydrolytic sol-gel route for the preparation of $MoO_3/SiO_2/Al_2O_3$ metathesis catalysts.

Xerogels were obtained in one step by reaction of $MoCl_5$, $SiCl_4$ and $AlCl_3$ with diisopropylether in dichloromethane. The adjunction of solvent is an efficient tool for the control of the final textural properties[1,2]. Our strategy was to provoke the migration of Mo species towards the catalyst surface by applying appropriate calcination conditions on the xerogels. This effect is evidenced by XPS measurements and leads to the production of well-dispersed Mo species as attested by XRD and Raman measurements. The resulting materials were mesoporous (mean pore size of ~12 nm) with high specific surface area (between 400 and 600 m²/g) and very high pore volumes (up to 2 cm³/g).

Various compositions were prepared in order to evaluate the effect of the Mo loading and of the Si/Al ratio on the properties of the materials and on their catalytic performances. These ternary systems are active in the self-metathesis of propylene. Specific activity is shown to be highly dependant on the MoO_3 loading but also on the Si/Al ratio. The performances of the catalysts in the self-metathesis of propylene are successfully correlated with their physicochemical properties. New insights on the nature of the metathesis active sites are also gained with this study.

[1] Lafond, V.; Mutin, P. H.; Vioux, A. *Chem. Mater.* **2004**, *16*, 5380.

[2] Vioux, A. *Chem. Mater.***1997**, 9, 2292.

16:00 Poster D11

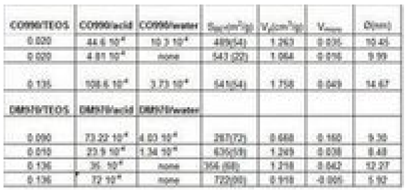
Synthetis of silica materials mesoporous with nonylphenyl ether

Hamaizi Hadj, Mama Benzine, Hadj Hamaizi, Abdelkader Tayeb, Abdelkader Bengueddach

Laboratoire de Chimie des Matériaux, LCM, Université Oran-Sénia, BP 1524, Oran 31000, Algeria

e-mail: hamaizimizou@yahoo.fr

The use of non-ionic surfactants in the synthesis of mesoporous solid leads to a porous texture offering properties in catalysis. In this work, we used non-ionic surfactants type Igépal CO-990 and MD-970, which under acidic, and in the presence of TEOS, give an amorphous texture with pores in the form of "wormhole" and whose dimensions are variable depending on the content of surfactant / silica and pH environment.A variety of materials silicic mesoporous is obtained by the sol-gel process from a source of silica (TEOS and silica fume) and non-ionic polyoxyethylenic surfactants (CO - and DM 990 - 970). The characterization by the measures adsorption of nitrogen and electron microscopy indicate a multi porous texture with very large pores whose diameters are between 7 and 20 nm. The table gives the molecular composition of each of reagents used in the synthesis and the textural parameters.



16:00 Poster D12

Self organized ensembles of LDHs particles supported with nanoparticles of Fe and Ti oxides - as new catalysts for the oxidative decomposition of chlorobenzene

Gabriela Carja, Gabriela Ciobanu, Nicolae Apostolescu

Technical University from Iasi (UTI), Bd.D.Mangeron 63, Iasi 700050, Romania

e-mail: carja@uaic.ro

Nanostructured catalysts derived from nanoparticles of iron and titanium oxides supported on the matrices of hydrotalcite-like anionic clays (LDHs) have been obtained and tested as new catalysts in the process of oxidative decomposition of chlorobenzene. A simple synthesis method based on the LDHs “memory effect” has been used to tune the synthesis procedure of Fe - Ti oxides - anionic clay nanostructures. XRD analysis is used to describe the structural characteristics of the studied samples. TEM analysis shows that on the typical LDH particles (average size equal to 110 nm) smaller nanoparticles (average size equal to 20 nm) are supported. XPS analysis gives information about the nature of the supporting nanoparticles pointing out the presence of mainly Fe_2O_3 and TiO_2 on the surface of the tested catalysts. A complete oxidation is reached around 340 °C and chlorine was the only chlorinated organic product.

Acknowledgments: This research work was supported by the PNCDI II contracts NATOEPA 71-020 / 2007 and the LaCaFiA Capacitati 134 / 2007.

16:00 Poster D13

Photocatalytic Characteristics of Zinc Oxide Particles Precipitated from Concentrated Solutions at Low Temperatures

Jean-Francois Hochepied[1], Ana Paula Almeida de Oliveira[1], Véronique Guyot Ferreol[2], Jean François Tranchant[2]

1. *Laboratoire de Systemes Colloidaux dans le Processus Industriels (SCPI), Ecole des Mines de Paris, Paris F - 75272, France* **2.** *LVMH Recherche, Parfums et Cosmetiques, Departement Innovation Materiaux et Technologies, Saint Jean de Braye 45804, France*

e-mail: hochepied@ensmp.fr

Zinc oxide particles of different morphologies (sand roses and prickly spheres) were directly obtained at soft conditions (T=25 °C, 40 °C, 60 °C) by double-jet precipitation using 0.5 mol.dm^{-3} zinc nitrate and 1.0 mol.dm^{-3} NaOH at two different pH values, 9.5 and 10.5. Increasing precipitation temperature changed continuously particle morphology from two-dimensional (sand roses, 12m^2/g) to three-dimensional (prickly spheres, 3m^2/g) features. The interest of the method, in spite of a relatively low surface area, is to provide a morphology control without templates nor surface treatments, facilitating further comparisons. Particles result from different oriented aggregation of similar nanocrystals, exhibiting in the final architecture more or less polar vs non polar crystal faces of the zincite structure. Phenol photodegradation / ZnO weight is superior for sand-roses morphology due to their higher specific surface area, whereas phenol photodegradation / ZnO specific surface area is superior for prickly spheres, which can be interpreted by a better activity of zincite non-polar surfaces for phenol photodegradation.

16:00 Poster D14

Thermal stability and acidic proprities of heteropolycompounds

Smain Hocine

University, Laboratoire de Chimie Appliquée et de Génie Chimique, Université Mouloud, Tizi-Ouzou 15000, Algeria

e-mail: shocine_univ_to@yahoo.fr

Abstract

The heteropolycompounds Keggin-type, modified by exchanging the acidic proton of the heteropolyacid $H_3PMo_{12}O_{40}$ by counterions NH_4^+ and Fe^{3+}, or by substituting the addenda atoms Mo^{VI} by V^V, Fe^{III}, were prepared and characterized by BET, XRD, IR, UV, SEM, TGA/DTA and ^{31}P solid-state NMR spectroscopy techniques. The acidic properties were evaluated in the oxidative of decomposition of isopropanol. The catalytic performances of those compounds were tested in the isomerisation of n-hexane and in selective oxidation of methane to C1-oxegenates.

The experimental data (IR, Raman and XRD) indicated that compounds possess the Keggin structure.

TG curve shows that there are three steps of weight loss. DTA curve shows that the salts are thermally stable than the pure $H_3PMo_{12}O_{40}$ acid. The surface area , the acidic and the catalytic proprieties of heteropolyoxometalates depend considerably on the reaction conditions, and specifically on the chemical composition of the catalysts.

16:00 Poster D15

A Monte Carlo Study and Optimization of Proximity Effect in a New Method of Electron-Beam Nano-Lithography using Scanning Electron Microscopy

Hadi Hosseinzadegan, Behjat Forouzandeh

University of Tehran (UT), North-Kargar, Tehran 14395-731, Iran

e-mail: hadiinfo@ieee.org

We present a new method of nanolithography, using scanning electron microscopy. We explore the effecting parameters on electron beam lithography and solutions to improve its quality. A tri-layer of PMMA/ Ni/ Si is simulated and being experimented using Scanning Electron Microscopy. Simulation is being done by Monte Carlo method with a minimum number of 20.000 electrons. The effect of various thicknesses of Ni and PMMA is studied in different voltages. Silicon is the most usual substrate in integrated circuits fabrication. Nickel is below the PMMA layer in order to absorb the radiated electrons by SEM. The thickness of nickel is varied during the simulation process to study its effect on proximity effect.

The silicon substrate, used in the simulation is p-type or n- type to decrease the charging effect with <100> orientation. For the second layer, two thicknesses of 10nm and 100 nm is considered. Simulation is also done for voltages ranging from 5 KV to 30 KV with 5 KV steps.

With increasing the beam voltage, backscattering coefficient of electrons increases. Due to minimum backscattering coefficient in 10KeV, it is the optimum voltage to perform the lithography process. Increasing the nickel thickness is also increases the backscattering coefficient in all conditions. Thus the minimum nickel thickness is preferred. In the other hand, more nickel thickness results in more absorption coefficient.

Also in more thicknesses of PMMA layer, the thickness of nickel layer is not as effective as its thin layer in proximity effect.

Considering the parameters above, optimum point from backscattering point of view is the voltage of 10K Volts, PMMA thickness of 1.5 microns, and nickel thickness of 10 nanometers and from diffusion depth point of view is the voltage of 10 K Volts, PMMA thickness of 0.7 microns, and nickel thickness of 100 nanometers.

16:00 Poster D16

Synthesis and structural peculiarities of Ce–Zr–La–O catalysts

Maria I. Ivanovskaya[1], Dzmitry A. Kotsikau[1], Elena Frolova[1], Vladislav A. Sadykov[2]

1. *Research Institute of physical-chemical problems (FHP), Leningradskaja 14, Minsk 220050, Belarus* **2.** *Boreskov Institute of Catalysis (BIC), pr. akad. Lavrentieva, 5, Novosibirsk 630090, Russian Federation*

e-mail: ivanovskaya@bsu.by

The effect of structural features of Ce–Zr–La–O complex oxides and electronic state of supported Pt on their catalytic activity in methane selective oxidation and steam reforming has been studied. Ce–Zr–La–O (1, 10 and 30 mol. % of La) fluorite-like oxides were prepared by inorganic sol-gel method. As it was shown earlier the indicated composites demonstrate a high and stable activity in CH_4 selective oxidation and steam reforming into syngas as well as high electrocatalytic performance as anode catalysts in solid oxide fuel cells. The structure of the samples was characterized by XRD, XPS, TEM, EDXA, EPR and FTIR-spectroscopy. The Ce–Zr–La–O samples annealed in the range of 600-1100 °C have cubic structure with particle size less than 10 nm. Detailed analysis revealed co-existence of the following nano-phases with similar crystalline structures: $Ce_{1-x}(La,Zr)_xO_{2-d}$ (solid solution), $La_2Zr_2O_7$, $La_{0.1}Zr_{0.9}O_{2-d}$, $Zr_{0.4}Ce_{0.4}O_2$, $Ce_{0.1}Zr_{0.9}O_2$. Their amount depends on La content and the annealing temperature. The phases can be arranged as fragments within a single nano-crystal and have shared crystallographic planes (CeO_2: a = 5.4113 Å, $Fm3m$; $La_2Zr_2O_7$: $a/2$ = 5.3965 Å, $Fd3m$; $Zr_{0.4}Ce_{0.6}O_2$: a = 5.3049 Å, $Fm3m$; ZrO_2: a = 5.09 Å, $Fm3m$). Both catalytic features and thermal stability of the nano-heterophased Ce–Zr–La–O material were found to depend on the character of interaction between the separate phases and between the phases and Pt(Ru).

A model of mixed active center consisting of various Pt (Pt^0, Pt^{2+}) states and [Pt^{d+}–$Zr^{(n-d)+}$] charge transfer complex has been proposed based on XPS study. Oxidized platinum states are important for the effective oxygen and CH_4 activation in the selective methane oxidation process and stabilizing small Pt clusters. The [Pt^{d+}–$Zr^{(n-d)+}$] complex is mainly localized at the surface of $La_xZr_{1-x}O_{2-d}$ fragments.
The work has been supported by ISTC Project No 3234

16:00 Poster D17

Analysis of catalytic properties of Ni_3Al thin foils in methanol decomposition

Paweł R. Jóźwik[1], Zbigniew BOJAR[1], Ryszard Grabowski[2]

1. *Military University of Technology (MUT), Kaliskiego, Warsaw 00-908, Poland* **2.** *Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences (ICSC), Niezapominajek 8, Kraków 30239, Poland*

e-mail: pjozwik@wat.edu.pl

Catalytic properties of fully dense Ni_3Al-based thin foils (thickness below 50µm) with nano- or microstructure were investigated. The material under examination - thin foils without any additional catalytic coating, was successfully produced from as cast coarse-grained sheet by heavily cold rolling and recrystalization at appropriate chosen set of parameters. The examination has concerned to methanol decomposition into H_2 and CO in a temperature range up to 530°C in a quartz reactor. Excepts these products a little amount (below 1%) CO_2 and dimethyl ether was observed. The catalyzed reaction has started effectively at about 400°C, with methanol conversion about 90% or higher. Results of our investigations confirmed that the refinement of structure up to nanostructure essentially improved catalytic properties of investigated Ni_3Al foils.

16:00 Poster D18

Comparison of Au/ZrO_2 materials prepared by precipitation and impregnation methods

Jarosław Kaszewski, Urszula Narkiewicz

Szczecin University of Technology, Institute of Chemical and Environment Engineering, Szczecin 70-322, Poland

e-mail: jaroslavuss@wp.pl

Noble metals supported on zirconium dioxide are well known catalysts of CO oxidation and 1,3-butadiene hydrogenation. High catalytic activity is reached, when gold particles are small enough to interact with oxide support. Effect is also stronger, when size of support nanoparticles matches with size of gold nanoparticles. Activity of Au/ZrO_2 catalysts is related to existence of both metallic and cationic gold. In present work comparison of different synthesis routes of zirconia-gold materials is presented. Samples were synthesized by impregnation of fine zirconia nanoparticles and microwave driven hydrothermal synthesis starting from zirconia hydrogel precipitate or zirconium hydroxide. The source of gold was $HAuCl_4$ compound. Au/ZrO_2 materials were prepared with different concentrations of gold: from 0,01%wt. to 5%wt. Obtained powders were characterized by SEM, TEM, XRD, XPS, BET, ICP-AES and helium pycnometry.

16:00 Poster D19

Study of the benzylation of benzene and other aromatics by benzyl chloride over chromium-mesoporous molecular sieves materials

Bachari Khaldoun, Touileb Ali, Halliche Djamila, Saadi Adel, Cherifi Ouiza

Centre de Recherche Scientifique et Technique en Analyse Physico-Chimique (CRAPC), BP248, Alger RP. Alger 16004,Algerie, Alger 16004, Algeria

e-mail: bachari2000@yahoo.fr

A series of chromium-containing mesoporous silicas with different Cr contents were prepared and characterized with chemical analysis, N_2 adsorption Measurements (BET and BJH theory), X-ray diffraction, diffuse reflectance UV–visible and H_2-temperature programmed reduction techniques. Excellent results in benzylation of benzene and substituted benzenes reaction employing benzyl chloride as the alkylating agent were obtained. The mesoporous chromium-containing materials showed both high activity and high selectivity for benzylation of benzene. The activity of these catalysts for the benzylation of different aromatic compounds is in the following order: benzene > toluene > p-xylene > anisole. Kinetics of the benzene benzylation over these catalysts have also been investigated.

16:00 Poster D20

Catalytic properties of Ga-HMS-n materials in the tertiary butylation of phenol

Bachari Khaldoun, Touileb Ali, Touati Mourad, Cherifi Ouiza

Centre de Recherche Scientifique et Technique en Analyse Physico-Chimique (CRAPC), BP248, Alger RP. Alger 16004,Algerie, Alger 16004, Algeria

e-mail: bachari2000@yahoo.fr

Abstract:

The gallium-incorporated mesoporous silica material Ga-HMS-n (where n is the Si/Ga ratio in the precursor gel = 30, 60, 90) was successfully synthesized at ambient temperature using hexadecylamine as the template agent. The obtained materials were analyzed by XRD, transmission electron microscopy TEM and nitrogen adsorption to determine the structural order and the textural properties. It has been observed by ^{71}Ga MAS-NMR spectroscopy that gallium atoms are exclusively in tetrahedral coordination for all samples. Temperature-programmed desorption of pyridine showed that Ga-HMS-30 has a higher number of strong acid sites. The catalyst Ga-HMS-30 showed bigger performance in the acid-catalyzed tertiary butylation of phenol employing tert-butanol as the alkylation agent. In fact, a high phenol conversion of 75.3% is observed for this catalyst at a reaction temperature of 433K. However, the 4-TBP yield amounts to 41.8% and the 2,4-DTBP yield corresponds to 30.3%. Furthermore, due to the large pore size, which allows a faster diffusion of reactants and products, catalyst deactivation of Ga-HMS-30 was not observed even after reaction for 5 h.

16:00 Poster D21

Activated carbon materials as a solid acid catalyst

Masaaki Kitano[1], Keisuke Arai[1], Kiyotaka Nakajima[2], Shigenobu Hayashi[3], Michikazu Hara[1,2]

1. *Kanagawa Academy of Science and Technology (KAST), 3-2-1 Sakado, Takatsu-ku, Kawasaki 213-0012, Japan* **2.** *Materials and Structures Laboratory, Tokyo Institute of Technology, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan* **3.** *National Institute of Advanced Industrial Science and Technology (AIST), Central 5, 1-1-1 Higashi, Tsukuba, Ibaraki 305-8565, Japan*

e-mail: hp_kitano@newkast.or.jp

In our previous work, amorphous carbon with high density of SO_3H groups was demonstrated to function as an efficient replacement for sulfuric acid catalyst. The carbon material can incorporate large amounts of hydrophilic molecules into the carbon bulk, due to the high density of the hydrophilic functional groups bound to the flexible carbon sheets. This incorporation provides good access by reactants in solution to the SO_3H groups in the carbon material, giving rise to high catalytic performance, despite the small surface area (2 m^2 g^{-1}). However, the hydrophilic functional groups prevent incorporation of hydrophobic molecules into the bulk, and thereby hydrophobic acid-catalyzed reactions proceed only on the surface, resulting in poor or no catalytic activity for the reactions. In this study, sulfonated activated carbon materials prepared at low temperatures were studied as solid acid catalysts. Activated carbon catalysts were prepared by sulfonation of activated carbon obtained by carbonization of wood powder with $ZnCl_2$ at 523-873 K. The surface areas of the activated carbon catalysts increased with increasing carbonization temperature, reaching a plateau at 773 K. The maximum surface area of the samples was 1560 m^2 g^{-1}. Structural analyses revealed that the activated carbon catalysts have sulfonic acid, carboxylic acid, and hydroxyl groups and these functional groups decreased with increasing carbonization temperature. The catalytic activity of the activated carbon catalysts was demonstrated through the esterification of acetic acid (343 K) and the alkylation of toluene (373 K). In the case of the esterification of acetic acid, the catalytic activity depended only on the acid amount. On the other hand, the alkylation of toluene on the carbon material depended on the surface area in addition to the acid amount. These results suggest that the activated carbon catalyst with high surface area act as a solid acid even for hydrophobic acid-catalyzed reactions.

16:00 Poster D22

Thermal stability of porous anodic titania films

Irina V. Kolesnik, Dmitry I. Petukhov, Dmitry A. Buldakov, Andrey A. Eliseev, Alexey V. Lukashin, Yuri D. Tretyakov

Faculty of Materials Science, Moscow State University, Lenin Hills, Moscow 119992, Russian Federation

e-mail: kolesnik@inorg.chem.msu.ru

Porous oxide films obtained by anodic oxidation attract a great deal of attention due to their unique microstructure. The structure of as-synthesized films can be characterized as an array of cylindrical channels in amorphous metal oxide with perpendicular orientation to metallic substrate and narrow size distribution. This feature makes anodic titania films promising elements of gas sensors, selective and catalytic membranes. However, these applications require high thermal and mechanical stability of anodic oxide membranes, and crystallinity of the pore walls.

In the present work we studied crystallization and evolution of the microstructure under thermal treatment. Anodic titania was obtained by anodic oxidation of metallic titania in 0.25% NH_4F ethylene glycol solution at 60V. According to thermal analysis mass loss (up to 11,5%) accompanied by two exothermal effects at 220^{o}C and 330^{o}C which is observed during heating to 375^{o}C can be ascribed to decomposition and removal of electrolyte from the pores. According to XRD data crystallization of amorphous titania into anatase begins at 300^{o}C and finishes at 420^{o}C. Crystallinity degree runs up to 85% and crystalline size runs up to 40 nm during heating to 375^{o}C . According to SEM data porous structure are stable up to 600^{o}C.

Thus the minimal temperature for crystallization of anodic TiO_2 is 420^{o}C and operating temperatures of membranes and sensors based on anodic TiO_2 can be varied form room temperature to 600^{o}C.

This work was supported by RFBR (grants 06-03-89507, 06-08-01443) and FASI (grant 02.523.12.3015)

16:00 Poster D23

Novel synthesis of ternary magnesium based transition metal hydrides as potential energy storage materials

Izabela S. Kunce, MAREK POLAŃSKI, Jerzy Bystrzycki

Military University of Technology, Faculty of Advanced Technology and Chemistry, Kaliskiego 2, Warszawa 00-908, Poland

e-mail: iza_kunce@tlen.pl

Ternary magnesium based transition metal hydrides such as Mg_2FeH_6, Mg_2CoH_5, Mg_2NiH_4, etc. are attractive materials for hydrogen or thermal energy storage. Unfortunately, most of them are rather difficult to synthesize. The traditional method for the synthesis of these ternary hydrides is the conventional metallurgical sintering at high temperature (350-550°C) under high hydrogen pressure (2-100 bar). However, in many cases this processing route does not lead to satisfactory results because the yield of the sintering is about 60% and the unreacted elements have to be removed through a complicated process. Therefore to overcome these problems, discovering simple and effective method of their synthesis is needed.

In our work we present a new method for rapid and effective synthesis of ternary Mg-based Fe, Co and Ni hydrides. The stoichiometric powder mixture of both magnesium hydride and transition metal was mechanically (ball) milled for 1h in a planetary mill under argon. Afterwards unique pressurizing and heating cycle was applied to obtain full phase transformation within no longer than 1,5 hour.

Structural investigations carried out by using X-ray diffraction revealed that almost all initial powder mixture transforms into ternary intermetallic hydride during first several minutes. The yield of the synthesis method is over 90%. However, traces of Fe and Co in the synthesized mixtures were found. Additionally, dehydriding properties of synthesized ternary hydrides were investigated by temperature programmed desorption and differential thermal analysis. The obtained results clearly shown that ternary magnesium based hydrides are formed via direct reaction of magnesium hydride with transition metal and hydrogen. Moreover, our results indicate that significant improvements to the phase transformation and reaction kinetics can be made by mechanical alloying of initial powder mixture due to reducing overall diffusion distances to the nanometer scale.

16:00 Poster D24

Synthesis and characterization of metal nanoparticles

Galif Kutluk[1], Masashi Nakatake[1], Sinya Yagi[2], Hirosuke Sumida[3], Masaki Taniguchi[1], Hirofumi Namatame[1]

1. *Hiroshima University, Synchrotron Radiation Research Center, 2-313, Kagamiyama, Higashi-Hiroshima 739-0046, Japan* **2.** *Garaduate School of Enginnering, Nagoya University (NAGOYAU), Nagoya university, Furo-cyo, Chikusa-ku, Nagoya 464-8603, Japan* **3.** *Mazda Motor Corporation, 3-1,shinchi,Fuchu-cho,, Aki-gun 730-8670, Japan*

e-mail: gkutluk@hiroshima-u.ac.jp

Gold highly dispersed on metal oxide supports has unexpectedly been found to be highly active for a number of catalytic reactions. However, the electronic nature of the gold species in active catalysts has not been fully elucidated. We have applied a modified version of the gas phase condensation combined with Arc plasma method for the metal nanoparticle synthesis. Which is not only convenient in synthesizing highly dispersive metal nanoparticle with cleaner surface but also is suitable for the size controlling. In addition, this method also shows advantage in synthesizing metal nanoparticle with simple shape on a supporting material (Si Ta, TaN, HOPG). The performance of the gas phase condensation and Arc plasma method for the size control has been confirmed in the earlier work [1]. In this study, we report the investigations of the thermal stabilities, crystallographic structure and the size dependence of electronic structures of Au ant Pt nanoparticles in range of 1.5 ~ 5nm in diameter. The Au nanoparticle were characterized by the TEM, AFM, XPS and UPS. Drastic change have observed in the 4f level photoemission spectrum when the size of Au particle down to 1.5nm. The spectrum is characterized by component of an oxidized doublet states of Au_2O_3 coexisting with the doublet states of pure Au. The vanishing of component of Au_2O_3 doublets has been observed with increasing the annealing temperature of the sample in the reduction atmosphere.

[1]. G. Kutluk, S. Yagi, H. Sumida, H. Namatame, M. Taniguchi, Mater. Res. Soc. Symp. Proc. Vol. 915 R06-18 2006

16:00 Poster D25

Influence of cycling on microstructure and hydriding/dehydriding properties of nanocrystalline magnesium hydride with nanosized niobium fluoride

Iwona E. Malka, Jerzy Bystrzycki

Military University of Technology, Faculty of Advanced Technology and Chemistry, Kaliskiego 2, Warszawa 00-908, Poland

e-mail: imalka@wat.edu.pl

Magnesium hydride (MgH_2) is a promising material for hydrogen storage applications because of its high gravimetric (7.6 wt.%) and volumetric (110 kg m^{-3}) densities and low cost. However, there are some drawbacks limited practical application of this hydride. First of all, it is too stable thermodynamically (H=-75 kJ/mol). It results in high desorption temperature (>400ºC). Moreover, the MgH_2 exhibits relatively poor absorption/desorption kinetics below 350ºC. Recently, it has been shown that the sorption kinetics of MgH_2 can be dramatically improved by ball milling of MgH_2 with some transition metals and their oxides or halides. Among them, NbF_5 additive seems most significantly enhance the sorption kinetics of MgH_2. However, it is still not clear how the NbF_5 promotes the dehydrogenation and hydrogenation reactions. Additionally, there is a lack of information about microstructure and sorption properties of MgH_2 with nanosized NbF_5 after cycling loading.

In our work we present the effect of cycling on microstructure and hydriding-dehydriding properties of nanocrystalline MgH_2 with nanosized NbF_5 prepared by mechanical milling. Commercial MgH_2 powder was mixed with NbF_5 powder (7 wt.%) and subsequently ball milled in an inert atmosphere in a planetary mill. The phase structure, morphology and chemical composition were investigated by XRD, SEM, EDS and DSC-TG. The hydrogen sorption properties and pressure composition isotherms were evaluated using a volumetric Sievert apparatus and temperature programmed desorption. Our results have shown a considerable catalytic effect of NbF_5 additive on both the dehydrogenation temperature and hydriding/dehydriding kinetics of MgH_2. The obtained nanocomposite exhibits good reversibility in the pressure composition isotherms at 325ºC. However, degradation of nanostructure and hydrogen storage capacity after prolonged cycling are observed, apparently related to the grain growth during cycling at elevated temperature.

16:00 Poster D26

Supported hydrotalcites for enhanced and stable CO_2 capture

Niels Meis, Harry Bitter, Krijn P. De Jong

Inorganic Chemistry and Catalysis, Utrecht University, Sorbonnelaan 16, Utrecht 3584CA, Netherlands

e-mail: n.n.a.h.meis@uu.nl

To alleviate the environmental concerns regarding the current CO_2 emissions into the atmosphere Carbon Capture & Storage (CCS) is investigated as one of the possible routes. Due to the acidic character of CO_2, basic oxides are expected to be suitable sorbents. We investigated the use of hydrotalcites (HT) as CO_2 sorbent. HT, e.g. $Mg_4Al_2(OH)_{12}CO_3.4H_2O$, has a structure similar to that of $Mg(OH)_2$. In the latter, Mg^{2+} is octahedrally coordinated by hydroxyl group, which are edge-shared to form a sheet-like structure. A net positive charge of the brucite-like layers originates from replacement of Mg^{2+} by Al^{3+}. This charge is compensated for by anions, typically carbonate, situated together with water molecules in the interlayer. In the current contribution we will report on the relation between CO_2 capture properties and HT platelet size. Two different series samples were prepared i.e., unsupported HTs with lateral size range from 40 nm to 2 mm, very small (~20 nm) supported HTs were deposit on carbon nanofibers (CNF).

The CO_2 absorption characteristics of unsupported HTs at 250 °C showed a low and invariant absorption capacity (0.1 $mmol{\bullet}g^{-1}$) for all samples regardless of the platelet size. However, small supported hydrotalcites showed a considerable higher uptake (1.3 $mmol{\bullet}g^{-1}$) of CO_2. Currently we tentatively relate this higher uptake to a higher density of defects in the $Mg(Al)O_x$ phase that binds CO_2. Moreover, supported hydrotalcites gave improved cycle stability. We speculate that by anchoring individual HT platelets on CNF their mobility is limited, resulting in less agglomeration and annealing of defects on the $Mg(Al)O_x$ phase, thus less deactivation upon cycling. These results indicate the advantage of supported hydrotalcites for the uptake of CO_2 capture. We improved not only the specific capacity by a factor 10 for the CO_2 capture material hydrotalcite, we also improved mechanical strength and cycle stability for these CO_2 capture materials.

16:00 Poster D27

Acidic Carbon Catalyst Prepared from Lignin

Kiyotaka Nakajima[1], Keiko Ichikawa[1], Hideki Kato[1], Shigenobu Hayashi[2], Michikazu Hara[1]

1. *Materials and Structures Laboratory, Tokyo Institute of Technology, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan* **2.** *National Institute of Advanced Industrial Science and Technology (AIST), Central 5, 1-1-1 Higashi, Tsukuba, Ibaraki 305-8565, Japan*

e-mail: nakajima.k.ae@m.titech.ac.jp

Lignin is one of the major components in woody-biomass and composed of aromatic and aliphatic carbohydrates with oxygen-containing functional groups. Conversion of lignin to important functional materials is important issue as plant-derived raw materials are increasingly used as a renewable source. Here, we present the unique strategy for the preparation of SO_3H-containing carbon catalysts from lignin and their catalytic properties for the acid-catalyzed reactions. Sulfonated carbon catalysts are obtained by imcomplete carbonization of lignin at around 673 K followed by sulfonation of the resulting carbon in concentrated sulfuric acid solution. The obtained material consists of mainly nanosized graphenes in size of ~ 1.5 nm. XRD, XPS, and solid-state NMR reveal that the resulting catalyst contains -SO_3H, COOH, and OH groups, which are attached to the graphene sheets. The amount of sulfonic acid groups, which are act as Brönsted acid sites in acid-catalyzed reaction, are estimated as 1.3 $mmol{\cdot}g^{-1}$. Acid catalysis of this catalyst is demonstrated through esterification of acetic acid with ethanol. The resulting catalysts produced ethyl acetate in high yield: the activity is comparable to those of conventional ion-exchangable resins (Nafion and Amberlyst-15). Catalytic activity and S content remains unchanged after reuse of this catalyst for three times, indicating the introduced sulfonic acid groups are stabilized on the carbon framework. Because of the presence of benzene ring, sulfonic acid groups are introduced in the bare lignin and sulfonated lignin also catalyzes the corresponding reaction. However, severe leaching of sulfonic acid groups occurs when the sulfonated lignin is repeatedly used as an acid catalyst. The lignin-derived solid acid also shows higher catalytic activity for esterification of stearic acid with ethanol than those of Nafion and Amberlyst-15. Therefore, the resulting carbon catalyst is suitable for solid material in acid-catalyzed reactions.

16:00 Poster D28

Structure and functional properties of ceramic oxygen-conducting membranes

Vladimir V. Pankov[1], Maria I. Ivanovskaya[2], Dzmitry A. Kotsikau[2], Vladimir A. Lomonosov[1], Leanid V. Makhnach[1], Vladislav A. Sadykov[3]

1. *Belarusian State University (BSU), F. Skaryna av. 4, Minsk 220050, Belarus* **2.** *Research Institute of physical-chemical problems (FHP), Leningradskaja 14, Minsk 220050, Belarus* **3.** *Boreskov Institute of Catalysis (BIC), pr. akad. Lavrentieva, 5, Novosibirsk 630090, Russian Federation*

e-mail: pankov@bsu.by

The oxygen-conducting membrane consists of $La_{1.8}Sr_{0.2}NiO_4$ gas-tight layer (100 mkm). The conditions of formation of the layer have been studied in order to optimize its micro-structure for effective oxygen transport. $La_{1.8}Sr_{0.2}NiO_4$ membranes were found to be promising materials for syn-gas ($CO+H_2$) generators. High effectiveness of conversion of hydrocarbons into syn-gas in TPO and TPSC processes is reached by covering the $La_{1.8}Sr_{0.2}NiO_4$ gas-tight layer with catalytically active Ce–Sm–O/Ru(Pt) or Ce–Zr–La–O/Ru(Pt) oxide nanocomposites. The catalytically active compounds were prepared by sol-gel approach using inorganic precursors. They were fabricated by repeated deposition of the corresponding co-precipitated metal hydroxides onto the membrane, and annealed at 600°C. It was found that the presence of $La_{1.8}Sr_{0.2}NiO_4$//Ce–Zr–La–O/Ru hetero-junction increases H_2 yield and enhances the selectivity of TPSC process (1% of CH_4 + 1% of H_2O, He). The deposition of the thin porous catalytic layers leads to the reduction of possible surface inhibition of oxygen diffusion.

The work has been partly supported by ISTC project No 3234

16:00 Poster D29

Novel synthesis methods of Co-doped ZnO Nanopowders

Robert R. Piticescu[1], Janusz D. Fidelus[2], Claude J. Monty[3], Liviu Giurgiu[4]

1. *Institute for Non-ferrous and Rare Metals, 102 Biruintei Blvd., Pantelimon 73957, Romania* **2.** *Polish Academy of Sciences, Institute of High Pressure Physics (UNIPRESS), Sokolowska 29/37, Warszawa 01-142, Poland* **3.** *CNRS laboratoire Procedes, Materiaux et Energie solaire (PROMES), BP5 Odeillo, Font-Romeu 66120, France* **4.** *National Institute of R&D for isotopic and Molecular Technologies (INCDTIM), Cluj-Napoca 3400, Romania*

e-mail: rpiticescu@imnr.ro

The properties of nanocrystalline oxides depend on the chemical and phase composition as well as the size and the morphology of crystallites, it is important to control all these characteristics during the synthesis process. In this paper zinc oxide powders doped with Co were produced in two ways: a microwave-driven hydrothermal process and vapour-condensation of the hydrothermal synthesized powders in a solar furnace. The combination of the two methods allows controlling both Co concentration (0.0079 wt% of Co in the hydrothermal powders and 0.0075wt% in vapour-condensation powders) and crystallite morphology from spherical nanoparticles to nanowhiskers. The influence of the synthesis process on the ESR spectra and magnetic properties are discussed.

In the absence of reliable phase diagrams for the studied system, thermodynamic simulations provided important information for controlling hydrothermal/solvothermal methods. The experiments confirm the high potential offered by solvothermal chemistry in producing semiconductor oxides with controlled dopant concentrations due to the in-situ nucleation of oxides, as observed from ESR spectra.

Acknowledgement

The paper is a result of a cooperation supported by EGIDE, France, in the frame of ECO-NET project "Fun-Nanos" and FP6 SOLFACE.

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16:00 Poster D30

Preferential oxidation of CO (CO-PROX) catalyzed by CuO/CeO_2 supported on zirconium containing mesoporous silica

Maurizio Lenarda[1], Loretta Storaro[1], Elisa Moretti[1], Aldo Talon[1], Enrique Rodriguez Castellon[2], Antonio Jimenez-Lopez[2]

1. *Diparimento di Chimica-Università Ca' Foscari, Venezia 30100, Italy* **2.** *Universidad de Malaga (UMA), Campus Teatinos, Malaga E29071, Spain*

e-mail: castellon@uma.es

Carbon monoxide is a typical by-product in the production of hydrogen by reforming of alcohols or hydrocarbons and must be reduced down to ppm levels in order to be used as feed for proton-exchange membrane fuel cells. Up to date, several options for CO removal have been studied and the selective oxidation (CO-PROX) is considered one of the most straightforward and cost-effective methods to achieve acceptable CO concentrations. The activity of $CuO-CeO_2$ supported on MCM-41 type mesoporous silica containing zirconium was evaluated in the preferential oxidation of CO in the presence of excess of H_2. As a reference, a Cu-Ce catalyst supported on a pure mesoporous silica was also synthesised. It is well known that the addition of ZrO_2 to CeO_2 matrix, with the formation of a solid solution, enhances the OSC capacity of the resulting mixed oxide $Ce_xZr_{1-x}O_2$, by increasing the oxygen vacancies that consequently improve the reducibility of copper. In this work we investigated the CO-PROX reaction over the Cu-Ce couple supported on a structurally organized SiO_2/ZrO_2 material, with the aim to obtain further information about the effect of zirconium in the catalyst structure when it is not in solid solution with cerium. The catalysts were characterised by elemental analysis, XRPD, H_2-TPR, TEM and XPS. All the catalysts displayed a very good performance in the 40-190°C temperature range. The catalyst containing 6 wt.% of copper and 20wt.% of cerium showed, in the technologically interesting 120-140°C range, a conversion near to 100% with a selectivity to CO_2 close to 90%.

16:00 Poster D31

Visible-Light active N-doped TiO_2 prepared by reaction of $TiO_2.nH_2O$

Samaneh Shadmehr, Nima Taghavinia

Sharif University of Technology, Azadi Avenue, Tehran 14588, Iran

e-mail: s_shadmehr@yahoo.com

Titanium Dioxide photocatalysis is now being used in practical applications such as self-cleaning, sterilization, deodorizing and air-cleaning. It is chemically and photochemically stable, but is only excited by ultraviolet light so that the light utilization efficiency to solar irradiation and a fluorescent lamp is very low. Therefore, attempts were made to extend the adsorption rang of titanium dioxide into the visible-light region by different methods. We prepared N-doped TiO_2 powders that respond to visible-light by high temperature reaction of $TiO_2.nH_2O$, prepared by the hydrolysis of Tetraisopropylorthotitanate with urea. We studied the effect of time and temperature and different weight ratios of urea/$TiO_2.nH_2O$ and we found that our best sample was the one with 500°C heat treatment for 2h and in this sample the weight ratio of urea/$TiO_2.nH_2O$ was 1. The absorption edge of the samples shifts toward a longer wavelength (about 550 nm). The nanoparticles had a relative specific surface area of about $51m^2g^{-1}$. The prepared N-doped TiO_2 nanopowders that respond to visible light ($400nm<\lambda<550nm$) showing better photocatalytic activity to that prepared by reaction of TiO_2 (P25-Degussa) with urea. We used Diffused Reflectance, XPS, XRD, SEM, FT-IR, CHN analyzer, TEM and EDS for characterization and we evaluated their photocatalytic activity.

Fig. 1 Light absorption spectra of samples prepared without urea as a reference (green curve) and with the weight ratio of urea/ $TiO_2.nH_2O$ of 1 and 2h annealing time in different temperatures.

Fig. 2 Photocatalytic decomposition of Methylene Blue under visible light. Blue under visible light)

Reference : "Visible-Light Photocatalysis in Nitrogen-Doped Titanium Oxides", R. Asahi, T. Ohkawa, K. Aoki, Y. Taga, Science, 293, 269(2001).)

16:00 Poster D32

The adsorption of amylase on mesoporous carbon and its hydrolysis property for starch

Wenzhong Shen

University Petroleum of China, Dongying 257061, China

e-mail: shenwzh2000@yahoo.com

Hierarchical mesoporous carbon was prepared using starch as precursor at 700 °C, then , it was used to adsorb the amylase and the hydrolysis property for starch was investigated. The mesoporous carbon was characterized by nitrogen adsorption-desorption isotherm, XRD, FTIR and SEM. The result showed that its had developed mesoporous structure, the pore size distribution in 3-5nm and 10-15nm, and plenty hydrophilic groups.The adsorption capacity of amylase was 80mg/g and it hydrolysis activity was kept as 95% after 6 runs due to the plenty hydrophilic groups, which could interact with the nitrogen group of amylase.

16:00 Poster D33

Peculiarities of non-conventional synthesis of V-Mo-O catalysts

Volodymyr Sydorchuk, Svitlana Khalameida, Valeriy Zazhigalov

Institute of Sorption and Problems of Endoecology NAS of Ukraine, 13 Gen Naumova Str., Kyiv 03164, Ukraine

e-mail: bilychi@online.com.ua

V-Mo-O compositions which are base of numerical oxidative catalysts are mostly prepared by heating of mixture of vanadium and molybdenum oxides or their ammonium salts. Recently some modern particularly hydrothermal (HTT) methods have been used thereto. However approaches of non-conventional chemistry are not enough attracted for synthesis of indicated catalysts. We investigated influence of mechanochemical (MChT), microwave (MWT) and ultrasonic (UST) treatment of nonporous coarsely dispersed V_2O_5/ammonium dimolybdate (ADM) (V/Mo=0,7:0,3) powders in aqueous medium on their chemical and phase composition, porous structure, surface morphology. It should be noted that at the heart of listed techniques underlie similar physico-chemical processes: local and impact increase of temperature and pressure, heating of whole system, intensive mechanical influence on solid and strengthening of mass transfer as a result. For comparison HTT of the same composition was also studied since hydrothermal conditions are simulated during MChT, MWT and UST. It was established that origination of meso-macroporous from non-porous substances occurs: total pore volume has maximal value after MWT (1,0-1,2 cm^3/g), minimal – after MChT (0,1-0,3 cm^3/g). Increase of duration or temperature of treatment leads to destruction of ADM to non-stoichiometric Mo-oxides and partial V_2O_5 amorphization. At MChT (1-2 h) intercalation of H_2O and NH_3 molecules into V_2O_5 structure with its transformation in ammonium hexavanadate (4-6 h) takes place. Solid solution of substitution Mo in V_2O_5 with crystallite size 6-12 nm is formed on base indicated phases at next calcination under 300-500˚C. At annealing of samples undergone MWT, UST, HTT solid solution wasn't found. However above 500˚C in all cases formation of V_2MoO_8 phase occurs. Thus non-conventional methods as well as HTT favor formation of V-Mo-O precursors which following calcination in essence leads to structuring of catalysts with changeable parameters.

16:00 Poster D34

Well-Defined Single-Site Heterogeneous Ru-NHC Catalysts for the metathesis of functionalized olefin Reaction via Surface OrganoMetallic Chemistry on Hybrid Organic-Inorganic Materials

Johan Alauzun[2], Jean-Marie Basset[1], Jean-Michel Camus[1], Christophe Coperet[1], Robert J. Corriu[2], Iyad E. Karame[1], Tarun Maishal[1], Ahmad Mehdi[2], Catherine Reyé[2], Laurent Veyre[1], Chloe M. Thieuleux[1]

1. *Chimie, Catalyse, Polymère, Procédé, UMR CNRS CPE UCBL (CCPP), 43 bd du 11 Nov. 1918, Villeurbanne 69616, France* **2.** *Institut Charles Gerhardt, CC15, Place eugène Bataillon, Montpellier 34095, France*

e-mail: thieuleux@cpe.fr

In the past ten years, olefin metathesis has become a key reaction in organic synthesis and material science because of the emergence of highly active and selective homogeneous ruthenium catalysts[1] tolerant to a large scope of functionalities. The best systems are currently based on Ru-complex having N-Heterocyclic Carbene (NHC) ligands. While several highly efficient homogeneous catalysts were developed, the corresponding heterogeneous catalysts have displayed poor efficiencies, despite numerous attempts.[2] The best Ru-based heterogeneous catalysts can only transform about 5000 equivalents of diallylmalonate through RCM, and this is probably due to the difficulty to generate well-defined systems.

In contrast to classical grafting methods on oxides or polymer supported systems, we have synthesized organic-inorganic hybrid nanostructured materials as supports for Ru-NHC-complexes in order to obtain catalysts having regularly distributed active sites throughout the oxide matrix. The imidazolium-containing nanostructured materials were prepared by a Sol-Gel process usingtemplating routes, and the thus-obtained materials contain regularly distributed imidazolium moieties, covalently bonded to the pores channels of the nanostructured silica framework, as evidenced by several characterization techniques (TEM, X-Ray, solid state NMR spectroscopy…).

Then, Ru-complexes were selectively coordinated on the imidazolium moieties of the materials to generate Ru-NHC alkylidene surface species. These new catalytic systems were fully characterized and displayed very good performances in the metathesis of ethyl-oleate compared to other reported Ru-based heterogeneous systems.

A deep understanding of the nature of the active site was obtained using the stereochemistry of ethyl-oleate self-metathesis reaction at very low conversion and it was further corroborated by spectroscopic datas (^{13}C Solid state NMR) performed on very similar material containing Ir-NHC ^{13}C labelled complexes.

16:00 Poster D35

Growth of Molybdenum Oxide Nano-Micro Structures by Thermal Annealing Process

Sajjad Tollabimazraehno[1], Seyed Mohammad Mahdavi[1], Azam Iraji zad[1,2], Seyad Ahmad Mahdavi Ardakani[3], Abas Azarian[1]

1. *Sharif University of Technology, Azadi Avenue, Tehran 14588, Iran* **2.** *Institute for Nanoscience and nanotechnology Sharif University of Technology, Azadi Avenue, Tehran 14588, Iran* **3.** *Aviation Technology College, Tehran, Iran, Tehran 00000, Iran*

e-mail: tollaby@gmail.com

The needle and planar molybdenum oxide structures on molybdenum foil were grown by thermal annealing process. The effects of different parameters such as oxygen flow rate, presence of oxygen, annealing temperatures and annealing time on structures, grain size and aspect ratio of nano/micro structures were studied. It is found that the density of structures is only function of oxygen flow rate and annealing temperature. The maximum density of MoO_3 nanorods were observed at annealing temperature 530ºC in air. The mechanism of the crystals growth was found for synthesized nanorods.

16:00 Poster D36

Starch Saccharification by Carbon-Based Solid Acid Catalyst

Daizo Yamaguchi[1], Michikazu Hara[2]

1. *Kanagawa Academy of Science and Technology (KAST), 3-2-1 Sakado, Takatsu-ku, Kawasaki 213-0012, Japan* **2.** *Tokyo Institute of Technology, Nagatsuda-Cho 4259,Midori-ku, Yokohama, Yokohama 226-8502, Japan*

e-mail: hp_yamaguchi@newkast.or.jp

SO_3H-bearing carbon material prepared from cellulose has been examined as a strong solid acid catalyst for the hydrolysis of corn starch into glucose. Sulfonation of incompletely carbonized cellulose results in amorphous carbon consisting of polycyclic aromatic carbon combined functional groups such as a sulfonic acid groups. The hydrolysis of starch into α-1,4 glucan and glucose in the presence of the carbon material was analyzed by factorial analysis (Taguchi Method) to identify the important factor for the process. A three-level-five-factor design was employed using L_{27} orthogonal array, and dependent value was glucose yield.

Analysis of variance (ANOVA) revealed that the contributions of reaction temperature (80-120 ºC) and time (1-5 h) to the reaction were estimated to be 70.8% and 3.7%, respectively, and that reaction temperature largely correlates reaction time (contribution: 18.5 %). This means that the reaction at high temperatures proceeds efficiently for short reaction time, suggesting that by-products forms with increasing reaction time at high temperatures. The reaction under optimal conditions proceeded at 120 ºC for 3 h (water, 0.8 ml; speed, 500 rpm; starch, 75 mg; catalyst, 0.3 g). The results of validation test demonstrated that liner model for the estimation of the process was useful and 100% of glucose yield would be achieved under the optimum conditions.

16:00 Poster D37

Fe-Co alloy catalyst for NH_3 decomposition to CO_x-free hydrogen

Weiqing Zheng, Jian Zhang, Robert Schlögl, Dangsheng Su

Fritz-Haber-Institute of Max-Planck-Gesellschaft, Faradayweg 4-6, Berlin D-14195, Germany

e-mail: zheng@fhi-berlin.mpg.de

In order to reduce the pollution arising from automobiles exhausts, hydrogen has been extensively studied as the ultimate clean energy carrier to replace fossil fuel. Nowadays, ammonia decomposition to provide CO_x-free hydrogen has attracted renewed interest due to its oustanding advantages over the conventional routes based on carbonaceous materials. In this study, we studied the microstructure and catalytic performances of Fe-Co alloy nanoparticles, with different Fe/Co ratios, supported on commercial carbon nanotubes for ammonia decomposition. Elemental mapping of energy filtered transmission electron microscopy (EFTEM), electron energy-loss spectroscopy (EELS) and powder X-ray diffraction (XRD) results suggest an almost complete alloy state between Fe and Co in all bimetallic samples. Catalytic activity and stability tests of different catalysts were carried out with 36000 ml/(h g_{cat}) NH_3 space velocity at given temperatures. Results indicated that replacing Co by less active but much cheaper Fe was found to keep the high activity but greatly improve the stability. We attributed these improvements to the electron donation effect of Co to Fe, which could assist the N adatoms to desorb from surface with a low activation barrier.

16:00 Poster D38

Nanoscale one-dimensional TiO_2 photocatalytic materials for hydrogen production by solar light activated water splitting

Shankar Muthukonda Venkatakrishnan, Mathieu Grandcolas, Olivier Rosseler, Nicolas Keller, Valérie Keller-Spitzer

CNRS, ULP, Laboratoire des Matériaux, Surfaces et Procédés pour la Catalyse (LMSPC), 25 rue Becquerel, Strasbourg 67087, France

e-mail: Shankar.Muthukonda@ecpm.u-strasbg.fr

Since the discovery of carbon nanotubes, extensive research also performed on the synthesis of metal and metal-oxide nanotubes. A wide range application for nanoscale 1D-TiO_2 has been explored, especially for targeting promising photocatalytic applications. They offer a larger surface area and enhanced electron transfer across the channel. Thus, the high adsorption capacity combined with efficient charge separation yielding to reduce the photogenerated electron and hole recombination, which is one of the limiting factors in photocatalysis, should have determinant roles in the surface redox reactions occurring in photocatalysis

Liquid-phase water splitting into hydrogen and oxygen using semiconductor photocatalysts – an uphill reaction belonging to the "artificial photosynthesis" reactions – has received much attention because of its potential application for direct production of hydrogen, a source of clean energy from solar light and water. This application is a promising target for new 1D TiO_2-based photocatalytic materials.

This communication reports use of Au, Pt or perovskite phases supported on nanoscale 1D-TiO_2 photocatalytic materials under solar light illumination. The role of the supported metal is to overcome the detrimental over potential related to the H_2O/H_2 redox couple and the TiO_2 conduction band location, and to increase the photogenerated charge separation. In addition, using Au is interesting compared to Pt, since Au avoids the restrictive back reaction between H_2 and O_2 that takes place at the platinum surface. By contrast, perovskite phases are interesting for extending the absorption to the visible-light range. Supporting those phases onto nanoscale 1D-TiO_2 materials helps both in reducing the recombination rate of photogenerated charges and in increasing the contact surface between water and the light-activated materials.

16:00 Poster D39

Nanostructural characterization and magnetic properties of pure and Fe, Co or Mn-doped TiO_2 nanopowders prepared by Solar Physical Vapor Deposition (SPVD)

Jules KOUAM[2], Janusz D. Fidelus[1], Larisa Grigorjeva[3], Alexei Kuzmin[3], Felipe SANDIUMENGE[4], Lluis BALCELLS[4], Marisol S. Martín-Gonzalez[5], Claude J. Monty[2]

1. *Polish Academy of Sciences, Institute of High Pressure Physics (UNIPRESS), Sokolowska 29/37, Warszawa 01-142, Poland* **2.** *CNRS laboratoire Procedes, Materiaux et Energie solaire (PROMES), BP5 Odeillo, Font-Romeu 66120, France* **3.** *Institute of Solid State Physics, University of Latvia, 8 Kengaraga, Riga LV-1063, Latvia* **4.** *Institut de Ciencia de Materials (ICMAB) - CSIC (ICMAB), Campus de la UAB, Barcelona 080193, Spain* **5.** *Instituto de Microelectronica de Madrid (CNM-CSIC), Madrid, Spain*

e-mail: jdf@unipress.waw.pl

It is well known that the incorporation of metal ions in TiO_2 powder may substantially change their bulk and surface properties such as magnetic properties or photocatalytic activity. The main parameters include the character and concentration of the dopant and the thermal treatments.

In this work we present results of the synthesis of transition metal (TM-) doped TiO_2 powders using the Solar Physical Vapor Deposition process (SPVD) in a 2kW solar reactor as well as the characterization using XRD, SEM, TEM and HRTEM, XPS and Raman spectroscopy.

Depending on the air pressure in the solar reactor during the vaporization-condensation process, Anatase or Rutile phase, or a mixture of both, was obtained. Average grain sizes were measured from XRD peaks width. For pure TiO_2 they vary in between 15 and 30 nm.

The Rutile phase is the major phase but the Anatase phase has an important contribution. We have found in $Ti_{1-x}Fe_xO_2$ targets, that the grain size of the nanopowders depends on the phase studied : the Rutile grain size increases with the metal content increasing (x=0.01 and x=0.02).

Magnetic measurements, performed by SQUID magnetometer, make evident the paramagnetic character of Fe, Co and Mn doped TiO_2 nanopowders.

Acknowledgements

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16:00 Poster D40

Application of expanded graphite in supported Ni catalysts

Dmytro Nasiedkin[1], Tetyana Levchenko[1], Igor Babich[2], Leon Lefferts[2], Yuri Plyuto[1]

1. *Institute of Surface Chemistry NAS of Ukraine, 17 General Naumov, Kyiv 03164, Ukraine* **2.** *University of Twente, Catalytic Processes and Materials, P.O. Box 217, Enschede 7500AE, Netherlands*

e-mail: nasiedkindm@gmail.com

The goal of the present work was to investigate applicability of the expanded graphite (EG) as novel catalyst support. EG was prepared by thermal shock of H_2SO_4 intercalation compounds at 900 °C for 10 s. Intercalation was carried out at room temperature using reagents weight ratio C : H_2SO_4 : H_2O_2 = 1 : 5.9 : 0.08. Expansion to graphitic layers of nanometer thickness increases the surface area of graphite from 1 to 52 m^2/g and creates the highly open spaces between layers which can host the metal nanoparticles. Ni/EG catalysts of different metal loading were synthesised by EG support impregnation with ethanol solution of $Ni(CH_3COO)_2$ followed by drying and reduction in H_2 flow at 450 °C for 2.5 h. The catalytic activity of Ni/EG in toluene to methylcyclohexane hydrogenation as model reaction was tested at atmospheric pressure. XRD shows the distinct diffraction patterns for Ni in metallic state starting from 1% of Ni on EG however no catalytic activity was detected even for maximum tested metal loading (20%). We supposed that this can be related to Ni poisoning by sulphur impurities existing in the EG support. Therefore additional purification of EG from sulphur traces in H_2 flow at 900 °C for 2 h was applied. In this case 20%Ni/EG catalyst exhibited the conversion below 50 °C with 100% performance at 150 °C. One can conclude that EG purification from sulphur compounds results in superior properties of the synthesised supported Ni catalysts.

Plasmonic nanostructures for application in the life sciences

Symposium E

Welcome

Plasmonic nanostructures for application in the life sciences

Plasmonic nanostructures have unique electronic, catalytic, and optical characteristics. The intense current interest in the properties of plasmonic nanostructures with view to their applications in chemical and biochemical sensors, medical diagnostics and therapeutics, as well as in biological imaging is fundamentally based on their enhanced optical absorption and scattering properties.

There has, however, been much less research on the direct application of nanomaterials to biomedical areas, such as labeling, drug delivery, or imaging, in which nanomaterials are deliberately placed in the body. The first published results showed that nanostructures can stimulate cell growth and that their compatibility with biological systems is determined by their surface chemistry. Modifying the surface and the morphology of nanomaterials can make them useful for numerous medical applications by harnessing their biocompatibility and their physical properties.

The unusual optical, magnetic, electronic, catalytic, and mechanical properties of nanomaterials make their application in nanobiomedicine possible. The similarity in size of nanomaterials compared to biological macromolecules, proteins, or peptides is also a very important parameter for their use in the life sciences. The interactions between biomolecules and nanomaterials have formed the basis for a number of applications including detection, biosensing, cellular and *in situ* hybridization, labeling, cell tagging and sorting, point-of-care diagnostics, kinetic and binding studies, imaging enhancers, and even as potential therapeutic agents. Noble metal nanoparticles/ nanostructures are, for example, interesting because of their unusual optical properties which arise from their ability to support surface plasmons. In this symposium, we plan to focus on biological applications and technologies that utilize nanomaterials with plasmonic properties.

Organisers

Prof. Dr. Michael Giersig
Helmholtz Centre Berlin for Materials and Energy
Glienicker Str. 100, Berlin D-14109, Germany
Ph: +49 30 8062 2753
e-mail: giersig@helmholtz-berlin.de

Prof. Dr. Stefan Jurga
Adam Mickiewicz University, Dept. of Macromolecular Physics,
ul. Umultowska 85, Poznan 61-614, Poland
Ph.: +48 61 8295216
e-mail: stjurga@amu.edu.pl

Programme

Monday, 15 September

Opening & Plenary Session

Czochralski Award Ceremony
Monday morning, 15 September, 10:00
Small Hall (237)

Lunch break

Monday afternoon, 15 September, 12:30
Inner Courtyards

CREATION OF PLASMONIC (DIFFERENT MATERIALS/COMPOSITION) NANOSTRUCTURES

Monday afternoon, 15 September, 14:00
Room 206
Chair: MICHAEL GIERSIG

14:00 Keynote lecture

Multi-dimentional metallic metamaterials and their coupling properties

Harald Giessen, Na Liu, Hongcang Guo

University of Stuttgart, Institute of Physics, Pfaffenwaldring 57, Stuttgart D-70569, Germany

e-mail: giessen@physik.uni-stuttgart.de

We report on the manufacturing and on the optical properties of 2D and 3D
metallic metamaterials. In the plasmonic picture, the resonances can be
well understood. Coupling several metamaterial resonators together, splitting of resonances can occur. The plasmon hybridization picture helps
to understand this behavior. Symmetric and antisymmetric modes are identified. Coupled metamaterial resonators with more than two constituents show intriguing behaviour that can be well explained in a
harmonic oscillator picture in a molecular physics framework.

14:40 Invited oral

Single plasmonic nanoparticles as biosensors

Jan Becker, Carsten Sönnichsen

Johannes Gutenberg Universität, Institut für Physikalische Chemie, Jakob Welder Weg, 11, Mainz 55128, Germany

e-mail: beckerja@uni-mainz.de

Dark-field optical microscopy allows the visualization of individual noble metal nanoparticles down to sizes around 20nm due to the excitation of plasmons. The color or resonance wavelength of such plasmonic nanoparticles depends on geometry, orientation, proximity to other particles and the refractive index of the environment, making them sensitive sensors for the nano-scale processes.

We report here on recent progress in our group among the three requirements for plasmonic nanosensors applications: parallel single particle dark-field spectroscopy [1], relevant biological functionalization, [2] and production of optimized plasmonic nanoparticles [3]. First, we developed a way to investigate many randomly deposited nanoparticles in parallel using a liquid crystal device as a spatially addressable electronic shutter. Secondly, we improved plasmon based biosensing by developing a membrane based functionalization (see figure). We coated the particles with a lipid bilayer which are easily bio-functionalized (many different headgroups are commercially available) and also block efficiently nonspecific binding. Testing this system by detecting Streptavidin binding to biotinylated lipids, we observe a spectral shift of 2.9 ± 1.8 nm. Finally, we produced the best known plasmonic structures by coating gold nanorods with a thin silver shell. The coating leads to a reduction of the single particle linewidth compared to uncoated gold rods at the same resonance wavelength.

[1] Becker, Schubert, and Sönnichsen, "Gold Nanoparticle Growth Monitored in situ Using a Novel Fast Optical Single-Particle Spectroscopy Method", Nano Letters **2007**, 7, 1664

[2] Baciu, Becker, Janshoff, and Sönnichsen, "Protein-Membrane Interaction Probed by Single Plasmonic Nanoparticles", Nano Letters, **ASAP Article**, DOI: 10.1021/nl0808051

[3] Becker, Zins, Jakab, et al. „Plasmonic Focusing Reduces Ensemble Linewidth of Silver-Coated Gold Nanorods", Nano Letters, **ASAP Article**, DOI: 10.1021/nl080720k

15:05 Oral

Self-organized metal nanowire arrays with plasmonic functionality and tunable optical anisotropy

Francesco Buatier de Mongeot, Daniele Chiappe, Corrado Boragno, Andrea Toma

Dipartimento di Fisica, Università di Genova (DIFI), Via Dodecaneso, 33, Genova 16146, Italy CNISM Unità di Genova (CNISM), Via Dodecaneso, 33, Genova 16146, Italy

e-mail: buatier@fisica.unige.it

We report on a self-organised approach for the physical synthesis of laterally ordered metallic nanowire arrays. The formation of periodic metal nanostructures is induced by defocused ion irradiation of polycrystalline metal films supported on glass and polymer substrates, providing a viable alternative to time consuming serial nanopatterning approaches.

These results qualitatively agree with the behaviour reported for off–normal sputtering experiments on single-crystal metals where periodic ripples in the 10 nm range are observed [1,2]. At variance with the latter case, we found that the sub-micrometric grain size distribution of the primitive films can play an important role in the wavelength selection process during the early stages.[3]

Far-field optical characterisation demonstrates that the nanostructured surfaces exhibit interesting optical and plasmonic properties in the visible range (e.g. spectrally selective dichroic absorption) due to the excitation of localised plasmon oscillations of the conduction electrons confined on the nanowires. The possibility to tailor the optical and plasmonic properties of the nanowire array in the visible range, has been demonstrated by finely tuning the morphological parameters of the arrays [4].

[1] U. Valbusa et al., J. Phys. Condens. Matter 14, 8153 (2002)

[2] A.Molle, F.Buatier de Mongeot, A.Molinari, F.Fuerkaiti, C.Boragno and U.Valbusa

Physical Review Letters, 93, 256103 (2004)

[3]A. Toma, D. Chiappe, B. Šetina Batič, M. Godec, M. Jenko, F. Buatier de Mongeot, submitted

[4]A. Toma, D. Chiappe, D. Massabò, C.Boragno, F. Buatier de Mongeot, submitted

Coffee break

Monday afternoon, 15 September, 15:30
Main Hall

Joint Poster Session 1

Monday & Wednesday
Monday afternoon, 15 September, 16:00
Main Hall

Tuesday, 16 September

CREATION OF PLASMONIC (DIFFERENT MATERIALS/COMPOSITION) NAN

Tuesday morning, 16 September, 9:00
Room 206
Chair: MICHAEL GIERSIG

9:00 Oral

Au nanoparticles array for in-vivo biosensing

Yongqi Fu, Shaoli Zhu, Fei Li, Chunlei Du

Sate Key Lab. of Optical Tchnologies for Microfabrication, Inst. of Optics and Electronics, CAS, Sichuan Province, ChengDu 610209, China

e-mail: ygfu@ioe.ac.cn

Au nanoparticles fabricated on glass substrate with coated Cr layer in 5 nm thickness under the Au as an adhesive layer. Two fabrication techniques were employed. One is chemical self-assembled monolayer (also called sphere lithography), and the other is focused ion beam direct milling. The former has advantages of low cost and simple operation facilities, but shortages of worse uniformity in both size and dimension. The latter has no limitation of shape, and thus more freedom for the particles design. An experimental biosensing system was designed and set up that can realize localized surface plasmon resonance (LSPR)-based immunoassay in-*vivo*. In other words, the detection can be carried out for the molecule such as antibody and antigen still involved/mixed in their original chemical solution instead of the conventional dried molecule on the biochips for the LSPR-based biosensing. Therefore, the detected results are reliable because the detection environment is the same as the actual case. Measurement error caused by variation of the biological environment is avoided accordingly. It can realize localized detection over a specific area as small as micron scale. Even single cell/molecular detection is possible in the case of the biosamples with low concentration and detected using the objective lens with large *NA*.

9:20 Oral

Possible biotechnology applications of seed mediated grown gold nanorods

Filip Novotny[1], Anton Fojtík[1], Michael Giersig[2]

1. *Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical Engineering, Department of Physical Electronics, Brehova str. 7, Prague 115 19, Czech Republic* **2.** *Helmholtz Centre Berlin for Materials and Energy, Glienicker Str. 100, Berlin D-14109, Germany*

e-mail: filip.novotny@fjfi.cvut.cz

Gold nanorods (GNR) are very promising material due to the appearance of localized surface plasmon resonance (LSPR). The LSPR is splitted into two modes where the frequency of the longitudal one is strongly dependent on the rod aspect ratio. Therefore one can tune the optical properties of sample by controlling the aspect ratio of the rods. As the gold nanomaterials also exhibit good chemical stability under various conditions and biocompatibility, they are interesting candidate for bioconjungation and usage in biological systems.

During past decades a number of methods of gold nanorod synthesis was explored and some of them were refined to the point, where one can grow large volumes of high yield samples directly in solution. Such colloidal aqueous solution is very convenient for further biofunctionalization. One of such methods, which is used in this work, is seed mediated growth of gold rods from monocrystalline spherical gold seeds using a specific surfactant.

Samples are studied by the means of absorption spectroscopy of LSPR bands and TEM imaging. Several experiments of covering the GNRs with thiol-like organic substances were conducted and the effect of adsorbed biologic material to the LSPR is discussed. An improvement of the nanorods growth process and yield is proposed by controlling the acidicity of the growth solution.

Such colloidal material can then be used for number of biomedicine and biotechnology applications including targeted drug delivery (TDD) and surface enhanced raman spectroscopy (SERS), which will be discussed in detail.

9:40 Oral

Structural and optical properties of gold nanolines

Piotr Patoka[1,2], Georgios Ctistis[1], Michael Giersig[1]

1. *center of advanced european studies and research (caesar), Ludwig-Erhard-Allee 2, Bonn 53175, Germany* **2.** *Max Planck Institute of Colloids and Interfaces (MPIKGF), Research Campus Golm, Potsdam 14424, Germany*

e-mail: patoka@caesar.de

During the last decades, a tremendous amount of experimental and theoretical work has been conducted, investigating the extraordinary structural and optical properties of metallic nanostructures. These properties are attributed to the excitation of surface plasmon-polaritons, making the materials exciting and promising for the use in opto-electronics and e.g. bio-sensing applications.

Here we will present our experimental results on the structural and optical properties of gold nanolines, which were produced by means of nanosphere lithography, providing a fast and simple method to reproducibly gain large and defect-free areas of the desired nanostructures.

The main focus of the investigations is on the structural characterization by means of atomic-force microscopy (AFM) and scanning-electron microscopy (SEM). They show that the width as well as periodicity of the lines depend on the production steps.

Furthermore we investigated the near- as well as far-field optical properties of the gold lines by means of scanning near-field optical microscopy and UV-vis spectroscopy (in the range between 0.5 and 6.2 eV) revealing a polarization dependent optical transmission, an evidence for SP generation. For these studies we used lines being 30nm thick, around 200nm broad and having a periodicity of 440nm.

Coffee break

Tuesday morning, 16 September, 10:30
Main Hall

OPTICAL AND STRUCTURAL CHARACTERIZATION

Tuesday morning, 16 September, 11:00
Room 206
Chair: HARALD GIESSEN

11:00 Keynote lecture

Plasmon polaritons in nanostructures

Krzysztof Kempa

Boston College (BC), Chestnut Hill, Boston, MA 02467, United States

e-mail: kempa@bc.edu

Interaction of light with matter involves various charge excitations. These, in turn couple to photons, and thus modify the light propagation, leading to polaritons. This process is enhanced in nanostructures, which due to their sizes provide necessary momentum for an efficient coupling. This talk will discuss various plasmonic effects in nanostructures, and the corresponding polaritons. Conceptually simplest are metallic nanoparticles, which support the Mie-type plasmon resonances. A much more complicated system is the carbon nanotube, which supports numerous plasmon modes, and in which a cross-dimensional (1D to 2D to 3D) cross-over occurs. To a special category belong polaritonic crystals, simplest of which is the 3D point dipole crystal, host to various polaritonic, plasmonic and photonic modes. Finally, the discretely guided effective medium will be discussed, based on nano-coaxial, subwavelength transmission lines. This medium allows for a remarkable manipulation of light, which could lead to optical lensing free of the diffraction limitation, image encoding, negative refraction, cloaking, etc.

11:40 Invited oral

SERS-Encoded substrates for ultrafast biodetection

Marcos Sanles-Sobrido, Laura Rodriguez-Lorenzo, Miguel A. Correa-Duarte, Ramon A. Alvarez-Puebla, Luis M. Liz-Marzan

University of Vigo, Campus Universitario Lagoas-Marcosende Vigo Spain, Vigo 36310, Spain

e-mail: ramon.alvarez@uvigo.es

An assay platform that is rapidly gaining prominence for a variety of applications from diagnosis and biodetection to combinatorial chemistry and drug discovery, are *encoded microparticles*. Such encoded particles address some of the limitations posed by conventional substrates. In this context, we present the use of surface-enhanced Raman scattering

(SERS) spectroscopy, as codifying alternatives. SERS offers unique advantages such as: a) ultrasensitive detection, down to the single molecule level,??? that decrease dramatically the deconvolution times, allowing for real-time applications such as high-throughput screening in flow-citometry or microfluidic systems; b) an unlimited number of barcodes since SERS spectra are essentially vibrational fingerprints, unique for each molecule, with the possibility of expanding the codified library to the infinite by combining different tags with similar SERS cross-sections;??? and, c) the use of the same hybrid systems as optical enhancing platforms for fluorescence in sandwich key-and-lock applications such as ELISA-like microarrays, with the subsequent decrease in the detection limits of pathogens or pathogen markers.???

??? Fenniri, H.; Alvarez-Puebla, R.A. *Nat.Chem Biol.***2007**, 3, 247-249

??? (A) Kneipp, K.; Wang, Y.; Kneip, H.; Perelman, L. T.; Itzkan, I.; Dasari, R. R.; Feld, M., *Phys. Rev. Lett.***1997,** 78, 1667-1670; (B) Nie, S.; Emory, S. R., *Science***1997,** 275, 1102-1106.

??? Fenniri, H.; Chun, S.; Ding, L. H.; Zyrianov, Y.; Hallenga, K. *J. Am.Chem. Soc.***2003**, 125, 10546-10560.

??? (A) Raez, J.; Blais, D.; Zhang, Y.; Alvarez-Puebla, R.A.; Bravo-Vasquez, J.P.; Pezacki, J.P.; Fenniri, H.
*Langmuir***2007**, 23, 6482-6485. (B) Bravo-Vasquez, J.P.; Alvarez-Puebla, R.; Fenniri, H. *Sensor Act. B***2007**, 125*,* 357-359

12:05 Oral

Morphological Studies of Gold Nanoparticles

Alison M. Funston, Carolina Novo, Paul Mulvaney

The Univeristy of Melbourne (UNIMELB), Grattan Street, Melbourne 3052, Australia

e-mail: afunston@unimelb.edu.au

The size and shape-dependent plasmon absorption of metal nanoparticles is due to the collective oscillation of electrons within the particle. For gold particles these absorption bands span the visible spectrum. Mie theory provides an exact solution for the surface plasmon resonance of spheres. However, for non-spherical particles, the optical spectra have to be calculated numerically using, for example, the Discrete Dipole Approximation (DDA). Within DDA, the target particle is divided into N polarizable point dipoles and the response of each dipole to an electromagnetic field calculated. DDA thus requires knowledge of the exact particle morphology.

Recently, single particle measurements utilising dark-field microscopy have been employed to avoid the effects of polydispersity on the measured ensemble surface plasmon resonance, allowing direct measurement of the homogeneous line width and position of the surface plasmon band of a single metal nanoparticle. The recently reported Focussed Ion Beam (FIB) Registration method allows the optical spectrum of a particle with known size and shape to be determined.1 Here, we present the first theoretical and experimental study of the effects of particle size, morphology and roughness on the optical properties of the same individual metal nanoparticles studied by dark field microscopy and SEM. Knowledge of the particle size and shape allows the construction of a target for DDA calculations, and the calculations can be compared to a single nanoparticle of exactly same size and shape. From the information garnered via SEM and TEM studies, a target consisting of ~ 20,000 dipoles was constructed as a model for the particle. We demonstrate that the surface plasmon peak position is extremely sensitive to tiny changes in morphology and surface roughness.

1) Novo, C., Funston, A. M., Pastoriza-Santos, I., Liz-Marzán, L. M., Mulvaney, P., Angew. Chemie. Int. Ed., 2007, 46, 3517-3520.

Lunch break

Tuesday afternoon, 16 September, 12:30
Inner Courtyards

OPTICAL AND STRUCTURAL CHARACTERIZATION

Tuesday afternoon, 16 September, 14:00
Room 206
Chair: HARALD GIESSEN

14:00 Keynote lecture

Surface Plasmon Spectroscopy of Single Metal Nanocrystals

Paul Mulvaney

The University of Melbourne, School of Chemistry, Parkville, VIC, Melbourne 3010, Australia

e-mail: mulvaney@unimelb.edu.au

In this talk I will provide an overview of our recent research into the spectroscopy and surface chemistry of single gold nanocrystals. In the first part, I focus on the possibility to study the optical properties of single metal particles using dark-field microscopy. It is now possible to routinely collect the scattered light from single metal nanocrystals and use this to study the effects of particle size and shape on the surface plasmon (SP) resonances. We show that the linewidth of the SP resonance is acutely sensitive to the particle end cap geometry, to the aspect ratio and to atomic roughness on the particle surface. In the second part I will discuss the possibilities to study catalysis on single nanocrystals and the ability to actively modulate the surface plasmon bands of single gold nanocrystals by electrochemical charging of the particles. This enables the reversible tuning of the band by some 15nm.

1. Electronic Tuning of the Surface Plasmon Resonance of Single Gold Nanorods, C. Novo, A. M. Funston, A. Gooding, P. Mulvaney, *submitted.*

2. Drastic Surface Plasmon Mode Shifts in Gold Nanorods due to Electron Charging, Paul Mulvaney, Jorge Pérez-Juste, Michael Giersig, Luis M. Liz-Marzán, Carlos Pecharromán, *Plasmonics*, 1, 61 (2006).

3. Gold nanorod extinction spectra, S.Prescott, P.Mulvaney*, J. Appl. Phys*. 99,123504 (2006).

14:40 Oral

Plasmonic resonance in diagnostics of processes for formation of nanosized silver

Galina P. Aleksandrova, Ludmila A. Grishchenko, Svetlana A. Medvedeva, Boris G. Sukhov, Boris A. Trofimov

Irkutsk Instutute of Chemistry (IRICH), 1 Favorsky Street, Irkutsk 664033, Russian Federation

e-mail: alexa@irioch.irk.ru

Distinctive optical properties of nanosized metals make them very promising for the development of new materials which stimulates search for new methods of their synthesis. Their particular features are connected with possibility to regulate their sizes and therefore their optical characteristics.

The approach to synthesis of nanosized silver composites with natural arabinogalactan polysaccharide as reducer and stabilizer is being developed at our laboratory. In the given work optical properties of the solutions during process of formation of silver nanoparticles have been studied. Nanosized mode of metals visually shows itself in absorption spectra as a plasmonic resonance. Thus, particle formation process can be spectrally controlled.

It has been established that optical properties of the particles strongly depend on the pH of medium. In electronic spectra of the solutions wide asymmetric bands of low intensity (l 420-470 nm) typical for initial metal silver clasters are observed starting from pH=5. At pH=9 the bands are transformed to characteristic plasmonic absorption (l_{max} 420 nm) conditioned by collective excitation of nanosized silver electrons supporting conductivity. Spectrum dynamics at pH>10 points to a gradual change of nanosized silver state parameters in the course of reaction. Observations upon solutions with various silver-arabinogalactan ratios have proved that it is possible to control the position of plasmonic absorption maximum. The shifts controlled in plasmonic absorption spectrum of nanoparticles demonstrate the interrelationship with size parameters. The results were obtained for solid samples of the composites by X-ray diffraction analysis data.

The determined principles of the process for nanosized silver formation are perspective for direct regulation of its optical properties which can be applied in development of new materials with controlled non-linear optical characteristics and optical markers in biology and medicine.

Coffee break

Tuesday afternoon, 16 September, 15:30
Main Hall

Wednesday, 17 September

Coffee break

Wednesday morning, 17 September, 10:30
Main Hall

BIOCOMPATIBILITY AND APPLICATION OF NANOSTRUCTURES IN BIOLOGY AND MEDICINE

Wednesday morning, 17 September, 11:00
Room 206
Chair: STEFAN JURGA

11:00 Keynote lecture

Fabrication of Nanoparticles and their Use in Materials and Life Sciences

Horst Weller

University of Hamburg, Institute of Physical Chemistry, Grindelallee 117, Hamburg 20146, Germany

e-mail: weller@chemie.uni-hamburg.de

This talk describes recent developments in the synthesis and characterization of semiconductor and metal nanoparticles using a preparative flow system. Results on the growth kinetics and the control of size, shape and surface chemistry will be addressed. We report on the non-covalent attachment of nanoparticles to carbon nanotubes and shape transformations induced by the attachment. Examples of applications in the area of optoelectronics, photovoltatics and catalysis will be given. We discuss the use of nanoparticles for biological and medical applications which includes a robust coating with biocompatible polymers and embedding nanoparticles in polymer vesicles. We also present experiments on the toxicity of nanoparticles using advanced optical microscopy for in-vitro cell culture studies. Examples on the improvement of magnetic resonance imaging using tailored superparamagnetic nanoparticles are given.

11:40 Invited oral

Laser-induced, reversible dehybridization of DNA attached to gold nanoparticles

Maximilian Reismann[1], Jan C. Bretschneider[2], Katrin Witten[2], Anne Buchkremer[2], Thomas Eckert[3], Walter Richtering[3], Ulrich Simon[2], Gero Von Plessen[1]

1. *Institute of Physics IA, RWTH Aachen University, Sommerfeldstraße 14, Aachen 52074, Germany* **2.** *RWTH Aachen University (RWTH), Landoltweg 1, Aachen 52074, Germany* **3.** *Institute of Physical Chemistry, RWTH-Aachen University, Landolltweg 2, Aachen 52074, Germany*

e-mail: Reismann@Physik.RWTH-Aachen.de

Noble metal nanoparticles show high light absorption at the frequency of the particle-plasmon resonance. When such nanoparticles are heated by absorption of laser light, they transfer their thermal energy to their environment. This heat transfer leads to a temperature increase in the vicinity of the surface of the metal nanoparticle and allows a spatially confined control of nearby (e.g. attached) temperature-sensitive objects. This concept of a nanoparticle-assisted photothermal heating has been investigated in several studies in the context of destructive processes, such as the hyperthermia of malignant cells. In contrast, the photothermal control of non-destructive, i.e. reversible, biomolecular reaction processes have rarely been studied.

In this study we investigated the reversible photothermal control of the dehybridization process of DNA. For this purpose, gold nanoparticle networks were synthesized using complementary single-stranded DNA as linker molecules. The well-known color change of the suspension that occurs upon disassembly or assembly of the nanoparticle networks is applied to continuously monitor the state of the networks using optical spectroscopy. A focused laser beam (c.w., 532 nm wavelength, 5 kW/cm^2 intensity, 100 µm focus size) is used to irradiate a DNA-nanoparticle network suspension. The spatially confined temperature increase that is induced by this photothermal treatment gives rise to the disassembly of the networks, indicating the dehybridization ('melting') of the DNA double strands. After the end of the laser irradiation, the networks reassemble, thus indicating the reversibility of the dehybridization process. It is shown that the DNA melting occurs predominantly within the 100 µm wide laser focus, where the intensity is highest, thus enabling a highly local control of the reaction.

Lunch break

Wednesday afternoon, 17 September, 12:30
Inner Courtyards

BIOCOMPATIBILITY AND APPLICATION OF NANOSTRUCTURES IN BIOLOGY AND MEDICINE

Wednesday afternoon, 17 September, 14:00
Chair: STEFAN JURGA

14:00 Keynote lecture

Biomedical Application of Metallic and Magnetic Nanoparticles

Anton Fojtík

Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical Engineering, Department of Physical Electronics, Brehova str. 7, Prague 115 19, Czech Republic

e-mail: ftk@fjfi.cvut.cz

Nanotechnology is getting still more attention and is becoming emerging topic of recent days. Its biological and medical approaches and applications are opening novel, unpredicted and efficient ways of solving health issues, that is why the extraordinary field of bionanotechnology is shaping into one of the leading sciences of the 21st century… Goal of the project is to functionalize Fe3O4 magnetic nanoparticles, which according to chemical groups attached at the surface, are able to bond to special pathogens (bacteria or virus) and being easily manipulated by magnetic field, they can be removed from the system taking the pathogens with them as well.

Nanoparticles are produced by 'wet' chemical way under special conditions. Final product is 10s of nanometers in diameter and possesses special superparamagnetic properties, which give it ability to be manipulated while working in complex biological systems such as human body. Shape and size of nanoparticles are evaluated using AFM, magnetic properties measured by Mössbauer Spectroscopy and Superconducting Quantum Interference Device (SQUID). Surface of the particles is stabilized and treated, so that they maintain their unique properties and remain stable and separated. Certain chemical groups, proteins or residues are attached onto the surface to functionalize it. Particles are then ready to play a key role in recognition of the pathogens bonding to the surface of nanoparticles and following applied magnetic field to get out of the system.

14:40 Oral

Study of Pd/InP interfaces for Hydrogen detection

Ondřej Černohorský[1], Karel Žďánský[2], Jiří Zavadil[2], Pavel Kacerovský[2], Anton Fojtík[1]

1. *Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical Engineering, Department of Physical Electronics, Brehova str. 7, Prague 115 19, Czech Republic* **2.** *Czech Academy of Sciences, Institute of Photonics and Electronics, Chaberská 57, Prague 18251, Czech Republic*

e-mail: oce@razdva.cz

For preparation good performance sensor it is necessary to prepare high-quality Pd/InP interface with high Schottky barrier. In this sense it is not convenient to prepare this interface by high energetic means of metal deposition because it leads to Schottky barrier decrease induced by Fermi level pinning explained by disorder-induced gap states (DIGS). Our effort is to develop reproducible method for preparation such interfaces with the highest Schottky barrier possible.

For the deposition we used electrophoretic deposition method which put Pd nanoparticles from colloid solution on the InP wafer. This process occurs in a presence of electromagnetic field, which accelerate Pd nanoparticles in the direction to the wafer.

We prepared several interfaces by this method. These structures were analyzed by current-voltage measurements, capacitance-voltage measurements, impedance measurements, AFM, and secondary mass spectroscopy. This measurements show the good rectifying character of this structure and the Schottky barrier high calculated from I-V curves was about 1eV. We also tried to improve properties of this interface by annealing which had positive impact on Schottky barrier high.

This talk is to refer about the progress in the project of central goal to find reproducible method for fabrication Pd/InP interfaces with high-quality properties.

Joint Poster Session 2

Wednesday afternoon, 17 September, 16:00
Main Hall

Posters

Monday, 15 September

Joint Poster Session 1

Monday & Wednesday
Monday afternoon, 15 September, 16:00
Main Hall

16:00 Poster E03

Large area corrugated plasmonic structures formed on a polyester film

Richard J. Winfield, Jing Rao

University College Cork, Tyndall National Institute (TYNDALL), Lee Maltings, Prospect Row, Cork, Ireland

e-mail: richard.winfield@tyndall.ie

The field of plasmonic nanostructures has attracted much interest since Ebbesen reported optical transmission through thin metallic films with submicron holes. Subsequent researchers showed that a similar transmission phenomenon can be demonstrated using corrugated metal films without subwavelength perforation. The fabrication process often uses a complex and expensive lithographic step that inhibits the usefulness of the technique in practical applications.

One technique of improving the speed of fabrication whilst reducing the cost is to use embossing as a way of making the template onto which the metallic structure can be deposited. This makes the realization of large area plasmonic structures possible. In this report we describe the successful use of an embossed polyethylene teraphtalate polymer film onto which a metal layer was evaporated. The films have a 250 nm pitch and are available in areas exceeding 500 cm^2. The transmission properties were measured and compared to the theoretical predictions of a RCWA code. The films show spectral features consistent with the interaction of light with the surface plasmons.

There are a number of applications under investigation including but the sensor area is particularly active and often comprises functionalized surfaces that modify the surface plasmon resonance. The fabrication route proposed here will facilitate large area detection techniques.

16:00 Poster E04

Surface Plasma Absorption in Systems Consisting of Nanoparticles Arrays on a Metallic Substrate

Vo-Van Truong[1], Bernard De Dormale[2]

1. *Concordia University, Department of Physics, 1455 de Maisonneuve West, Montreal H3G1M8, Canada* **2.** *Université de Moncton, Département de mathématiques et de statistique, Moncton E1A3E9, Canada*

e-mail: truong.vo-van@concordia.ca

Surface plasma oscillations in metallic particles as well as in thin metallic films have been studied extensively in the past decades. New features regarding surface plasma excitations are however constantly discovered, leading, for example, to surface-enhanced Raman scattering studies and enhanced optical transmission though metal films with nanohole arrays. In the present work, the role of a metallic substrate is examined in two cases, one involving an overcoat of dielectric nanoparticles and the other, an overcoat of metallic nanoparticles. Theoretical results are obtained by modeling the nanoparticles as forming a two-dimensional, hexagonal lattice of spheres. The scattered electromagnetic field is then calculated using a variant of the Green function method. Comparison with experimental results is made for nanoparticles of tungsten oxide, tin oxide and titanium oxide deposited on either gold or silver substrates, giving qualitative agreement on the extra absorption observed when the dielectric nanoparticles are added to the metallic surfaces. Such absorption would be attributed to the mirror-image effects between the particles and the substrate. On the other hand, calculations of the optical properties of silver or gold nanoparticle arrays on a gold or a silver substrate demonstrate very interesting features in the spectral region from 400 nm to 1000 nm. Interactions between the nanoparticle arrays surface plasmons and their images in the metallic substrate would be responsible for the red shift observed in the absorption resonance. Moreover, effects of particle size and ambient index of refraction are studied, showing a great potential for applications in biosensing with structures consisting of metallic nanoparticle arrays on metallic substrates.

16:00 Poster E05

Investigation of polyvinylpyrrolidone/Ag nanocomposite films prepared by UV irradiation

Valentinas Baltrušaitis[1], Judita Puišo[1,2], Igoris Prosyčevas[1], Asta Guobienė[1]

1. *Kaunas University of Technology, Institute of Physical Electronics, Savanoriu 271, Kaunas LT-3009, Lithuania* **2.** *Kaunas University of Technology, Department of Physics, Studentu 50, Kaunas, Lithuania*

e-mail: judita.puiso@ktu.lt

Silver nanoparticles layers were fabricated using spin coating and UV irradiation of polyvinylpyrrolidone/Ag nanoparticle composite thin films on glass. The spontaneous aggregation of Ag nanoparticles was accompanied with the absorption peak due to surface plasmon resonance (SPR) at 410 nm. Longer irradiation leads to partial coalescence of the nanoparticles with a corresponding shift of SPR towards longer wavelengths. The dependence of the shape, size, and absorbance spectra of these aggregates on UV irradiation time and silver salts concentration were investigated by UV-VIS spectroscopy, XRD and AFM.

16:00 Poster E06

Synthesis of silver nanoparticles by gamma irradiation

Judita Puišo[1,2], Jurgita Laurikaitienė[1], Diana Adliene[1], Igoris Prosyčevas[2], Sigitas Tamulevičius[1,2]

1. *Kaunas University of Technology, Department of Physics, Studentu 50, Kaunas, Lithuania* **2.** *Kaunas University of Technology, Institute of Physical Electronics, Savanoriu 271, Kaunas LT-3009, Lithuania*

e-mail: judita.puiso@ktu.lt

Silver nanoparticles have received considerable attention due to their attractive physical and chemical properties. The surface plasmon resonance and large effective scattering cross section of individual silver nanoparticles make them ideal candidates for molecular labelling. In additional silver nanoparticles have recently been shown to be a promising antimicrobial material. Silver nanoparticles were synthesized by gamma - irradiation of aqueous silver nitrate solution with sodium citrate as reduction and stabilization agent. Silver nanoparticles and their aggregates were monitored by UV-vis spectroscopy. By varying the irradiation dose and ratio of silver salts and stabilisator concentrations, silver nanoparticles with different size and shape could be obtained. The formation of spherical silver nanoparticles and silver nanorods were confirmed by appearance surface plasmon resonance peak at 410 nm and 660 nm. The silver nanoparticles with selective light properties as a result of SRP shifting in the UV-VIS wavelength region were produced.

16:00 Poster E07

The template synthesis of ensembles of isolated Au nanocrystals in silicium dioxide shell

Yuliya I. Pazura, Neonila A. Matveevskaya, Iuliia V. Iermolaieva, Yuriy N. Savin

Institute for Single Crystals NAS of Ukraine (ISC), 60 Lenin Ave., Kharkov 61001, Ukraine

e-mail: pazura.yu@isc.kharkov.ua

Development of new functional optical materials based on the ordered ensembles of monodisperse semiconductor and metal nanocrystals (NCs) is an actual problem. One of the effective methods of formation of NCs ensembles is template synthesis which allows to control density of filling of the modified substrate (template) by nanocrystals and provides the high uniformity of their sizes. To present day the prevention of isolated nanocrystals aggregation on substrates at ensembles formation is one of the unsolved problems. The purpose of the present work is to obtain the ensembles of isolated gold NCs in an environment from silicium dioxide with controlled thickness by the template synthesis method on the modified substrates (glass, quartz). The ensembles of monodisperse gold NCs in diameter of 20 nanometers in an environment from silicium dioxide with thickness 5 - 100 nanometers are synthesized. The characterization of NCs ensembles (structure, sizes, optical properties) was done by methods of electronic diffraction, photoelectronic and optical spectroscopy, electronic microscopy. It is established, that Au NCs have FCC crystal structure with lattice parameters, corresponded to bulk gold. It is shown, that creation of the protective environment from silicium dioxide prevents the aggregation gold nanocrystals on a substrate. The absorption spectra of the ensembles of Au NCs with an SiO2 shell with thickness 5-15 nanometers are characterized by a maximum of plasmonic resonance peak at the 540 nanometers. The increase of shell SiO2 thickness leads to peak broadering and shifting in long-wave region. Thus, changing the thickness of SiO2 shell it is possible to verifying the optical properties of nanostructures studied.

16:00 Poster E08

Towards label-free and highly-sensitive biosensors based on localized surface plasmon resonance

Si Chen, Linda Gunnarsson, Mikael Käll

Chalmers University of Technology, Göteborg S-412 96, Sweden

e-mail: bt03chsi@chestud.chalmers.se

The successful treatment of patients and early preventing of a disease outbreak often require rapid and reliable pathogen detections. This study is a first step to achieve a cost effective and highly sensitive label-free biosensor based on the localized surface plasmon resonance phenomenon. Gold nano disks supported on a glass substrate with diameter of 100 nm and height of 70 nm are fabricated with the in house developed method, hole mask colloidal lithography (HCL). The diameter and height of the nano-disks are chosen so that the optical scattering and absorption of the nano disks match the visual light region 550 - 700 nm with an extinction maximum at around 600 nm.

The sensitivity and the electric field decay length of the nano disks are characterized by deposit thin layers of SiO_2 with different thickness. Biorecognition systems such as biotin - streptavidin and anti-prostate specific antigen antibody (anti-PSA) - PSA have been used to verify the biosensing application of such nano disks. With a noise level of 0,02 nm peak shift, the detection limit for the first layer of protein absorbed on the surface of nano disks is 10 ng/cm^2. A biosensing experiment with antibody and vaccine was also performed to demonstrate and simulate the pathogenic sensing ability of this kind of biosensors.

16:00 Poster E10

Bactericidal effect of metal nanoparticles and their characterization

Kateřina Štyndlová[1], Anton Fojtík[1], Marie Weiserová[2]

1. *Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical Engineering, Department of Physical Electronics, Brehova str. 7, Prague 115 19, Czech Republic* **2.** *Czech Academy of Science, Institute of Microbiology, Vídeňská 1083, Prague 14220, Czech Republic*

e-mail: katerina.styndlova@fjfi.cvut.cz

Nanotechnology is expected to open new avenues to fight and prevent disease using atomic scale tailoring of materials. Rapid development of bio-nanotechnology and material research lead to the new way in the combating of bacteria and to searching specific properties of nanomaterials. The study of bactericidal nanomaterials is particularly timely considering the recent increase of new resistant strains of bacteria to the most potent antibiotics.

The present work studies the bactericidal effect of silver nanoparticles in the range of 7-50 nm on Gram-negative bacteria and Gram-positive bacteria. The colloid silver nanoparticles was prepared by the modified Türkewitsch´s method. This colloid particles has the specific properties which have bactericidal effect.

Relations between bactericidal effects and physical properties of nanoparticles shall be discuss.

Acknowledgements:

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Nano Composite Materials

Symposium F

Nanocomposite materials constitute a rapidly evolving field of science and technology where the first applications are already on the market and many more are expected to follow. The admixture of relatively low amounts of nanoparticles (by definition any morphology having at least one dimension in the nano-range, i.e. particles, fibres, plates) in a matrix of polymer, ceramic or metal has dramatic increasing effects on the resulting properties (volume, surface and functional properties). Unusual property combinations can be realized, resulting in a new class of materials for almost every application.

But before these exciting prospects can be fulfilled, a large number of unresolved questions still need to be answered by science and technology: the understanding of the true nature of such composites, the interaction of the enormously large interface of the nanoparticles with the matrix, the composition/structure/processing/property relationship, the reproducible production routes, the making and source of nanoparticles, and questions on cost, health, sustainability and standardization.

Symposium F on nanocomposite materials aims to provide an overview of the various aspects of nanoparticle composites and thus to intensify the networking and cross-fertilization of ideas between the geographically distant groups working on nano-reinforced polymers, ceramics and metals.

The various oral and poster sessions will last five days and are organized with the help and sponsorship of ENMAT - the European Network of Materials Research Centres and the Cost action NMP0701 on Polymer Nanocomposite Materials.

Specifically, the various sessions will concentrate on the following scientific topics:

- Gaining a better understanding and control of the behaviour of the enormously large interfaces between nanosized particles and the matrix
- Methods for improved uniform dispersion and exfoliation at nanoscale
- Formation of controlled, patterned or hierarchical structures
- Developing advanced nanomechanical modelling and simulation tools
- Effective bonding of nanosized particles to the matrix
- Setting up novel improved processing methods for nanocomposite materials
- Process control to ensure reproducible results
- Developing cost-effective processing methods
- Elaborating, understanding and using the composition/process/property relationships
- Development of adapted or new characterization methods
- Utilizing new, alternative nanoparticles in nanocomposites.

Welcome

The idea of organizing this symposium on nanocomposite materials first came to me at one of the regular meetings of ENMAT in Nuremberg in September 2007 and was inspired by a suggestion from Wolfgang Faul and Paul Kiekens, former chair and vice chair of ENMAT in 2007. Nanocomposites, in particular polymer matrix nanocomposites, provide ample opportunities to develop revolutionary materials for potential applications in electronics, catalysis, ceramics, magnetic data storage and much more.

We had at this time already initiated and prepared a proposal for a networking activity in the field of polymer nanocomposites as we believed that this technical and scientific field, which attracts great interest throughout Europe, could greatly benefit from closer cooperation between the scientists involved. This proposal was submitted to COST and was finally awarded in March 2008.

When the proposal for a scientific symposium to be held at the EMRS fall meeting in Warsaw in cooperation with the COST action was accepted, I had only modest expectations about the number of abstracts that would be received and I was expecting to have at least enough presentations to organize a one day symposium. Shortly afterwards, I was overwhelmed by the large number of abstracts that I had received: 128 in total, more than we could handle in a symposium lasting for a full five days. We were therefore only able to accept 105 of these abstracts: not due to any lack of quality but simply because of time and space limitations and the need to focus the symposium content. I apologize to and ask for understanding from all those authors whose abstracts were not accepted for these reasons.

The oral presentations are grouped in thematic sessions covering polymer matrix based nanocomposites, ceramic and metal matrix nanocomposites as well as the generation and use of nanoparticles and applications of these nanocomposites. The oral presentations are also supported by a great number of poster presentations in two parallel poster sessions.

I believe that this symposium will provide a great opportunity for networking, meeting old and new friends, exchanging ideas and planning future collaborations and joint undertakings.

All of you, authors and participants, will play a key role in the success of this symposium on polymer nanocomposites and I would like to thank you for coming, participating and contributing!

Erich Kny

Chair of Symposium F

Organisers

The various oral and poster sessions of Symposium F will last the full five days of the EMRS fall meeting 2008 and are organized with the help and sponsorship of ENMAT - the European Network of Materials Research Centres and the Cost action MP0701 on Polymer Nanocomposite Materials.

Proceedings

The oral and poster presentations of Symposium F on nanocomposite materials will be published in a special volume on Solid State Phenomena. Only papers that have successfully passed the peer review process will be accepted for the proceedings. It is expected that this special edition of Solid State Phenomena, containing the full texts of all papers presented at Symposium F, will be available towards the end of 2008. The cooperation of all authors in the timely submission of their papers is appreciated in order to meet the expected date of publication.

Each registered symposium participant will receive a paper bound copy of the proceedings. Authors will also receive free online "author access" via their email address (as it appears in the paper) and a supplied password. This access will enable them to download their papers in PDF format and to order reprints online. In addition, participants will receive full online access to the entire proceedings.

Acknowledgements

Right from the very start, when I first had the idea of organizing a symposium on polymer nanocomposites, and throughout the planning and preparation stages of this symposium, I received a great deal of encouragement and help from a number of people and organizations. I would like to greatly thank the following people, in no particular order: Sebastian Vaucher of EMPA, Monika Pilz of SINTEF, Christopher Plummer of EPF Lausanne, Clara Sylvestre of CNR in Italy, Alexandru Morega of the University of Bucharest, Celeste Perera of INEGI, Francesco Branda of Federico II di Napoli, Wolfgang Faul, Mathias Schweinsberg of SusTech and Tassilo Moritz of Fraunhofer, IKTS for their kind, continuous support and their much appreciated willingness to take on various functions in the COST action MP0701. I would like to thank Malgorzata Lewandowska of Warsaw University of Technology and Paul Kiekens, Ghent University, president of ENMAT and vice chairman of the Cost action MP0701, for their continuous encouragement and assistance in the planning and development of this scientific undertaking. Many thanks go to Els van der Burght, representative of ENMAT, Agnieszka Rytel of EMRS and Julia Käfinger of ARCS for their continued support in all organizational and secretarial issues. Last but not least, I would like to greatly thank Milena Stoyanova, Caroline Whelan and Piotr Swiatek, the representatives of the COST office in Brussels, for their financial support, patience and assistance.

Erich Kny

Chair of Symposium F
Chair of Cost action MP0701
Vice president of ENMAT
e-mail: erich.kny@arcs.ac.at
Tel.: +43 50 5502003
Fax: +43 50 5502131
ARC Seibersdorf research GmbH
A-2444 Seibersdorf
Austria

Programme

Monday, 15 September

Opening & Plenary Session

Czochralski Award Ceremony
Monday morning, 15 September, 10:00
Small Hall (237)

Lunch break

Monday afternoon, 15 September, 12:30
Inner Courtyards

afternoon session

Introduction, invited lectures
Monday afternoon, 15 September, 14:00
Room 219
Chair: Kny, Erich

14:00 Invited oral

Principles, applications, and limitations of polymer nanocomposites, cutting-edge materials for innovative engineering uses.

Erich Kny

Austrian Research Centers Seibersdorf (ARCS), Seibersdorf A-2444, Austria

e-mail: erich.kny@arcs.ac.at

Polymer nanocomposites are blends of different polymer matrices with nanometre sized functional particles. The properties of such nanocomposites are remarkably different compared to conventionally filled polymers. The incorporation of only a few percent of nanosized particles can make both dramatic property changes and formerly unachievable property combinations possible. Polymer materials reinforced with nanoscale components are therefore adding new dimensions to composite materials and major improvements in functional and structural properties are within reach. Offering improved barrier properties, fire resistance, and strength, polymer nanocomposites are increasingly desirable as coating, structural, and packaging materials and are of great importance for a multitude of industrial uses in automotive, health care, electronics, aerospace, mechanical engineering, construction and building and consumer products with great economical and ecological benefits. This new technology constitutes a driving force for new employment opportunities in Europe.

Despite such property improvements and despite a large amount of research being undertaken in industry, research laboratories and universities, nanocomposites is still a nascent field of materials science and technology which is in the development stage with tremendous potential growth prospects in the future.

To improve this situation in Europe, and making the best out of what is available requires top level research but also intensified networking and concentration in order to form a critical mass of expertise. The COST Action MP0701 on polymer nanocomposites will be innovative in that sense that a critical mass of expertise can be formed targeting many different areas of application and facilitating the fast exchange of information between different areas of expertise and applications.

14:30 Invited oral

Polymer nanocomposite development for electronic industry needs

Mikko Karttunen, Jari J. Koskinen, Mika Paajanen, Juha Sarlin, Jouni Enqvist, Satu Kortet

e-mail: jari.koskinen@vtt.fi

The properties of polymeric materials have been enhanced by developing nanocomposites in several projects at the Technical Research Centre of Finland VTT. The improvement of conductivity, dielectric, mechanical properties and the thermal stability of polymer materials opens new application potential in electronic industry. In this paper the results of several projects are presented. By applying nano-POSS particles in epoxy the break down voltage was increase by over 20%. The thermal stability of electret materials were improved by adding nano-POSS particles to PP and COC. The use of carbon nanotubes in polyaniline enhanced the conductivity by two decades compared to the commercially available polymers. Isotropic LCP with excellent thermal and chemical properties required in electronic packaging was developed by stabilising the polymer by nanoflakes of magnesium silicate.

15:00 Invited oral

New method for improving properties of polymer composites by using organic inorganic hybrid polymers

Monika Pilz

SINTEF (SINTEF), Forskingsveien 1, Oslo N-0314, Norway

e-mail: Monika.Pilz@sintef.no

Polymer materials are utilized in an increasing number of categories of products, such as components for cars, boats, airplanes, within the electronics industry and other advanced industry as well as in paints and other coatings, for special packaging etc. The uses of polymer materials in new categories of products are only limited by the product properties. It is thus a continuous need for development of polymer products with improved properties e. g. with respect to increased scratch resistance, improved weather resistance, increased UV resistance, increased chemical resistance and improved properties with respect to antioxidation, anticorrosion etc.

In addition to pure polymer materials there has also been developed products based on materials that may be described as hybrids between inorganic and organic materials, which means that these materials are macro molecules that may have an inorganic core and organic branches.

Organic/inorganic hybrid polymers (HP) are prepared based on a SINTEFs well-defined technology (WO2005100450) corresponding to properties of hyperbranched polymers and are used e.g. as additives for polymer products like thermoset plastics and in lacquers and other types of coatings for surface protection. Used in appropriate amounts and with convenient particle size such hybrid polymers may contribute to a significant improvement of the properties of the plastic material or the lacquer, hereunder an increased wear resistance/scratch resistance and/or weather resistance.

It will be shown that the HP additives are suitable for a number of applications within organic chemistry and in particular within polymer chemistry and that they can provide a stabilizer for thermoplastics with a broader range of utility than that known, mono-functional stabilizers exhibit.

Coffee break

Monday afternoon, 15 September, 15:30
Main Hall

Joint Poster Session 1

Polymer matrix nanocomposites
Monday afternoon, 15 September, 16:00
Main Hall

Tuesday, 16 September

Parallel Session

Polymer Nanocomposites I
Tuesday morning, 16 September, 9:00
Room 219
Chair: Kny, Erich

9:00 Invited oral

Silsesquioxane-based hybrid nanocomposites of polymethacrylate type with self-assembling properties

Mihaela A. Olaru[1], Ana-Bogdana Simionescu[2], Magdalena Aflori[1], Emil C. Buruiana[1], Corneliu Cotofana[1]

1. *Petru Poni Institute of Macromolecular Chemistry of the Romanian Academy, Aleea Grigore Ghica Voda 41A, Iasi, Romania* **2.** *University of Oviedo, Dept. of Geology, Calle Jesus Arias de Velasco, Oviedo 33005, Spain*

e-mail: olaruma@icmpp.ro

The aim of this study was to synthesize and characterize new types of silsesquioxane-based hybrid nanocomposites with self-assembling properties. Through radical polymerization of the polymeric matrix (3-(trimethoxysilyl)propyl methacrylate) that contains both methacrylate and silica phases in or without the presence of a surfactant (dodecylamine), new type of hybrid nanomaterials were obtained in which silica was dispersed in the form of domains with typical sizes in the nanometer range. The self-assembling properties of the synthesized composites have been ascribed to formation of polyhedral structures or a combination of linear, ladder, and cagelike fragments of silsesquioxane type. Such materials could find application in stone conservation and water-repellence, as well as drug delivery.

9:35 Oral

An innovative application of polymers swelling by $scCO_2$: their nanostructuration with inorganic nanoparticles

Pauline Vitoux[1], Cyril Aymonier[1], François Cansell[1], Thierry Tassaing[2], Jean Jacques Letourneau[3]

1. *Institut de Chimie de la Matière Condensée de Bordeaux, ICMCB-CNRS ENSCPB, Université Bordeaux, 87 Avenue du Docteur Schweitzer, Pessac 33608, France* **2.** *Institut des Sciences Moléculaires, CNRS-Université Bordeaux, 351 Cours de la Libération, Talence 33405, France* **3.** *Centre RAPSODEE-CNRS, Ecole des Mines d'Albi Carmaux, Route de Teillet, Albi 81013, France*

e-mail: vitoux@icmcb-bordeaux.cnrs.fr

Polymer swelling by $scCO_2$ was mainly studied to understand many industrial processes, especially in the field of pharmacy for drug delivery or polymer processing by CO_2-assisted extrusion. Curiously, the approach of polymer swelling by $scCO_2$ was just occasionally used to functionalize polymer matrixes with inorganic nanoparticles to produce organic-inorganic nanocomposites. Based on the numerous application fields of these organic-inorganic nanocomposites (automotive, aeronautic, pharmacy, chemistry...), we have developed a simple and direct method using supercritical fluids for the synthesis of polymer / metal nanocomposites. The incorporation of copper nanoparticles into two kinds of polymer matrixes (HydroxyTelechelic Polybutadiene (HTPB) as hydrophobic material and PolyEthylene Glycol (PEG) as hydrophilic one) is proposed as model system to study:

- the swelling of these polymers by $scCO_2$
- the viscosity of the polymer / CO_2 systems
- the nucleation and growth of copper nanoparticles into the polymer matrixes

After a brief overview on the potential application of organic-inorganic nanocomposites, we will describe the swelling of both polymers (HTPB and PEG) by $scCO_2$ based on *in situ* IR spectroscopy. The interpretation of these results will be discussed thanks to *ab initio* calculations. The viscosity dependence of both polymers with CO_2 density will be also investigated. Finally the formation of copper nanoparticles in HTPB and PEG matrixes will be studied, especially with *in situ* UV-visible spectroscopy and High Resolution Transmission Electron Microscopy. A good knowledge of the system will allow proposing a correlation between the thermodynamical behaviour of the polymer / CO_2 systems and the nucleation and growth phenomena of formation of copper nanoparticles.

9:55 Oral

Mechanical properties of highly filled latex based polystyrene-laponite nanocomposites.

Riccardo Ruggerone[1], Christopher J. Plummer[1], Elodie Bourgeat-Lami[2], Norma Negrete-Herrera[2], Jan-Anders E. Månson[1]

1. *Ecole Polytechnique Federale de Lausanne (EPFL), Ecublens, Lausanne 1015, Switzerland* **2.** *Chimie, Catalyse, Polymère, Procédé,LCPP, UMR CNRS CPE UCBL, Bât. 308F, BP 2077- 43, Bd. Du 11 Nov. 1918, Villeurbanne 69616, France*

e-mail: riccardo.ruggerone@epfl.ch

Emulsion polymerization provides a convenient route to well disperse polymer/clay nanocomposites. This technique exploits the natural swelling of clay in water and may lead to significantly higher loadings than generally obtained by other techniques (melt blending or in situ polymerization). The present work has focused on nanocomposite films with laponite clay loadings of up to 50 wt %, based on emulsion polymerized polystyrene (PS)/laponite clay latexes in which the laponite platelets are attached to the surfaces of the PS latex particles. Two regimes of reinforcement were identified: below the glass transition (T_g) of the PS matrix, the observed stiffness increases are accounted for in terms of the degree of exfoliation and classical micromechanical models for mechanical reinforcement, whereas above T_g the stiffness increases were correlated with the total clay content and were underestimated by more than two orders of magnitude by these same micromechanical models. Secondary transitions at $T > T_g$ in dynamic mechanical spectra from specimens with clay contents above 20 wt. % implied part of the matrix to show limited chain mobility in this regime. A mechanical model has therefore been proposed to explain the mechanical behaviour in the rubbery state, in which laponite and PS with locally reduced mobility form a cellular network, consistent with TEM observations of the morphology of the nanocomposites and the latexes. This cellular arrangement has also been shown to have important consequences for the microdeformation mechanisms and bulk mechanical properties at high strains, resulting in a transition from crazing to relatively coarse matrix cavitation at the scale of the original latex particles as the laponite content increases. TEM has been used to demonstrate an accompanying decrease in local matrix drawability, accounting for the strong decrease in fracture resistance observed at high laponite contents.

10:15 Oral

Development of polymer matrix clay nanocomposites for industrial applications using high throughput methods

Ignacy Jakubowicz, Nazdaneh Yarahmadi

SP Technical Research Institute of Sweden (SP), Brinellgatan 4, Boras 50115, Sweden

e-mail: ignacy.jakubowicz@sp.se

In the pursuit of improved properties offered by polymer-layered silicate nanocomposites (PNC) a wide variety of concerns must be addressed and a large number of parameters that influence PNC performance must be taken into consideration. Parameters such as polymers, nano-fillers, co-additives, and processing variables generate thousands of combinations/formulations that are worth to be investigated. Consequently, a fairly extensive research and development work is necessary to perform. Often this work is too broad, complex, expensive, long-term and risky for industry to undertake which constitutes an obstacle in the commercialization of nanotechnology. This paper, which is based on the experience from a R&D work for an industrial application, presents a procedure composed of high throughput (HT) screening methods for speed up the development of PNC. Our task was to replace existing conventional glass fibre reinforced polypropylene (PP) used in manufacturing of pallets by PP/montmorillonite nanocomposite. One of the most important HT tools was a 15 cc laboratory-scale twin-screw micro-compounder equipped with 3,5 cc shot volume injection moulder. The HT nature of the micro-compounder was derived from three important abilities viz. the ability to quick alterations of the formulation, the ability to easily change the processing conditions and direct extrusion of the test samples suitable for the evaluation. Equally important was to determine the overall order and morphology of the system to provide a basic understanding of these materials. Wide Angle X-ray Diffraction (WAXD) was used to investigate the intercalation effects due to ease and availability. The shape and dispersion of clay platelets in the polymer was made visible by High Resolution Scanning Electron Microscopy (HR-SEM) but the big advantage with this technique was the possibility to observe the compatibility between the clay particles and the polymer matrix.

Coffee break

Tuesday morning, 16 September, 10:30
Main Hall

Parallel Session

Polymer Nanocomposites II
Tuesday morning, 16 September, 11:00
Room 219
Chair: Plummer, Christopher

11:00 Invited oral

Melt spinning of carbon nanotube modified polypropylene for electrically conducting nanocomposite fibres

Mikael Skrifvars, Azadeh Soroudi

University College Boras (UCB), Allegatan 1, Boras 50190, Sweden

e-mail: mikael.skrifvars@hb.se

Conductive textile fibres find interesting applications in technical and smart textiles. The combination of electronic components such as sensors and actuators into wearable textiles is an on-going effort in the textile R&D. These smart textiles find applications such as monitoring physiological parameters during medical treatment among patients, monitoring elderly people, or personnel working under dangerous conditions such as firemen. Conductive fibres that can be integrated into the textile fabric are of high interest, both for information transfer and for power supply. There are several reported concepts for conductive or semiconductive fibres. Carbon nanotubes (CNTs) are a novel class of materials with potential applications in polymers and plastics. It is well documented that CNTs can be used to make electrically conductive nanocomposites.

This presentation will discuss some recent and on-going efforts regarding the melt spinning of carbon nanotube-polypropylene blends. A commercial single wall CNT-PP master batch (15 wt-% CNT content) was used for the preparation of melt spun fibre filaments. The blends were compounded in a DSM Explore twin screw microcompounder, and further spun into a fibre by using a 0.2 to 0.4 mm spinneret. The spinning temperature was around 180 to 200 °C. The filaments were further drawn (2 – 6 times) at a temperature above the Tg of the PP used, in order to orient the polymer chains and increase crystallinity. The filament drawing was done by using twin Godget rolls, heated to a temperature above the Tg of the PP used. The filament was finally collected on cardboard bobbins.

The resulted fibre filaments were characterised regarding electrical conductivity, mechanical strength, thermal properties and microscopic morphology. The possibility to insert these fibres into fabrics will further be discussed.

11:35 Oral

Functionalisation of multi-walled carbon nanotubes (MWCNT) using 1,3,5-triazine: Characterisation of thermal stability and chemical structure and effect of thermal properties of epoxy resins

Luis Antonio S. De Almeida Prado, Alejandra de la Vega, Jan Sumfleth, Karl Schulte

Technical University Hamburg-Harburg (TUHH), Denickestr. 15, Hamburg 21073, Germany

e-mail: L.Prado@tuhh.de

In the present communication we report the functionalisation of MWCNT using a 1,3,5-triazine, namely melamine. The MWCNTs (Baytubes, Germany) were dispersed in ethanol for 16 hours and allowed to react with melamine at 80°C for 1 hour or 16 hours. The resulting MWCNT-melamine adducts were heated at 250°C under vacuum in order to remove the non-chemisorbed melamine. Thermogravimetric and elemental analyses indicated that a 16 hour vacuum treatment was enough to remove almost 95% of the melamine present in the original adduct. The nitrogen-content of sample decreased from 0.017 mol/gram (for the MWCNT-melamine adduct) to 0.002 mol/gram (the adduct was heated for 16 hours under vacuum). During the treatment at 250°C the melamine can also interact further with the MWCNT yielding either to a physical mixture, or the product of cycloaddition reactions between the 1,3,5-triazine rings and the MWCNTs. Based on the strong resemblance of the Raman spectra of the pristine MWCNTs with that of the MWCNT-melamine, i.e. all samples have spectra with the same intensity for the D and G bands, we suppose that the 1,3,5-triazine rings interact with the graphene layers of MWCNTs by the so-called p-p interactions. Therefore all materials prepared in this work can be regarded as non-covalently functionalised MWCNTs.

The functionalisation of MWCNTs with melamine can bring about enhanced interactions with polymeric matrices. For instance, differential scanning calorimetry results indicated a +10°C shift of the glass transition temperature of an epoxy resin based on bisphenol A (DER 331, Dow Chemical, Germany) and an amine hardener (A2954, Huntsman, Germany) at loading close to 0.10 wt-%. The similar nanocomposite containing 0.10-wt% of pristine MWCNT has a glass transition temperature slightly lower than the neat resin, which is in accordance with previous publications of our group [1].

References:

[1] J. Sumfleeth, L. A. S. A. Prado, M. Sriyai, K. Schulte Adv. Funct. Mater. 2008 (submitted)

11:55 Oral

SWCNT as cure-induced stress sensors in epoxy nanocomposites

Alejandra De la Vega[1], Luis Antonio S. De Almeida Prado[1], Josef Kovacs[2], Wolfgang Bauhofer[2], Karl Schulte[1]

1. *Technical University Hamburg-Harburg, Institute of Polymers and Composites (TUHH), Hamburg 21073, Germany* **2.** *Technical University Hamburg-Harburg, Institute of Optical and Electronic Materials (TUHH), Eissendorferstraße 38, Hamburg 21073, Germany*

e-mail: delavega@tuhh.de

Thermoset composites with improved mechanical properties can be obtained with the addition of homogenously dispersed, well adhered to the matrix carbon nanotubes. Under these constraints, the existence of an effective load transfer mechanism in combination with the electronic and vibrational properties of CNT enables their utilisation as stress sensors in addition to reinforcing elements in the polymeric matrix. In the present work, well dispersed single-walled carbon nanotubes (SWCNT) at concentrations slightly above the percolation threshold (~0.1 wt%) were incorporated to different epoxy resins and utilised to characterise internal stresses arising from the curing process. The curing reaction of the neat and SWCNT-modified epoxies was investigated by differential scanning calorimetry and parallel plates rheometry. The effect of the nanotubes on the cure parameters (i.e. gelation and vitrification times) and glass transition temperature of the neat resins were found to be negligible at this concentration. In-situ Raman and dielectric spectroscopy were performed in parallel on the SWCNT-modified resins, and the ongoing changes at both spectra yield information of the chemical or thermal induced stresses arising at the cure cycle, and which can be responsible for a) the detriment of the mechanical performance of the composite or b) the disruption of the growing SWCNT conductive network. It was found that chemical shrinkage effects are almost negligible in contrast to thermal stresses induced by cooling of the sample below its glass transition temperature (T_g). No stresses were detected for temperatures above T_g of the fully cured composites, pointing at a relaxation effect. Additionally, Raman shift rates of the composites cooling from their ultimate processing temperature were found to be strongly dependent on the chemistry of the epoxy system, pointing at the role of the interfacial interactions of the SWCNT with the matrix upon their shrinkage behaviour.

Lunch break

Tuesday afternoon, 16 September, 12:30
Inner Courtyards

COST MP0701 Meeting

Tuesday afternoon, 16 September, 14:00

Coffee break

Tuesday afternoon, 16 September, 15:30
Main Hall

COST MP0701 Meeting

Tuesday afternoon, 16 September, 16:00

Wednesday, 17 September

Parallel Session

Polymer Nanocomposites III
Wednesday morning, 17 September, 9:00
Room 219
Chair: Skrifvars, Mikael

9:00 Invited oral

Deformation and fracture in isotactic polypropylene glass mat thermoplastic composites modified with montmorillonite clay

Christopher J. Plummer, Sara Dalle Vacche, Chrystèle Houphouët-Boigny, Jan-Anders E. Månson

Ecole Polytechnique Federale de Lausanne (EPFL), Ecublens, Lausanne 1015, Switzerland

e-mail: Christopher.plummer@epfl.ch

The presence of well dispersed montmorillonite (MMT) clay in glass mat thermoplastic (GMT) grade isotactic polypropylene (iPP) results in significant increases in the melt viscosity at low shear rates, and this is shown to reduce the rate of impregnation of glass fibre mats in model experiments [1]. Satisfactory impregnation has nevertheless been obtained with iPP/MMT under conditions comparable to those used in industrial processing, and the flexural modulus of consolidated specimens prepared from the modified GMT has been found to show much greater increases than expected from the measured increases in the matrix stiffness on MMT addition. By using a combination of etching and optical and atomic force microscopy it has been demonstrated that the MMT is relatively homogeneously distributed within the matrix, i.e. that there is little filtering by the fibre bed, and that its presence significantly influences relaxation of the glass mat during impregnation, leading to modified through-thickness glass fibre distributions in the consolidated specimens. Thus, depending on the initial lay-up and overall glass fibre content, the bending modulus and strength of the consolidated specimens may either increase or decrease with increasing matrix MMT content, whereas the tensile properties are more consistent with the predictions of simple micromechanical models based on the assumption of a uniform glass fibre distribution. Results from fractographic analyses are used to show that the presence of matrix rich layers at the specimen surfaces may also lead to premature crack initiation and effective failure in flexion and under impact.

[1] Houphouët-Boigny, C., Plummer, C.J.G., Wakeman, M.D., Månson, J.-A.E., “Glass fiber reinforced thermoplastic nanocomposites” Journal of Thermoplastic Composite Materials.2008; 21: 103-118.

9:35 Oral

Immobilized fraction in crystallizable polymer nanocomposites

Andreas Wurm[1], Mohamed Ismail[1], Bernd Kretzschmar[2], Doris Pospiech[2], Christoph Schick[1]

1. *University of Rostock, Inst. of Physics, Polymerphysics, Rostock 18051, Germany* **2.** *Leibniz Institute of Polymer Research Dresden, Dresden 01069, Germany*

e-mail: andreas.wurm@uni-rostock.de

During isothermal crystallization of numerous polymers the base-line heat capacity decreases below the expected value when a two phase model is applied, where only rigid crystalline and mobile amorphous regions are assumed. It can be shown that the formation of a rigid amorphous fraction, which can be quantified by the heat capacity step at glass transition satisfies the obtained value. In some polymers, the rigid amorphous fraction is developed simultaneously with the crystal formation and not upon further cooling [1]. On the other hand, it was found that polymer composites based on inorganic nano-sized fillers distributed in an amorphous polymer matrix show a rigid amorphous fraction, too [2]. In this contribution we will discuss rigid amorphous fractions in crystallizable polymer nanocomposites. The rigid amorphous material in this class of polymers originates simultaneously from two different interaction mechanisms: (i) rigid amorphous due to interaction of the polymer with the crystals and (ii) rigid amorphous due to interaction of the polymer with the nanofillers. We present heat capacity data which allow determining fractions of different mobility for different filler contents (see fig. 1).

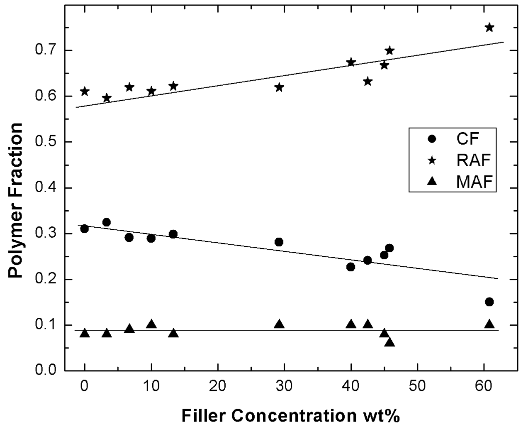


Fig. 1: Rigid amorphous fraction (RAF), crystalline fraction (CF), and mobile amorphous fraction (MAF) in semicrystalline Polyamide-6.6, filled with organophilically modified layered silicate Nanofil919 as a function of filler concentration. MAF was determined from heat capacity step at TG, CF from the melting enthalpy, and RAF as the remaining.

The remaining mobile amorphous fraction in polyamide-6.6/Nanofil 919 nanocomposites seems to be independent on the filler content as well as on the total rigid fraction (RF = CF + RAF). Only the distribution of crystalline and rigid amorphous fraction changes as a function of filler content.

1. Schick C, Wurm A, Mohammed A. Therm. Acta 2003:396(1-2):119

2. Sargsyan A, Tonoyan A, Davtyan S, Schick C. Europ. Polym. Jour. 2007:43:3113

9:55 Oral

Novel segmented polyurethane-based nanocomposites

Geta David[1], Mihaela A. Olaru[2], Bogdan C. Simionescu[1,2]

1. *Technical University from Iasi (UTI), Bd.D.Mangeron 63, Iasi 700050, Romania* **2.** *Petru Poni Institute of Macromolecular Chemistry of the Romanian Academy, Aleea Grigore Ghica Voda 41A, Iasi, Romania*

e-mail: geta_david2000@yahoo.com

Novel segmented polyurethane/organically modified montmorillonite nanocomposites were prepared, covering a wide range of inorganic composition. The influence of structural and compositional variety on constituent interactions, especially on the polymer ability to exfoliate the nanometer scale silicate layers of the organoclay, was studied by comparing nanocomposites with varying degrees of polarity, hydrophilicity, H-bonding ability of the soft polyurethane segments and clay loading.

The effect of nano-sized silicate layers of montmorillonite on glass transition, dynamic mechanical and thermal degradation properties of segmented polyurethane was investigated. X-ray diffraction analysis, thermal (differential scanning calorimetry, thermal gravimetric analysis) and spectral techniques (Fourier transform infrared measurements, solid-state nuclear magnetic resonance), optical observation (transmission electron/scanning electron microscopy) as well as mechanical and dynamic-mechanical analysis were used for the characterization of the newly prepared materials.

10:15 Oral

Setting up research-intensive clusters across the EU on characterization of polymer nanostructures - NaPolyNet

Clara Silvestre

Istituto di Chimica e Tecnologia dei Polimeri (ICTP-CNR), via Campi Flegrei, 34, Napoli 80078, Italy

e-mail: silvestre@ictp.cnr.it

On the First of April the new project "NaPolyNet" is started. It is a 36 month project involving 15 partners from 10 European countries. The objective are: 1) to network at regional, national and international level with experts on the characterization of polymer nanostructured materials in the field of packaging, textiles and membranes, bridging the gap between scientific and engineering approaches for the improved understanding of the structure-performance correlation in polymer devices; 2) to facilitate transnational access to important and unique equipment and to train young scientists and SMEs technologists; 3) to harmonize the work necessary for new standards in the field of characterization of polymer nanostructures for packaging, textiles and membranes. NaPolyNet will also focus on latest findings for managing the safety implications of polymer nanostructure along the life-cycle of those products. The activities are grouped into 7 work-packages (WP). After setting up the procedures for managing the project, the team will map the competences in the different field of characterization of polymer nanostructures and will set up a European Open Laboratory (EOL) which is open to partners outside of the consortium incorporating the best and novel characterization methodologies and expertises. The EOL will allow average trained users of equipment for thermal, structural, morphological, mechanical characterization to produce reliable data on nanostructured materials and correctly interpret them. An international Workshop is planned on processing-structure-dynamics-and-properties of polymer nanostructures in order to further support development and design of intrinsically safe nanomaterials. The last part of the project will be dedicated to harmonize the work for preparation of new standards for polymeric nanomaterials characterization and to overcome barriers to the industrial application of polymer nanostructured materials especially in SMEs.

Coffee break

Wednesday morning, 17 September, 10:30
Main Hall

Parallel Session

Applications I
Wednesday morning, 17 September, 11:00
Room 219
Chair: Pereira, Celeste

11:00 Oral

Electrical properties of electro spun nano- fibres of PEO/carbon black composite

Wai Kit Li, Yuen Wah Wong

Department of Applied Physics and Materials Research Centre,The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong 00-852, China

e-mail: 07900613r@polyu.edu.hk

Electro spinning is an efficient technique for the fabrication of polymer nano-fibres. The charges inside the polymer jet tend to repel each other so as to stretch and reduce the diameter of the polymer fibres. By rotating the collector at a fast angular speed, nano- fibres with specific orientation can be obtained. In this study, nano- fibres of Polyethylene oxide (PEO) with carbon black were prepared by electro spinning. PEO was dissolved in a mixture of water and ethanol. PEO is known as an electrolytic polymer. By blending with carbon black powders, its electrical properties along the fibre direction were improved. The fibre morphology and characteristics were studied by SEM and polarized FTIR.

11:20 Oral

Chemical Assembly of Semiconductor Nanocrystals in Solution

Isabella R. Franchini[1,2], Albert Figuerola[1,2], Angela Fiore[1,2], Rosanna Mastria[2], Roberto Cingolani[1,2], Liberato Manna[1]

1. *National Nanotechnology Laboratory of CNR-INFM (NNL), via per Arnesano Km 5, Lecce 73100, Italy* **2.** *Scuola Superiore ISUFI, Distretto Tecnologico ISUFI, Via per Arnesano Km.5, Lecce 73100, Italy*

e-mail: isabella.franchini@unile.it

Controlled assemblies from 0 to 3D of colloidal nanocrystals (NCs) have recently attracted growing interest as a result of their potentially novel electronic and optical properties, which might be different from those of a corresponding collection of non-coupled NCs or from the bulk.[1,3]

One issue that has been mainly addressed in this field is the control of the interparticle distance in the assembly which allows the tuning of the properties of the NC superstructure. In our work different CdX materials (X stands for S^{2-}, Se^{2-} or Te^{2-}) of various sizes and shapes, synthesized by a seeded-growth approach,[4] have been assembled giving rise to only inorganic NC-based superstructures with different branching degrees by easily processable solution-based reactions.

One general assembling strategy has been used for the organization of Type IV-VI semiconductor NCs independently of their nature. The aim of our work is the formation of an inorganic junction between NCs by means of a previous selective nucleation of gold dots (Au) on the tips of the semiconductor nanostructures. Trace amounts of iodine (I_2) were able to glue the Au domains that had nucleated at the tips of the

NCs, as previously observed by Cheng et al.[5]when iodide was added to a colloidal Au solution.

In the solution the final size of the assembly can be controlled by the ratio between NCs and aggregator agent (I_2). The selective nucleation of Au domains in just one or both tips of the chalcogenide NCs introduces preferential anchoring points that allow tuning the assembling freedom degree of the heterostructures.

Semiconductor NCs are interesting candidates for electronic and photovoltaic devices.[6, 7, 8] In addition, zero interparticle distances in the net are expected to improve optical and electronic properties of the assemblies with respect to those of individual NCs. In this sense, the use of continuous and solely inorganic-based semiconductor “polymers” could improve the performance of the final device.

11:50 Oral

Synthesis and characterization of novel proton exchange nanocomposite membranes based on chitosan biopolymer and molecular sieves

Erfan Dashtimoghadam, Mohammad M. Hasani-Sadrabadi

Amirkabir University of Technology (AUT), Hafez, Tehran 15914, Iran Young Researcher Club, Tehran 15655-461, Iran

e-mail: mahdi.hasani@gmail.com

Fuel cells are an attractive alternative to many energy conversion or storage devices. Among the various types of fuel cells, direct methanol fuel cells (DMFCs) are suitable for portable devices or transportation applications. The proton exchange membrane (PEM) material is a key component of the DMFCs. It is work as media for conducting protons from the anode to the cathode. They also provide a barrier against methanol cross-over between electrodes. Hydrophilic membranes based on chitosan are widely used in membrane applications due to its high hydrophilicity, good chemical/thermal resistance and high mechanical strength properties. So our aim in this study was to develop a novel high performance and also low cost proton conducting membranes based on chitosan. To reduce methanol crossover of membrane while maintaining essential proton conductivity, we have investigated the preparation of polymer-zeolites nanocomposite membranes. Nanocomposites were prepared by incorporating of nanoscale ZSM-5 zeolite (SiO_2/Al_2O_3=25) into chitosan biopolymer. Membranes were fabricated by solution-casting technique. Synthesized membranes were cross linked for improved dimensional stability in aqueous environments. Morphology of composites was studied by X-ray diffraction (XRD) and scanning electron microscopy (SEM). Sorption studies indicated that the degree of swelling for ZSM-5 filled membranes increased with zeolite content. The transport properties were characterized by measuring the methanol diffusion coefficient and proton conductivity as functions of nanoparticle loading weights. Fabricated membranes from cross-linked chitosan with ZSM-5 showed higher membrane selectivity (ratio of proton conductivity to methanol permeability) compared to Nafion117 as a commercial PEM. According to results, the nanocomposites based on chitosan biopolymer and zeolitic molecular sieves are excellent candidate for fuel cells applications.

12:10 Oral

High Dielectric Permittivity and Low Percolation Threshold in Nanocomposites Based on Poly(vinylidene fluoride) and Exfoliated Graphite Nanoplate

Jintu Fan[1], Fuan He[1], Sienting Lau[2]

1. *Institute of Textiles and Clothing, The Hong Kong Polytechnic University, Hung Hom Kowloon, Hong Kong* **2.** *Department of Applied Physics and Materials Research Centre, The Hong Kong Polytechnic Universit, Hunghom, Kowloon, Hong Kong, China, Hong Kong 0852, Hong Kong*

e-mail: tcfanjt@inet.polyu.edu.hk

A novel poly(vinylidene fluoride)/exfoliated graphite nanoplate (PVDF/xGnP) nanocomposite was successfully fabricated by a solution-cast and hot-press method. It was found that the homogenous dispersion of xGnP in the PVDF matrix could significantly improve the dielectric constant of PVDF/xGnP nanocomposite with extremely low percolation threshold. The high dielectric constant of more than 200 and 2700 could be obtained in the PVDF/xGnP nanocomposite near the percolation threshold (1.01 vol%) at 1000 Hz and 100Hz, respectively, which is 20 and 270 times more than that of PVDF matrix. When above the percolation threshold, the dielectric constant kept on increasing and the maximum value was as high as 4.5×10^7 with a high dielectric loss of 229 at 1000 Hz (2.34 vol%).The giant increment of dielectric permittivity can be explained by the combination of the micro-capacitance structure model and MWS effect. These flexible PVDF/xGnP nanocomposites with such high dielectric performance make them potential materials for practical applications in high charge-storage capacitors and electromagneticwave absorption.

Lunch break

Wednesday afternoon, 17 September, 12:30
Inner Courtyards

Parallel session

Application II
Wednesday afternoon, 17 September, 14:00
Room 219
Chair: Koskinen, Jari

14:00 Invited oral

Flame retardancy of thermoset polymer nanocomposites based on nanoparticles and carbon nanotubes

Celeste M. Pereira

Instituto de Engenharia Mecânica e Gestão Industrial (INEGI), Rua Doutor Roberto Frias, 378, Porto 4200Porto, Portugal

e-mail: cpereira@inegi.up.pt

An increasing number of structures are being made from fibre reinforced composites. For example, on aircraft, some crucial components are generally made from carbon fibre reinforced composites using an insulating thermoset polymer matrix. Furthermore, standard thermoset resins, i.e. epoxy and unsaturated polyester, are highly flammable and produce large quantities of smoke and toxic gases. Their increasing commercial utilization may bring these polymers into fire situations at any time, adding urgency to the development of effective and environmental friendly flame retardant systems to reduce fire hazards.

Commercially available flame retardants for these polymers can be highly effective but they have some important disadvantages, like, negatively affecting the resin workability, the quality (physical and mechanical properties) of the final product, in addition to being harmful. The concept of nanoscale reinforcement and flame retardancy provides opportunity for synthesis of new polymer materials with unique properties. Several nanoparticles, that is nanoclays and nano-$Mg(OH)_2$, and carbon nanotubes could also represent a rational alternative to the conventionally filled thermoset polymers because they have distinct advantages over traditional flame retardants on its related problem areas.

The purpose of this paper is to present the effects of different nanoscale flame retardants on flammability properties, such as the time-to-ignition, heat release rate, and smoke production.

14:35 Invited oral

Magnetically responsive nanocomposite materials

Ivo Safarik, Mirka Safarikova

Institute of Systems Biology and Ecology (USBE), Na Sadkach 7, Ceske Budejovice 37005, Czech Republic

e-mail: ivosaf@yahoo.com

Magnetic nano- and microparticles have already found many important applications in various areas of biosciences, medicine, biotechnology, environmental technology etc. Magnetic particles belong to the group of “smart materials” or “stimuli responsive materials” which exhibit response to external magnetic field. In most cases magnetic composite particles, prepared from biocompatible synthetic polymers or biopolymers have been used. These particles can be efficiently separated from difficult-to-handle samples and targeted to the desired place, used as contrast agents for magnetic resonance imaging, to generate heat during exposition to alternating magnetic field, to modify bio molecules and biological structures etc.

Different areas of biosciences and biotechnology have already benefited from the application of biologically active compounds (antibodies, enzymes, lectins, nucleic acids, oligonucleotides, specific affinity ligands) immobilized to magnetic nano- and microparticles (e.g., immunomagnetic assays of target compounds, affinity separation of cells, cell organelles or molecules, molecular biology applications, magnetofection, etc.). Biocompatible and biodegradable magnetic materials have been used as contrast agents during MRI, for magnetic drug targeting and magnetic fluid hyperthermia. Magnetically responsive microbial cells or lignocellulose, useful for xenobiotics removal, can be prepared by ferrofluid modification.

Both biosciences and nanotechnology can have enormous benefit from close mutual cooperation.

14:55 Oral

Cellulose acetate butyrate long fibre polyvinyl alcohol nanofibrecomposites

Nick Tucker[1], Lasse T. Hansen[2], Jon J. Stanger[1], Kathleen Hofman[1], Mark Staiger[3], Nigel G. Larsen[1]

1. *The New Zealand Institute for Crop and Food Research Ltd (CFR), Private Bag 4704, Christchurch 8140, New Zealand* **2.** *University of Southern Denmark (SDK), Niels Bohrs Allé 1, 5230 Odense M, Odense 5230, Denmark* **3.** *Dept. mechanical Engineering, University Canterbury (ME-UOC), Private Bag 4800, Christchurch 8140, New Zealand*

e-mail: tuckern@crop.cri.nz

Cellulose acetate butyrate (CAB) has long been used as a composite matrix as part of fabric coatings in the aerospace industry. It also has the ability to form thin tough films by casting. This property can be exploited to make experimental long nanofibre composites. Polyvinyl alcohol (PVoH) fibres were electrospun to use as the reinforcing element, these fibres were cast into CAB films to produce composite test specimens.

The electrospinning machine used for this work has a constant head device to feed the spinning head (a standard micropipette tip). The use of this type of constant pressure feed allows the user to establish a stable meniscus for the formation of the Taylor cone, and consequent drawing of fibre, the rate of meniscus replenishment is automatically matched to rate of fibre removal. A passive method was used to produce fibres with a high degree of orientation, and random orientated fibre was also manufactured.

The material properties of the composites were examined using an Instron Universal Tester, and the mode of failure of the composites was examined by scanning electron microscopy (SEM).

15:15 Oral

Synthesis & Characterization of Silicon Hybrids Nano Composites Containing Non-linear Optical Dyes

Yasaman Aghili[1], Mohsen Mohseni[1], Ezzeddin Mohajerani[2], H. R. Shirvani[2], Siamak Moradian[1], Alireza Khosravi[1]

1. *Amirkabir University of Technology (AUT), Hafez, Tehran 15914, Iran* **2.** *Shahid Beheshti University, Laser Research Institute, Tehran 15914, Iran*

e-mail: aghiliyas@gmail.com

A stable host-guest system was prepared to improve the nonlinear optical (NLO) effects as well as the mechanical and morphological properties of the polymeric host matrices. A hybrid organic-inorganic nano composite synthesized via the sol-gel process in our previous work and Disperse Red 1 (DR1) were utilized as the host and the guest, respectively. Thin films were deposited on glass slides using a dip-coater rig. Dichroism measurements were carried out to gain information on the aggregation of the dye molecules and also the orientation mechanisms. In addition, birefringence studies were performed to determine the desired variations of the refractive indices. The diagrams analyses were especially focused on the changing tendency of three parameters in different samples; the signal level, the rise time and the fall time.

References:

1. R.Ugo et al., Coordination Chemistry Reviews, 250 (2006) 1210-1233.

2. V. Ross et al., Journal of Non-crystalline Solids, 342 (2004) 140-145.

Coffee break

Wednesday afternoon, 17 September, 15:30
Main Hall

Joint Poster Session 2

Metal/ceramic matrix nanocomposites
Wednesday afternoon, 17 September, 16:00
Main Hall

Thursday, 18 September

Parallel symposia

Application III
Thursday morning, 18 September, 9:00
Room 219
Chair: Branda, Francesco

9:00 Oral

Development of Fe_xO/chitosan meso-porous "nano-rise" for organ-specific drug delivery vessels

Oleg Vasylkiv, Hanna Borodianska, Taras Kolodiazhnyi

National Institute of Material Science (NIMS), Tsukuba, Japan

e-mail: oleg.vasylkiv@nims.go.jp

The size dependent properties and biocompatibility of magnetic nano-Fe_xO are extremely promising for assembling of the drug delivery vessels. Drug delivery vessels should provide minimally invasive solutions to achieving organ-specific delivery, minimize toxic side effects, and signify efficiency of drugs (including chemotherapeutic agents, and gene therapies) to the pathologic tissues. We report on the engineering of rice seeds-like iron oxide-based nanoaggregates uniformly covered with chitosan and its physical properties. Nano-aggregates of highly ordered 7-12 nm crystallites with exact composition are shown to become stable and chemically inert drug carriers. Advanced features of Fe_xO –based nanoseeds will allow their use as new reliable and effective targeted delivery media instead of standard therapeutical treatment. Magnetic properties of seed-like Fe_xO/chitosan nanocomposites including magnetic moment, saturation magnetization, coercive field and remanence magnetization of FexO were studied in the temperature range of 10 – 400 K.

9:17 Oral

Biomimetically synthesized silica-carbon nano-fibre architectures for the development of highly stable electrochemical biosensor systems

Nikos Chaniotakis, Vicky Vamvakaki, Maria Hatzimarinaki

University of Crete, Chemistry Department, Voutes P.O Box 2208, Heraklion 71003, Greece

e-mail: vickyvam@chemistry.uoc.gr

Biomimetically synthesized silica, and conductive activated carbon nano fibres (CNFs) are used in a synergetic manner for the development of a novel electrochemical biosensor system. Poly(L-lysine) templated silica grows and encapsulates the CNF immobilized enzyme generating a highly stabilizing nanostructured environment for the underlying protein. Concurrently, CNFs provide both the required surface area for the high capacity enzyme immobilization required in biosensors as well as direct electron transfer to the inner platinum transducer. As a result, this silica/nano fibre superstructure is an ideal architecture for the development of electrochemical biosensor systems that can withstand exposure to extreme operational conditions, such as high temperatures, or the presence of proteases. AChE is used as the model catalyst, and with the aid of spectroscopic data it is proven that the observed high operational stability of the biosensor is due to the direct interaction of the protein with the silica backbone, as well as due to the nanostructured enzyme confinement.

9:34 Oral

Ag/polystyrene nanocomposite formation for anti bacterial applications

Maryam Raftari[1], Azam Iraji zad[1,2], Akhtarolmelook Kazemi Veisari[3], Seyed Mohammad Mahdavi[1], Reza M. Tilaki[1]

1. *Physics Department Sharif University of Technology, Azadi Avenue, Tehran 14588, Iran* **2.** *Institute for Nanoscience and nanotechnology Sharif University of Technology, Azadi Avenue, Tehran 14588, Iran* **3.** *Biochemical and Bioenvironmental Engineering Research Center, Sharif University of Technolog, Azadi Avenue, Tehran 14588, Iran*

e-mail: astromaryam@gmail.com

Silver nanoparticles/polystyrene nanocomposites were prepared via casting the solution of polystyrene in a mixture of carbon tetrachloride and acetone containing silver nanoparticles. Colloidal silver nanoparticles in acetone were synthesized by pulsed laser ablation (PLA) of pure bulk silver. Casting of the colloidal silver nanoparticles in a solution of polystyrene results in a yellowish transparent polymeric sheet. We study size and stability of particles in the polymer solvent (acetone). TEM images show rather spherical nanoparticles with mean diameter of 5 nm. Ag/PS nanocomposites were characterized by UV-VIS spectroscopy. In this study, we also investigated the antimicrobial activity of silver nanocomposites against Escherichia coli (E.coli) and Staphylococcus aureus (S.aureus) as a model for Gram negative and Gram positive bacteria. Bacteriological tests were performed in Luria bertani (LB) medium on solid agar plates and Nutrient broth in liquid system. These nanocomposites were shown to be an effective bactericide. Antibacterial tests were performed against E. coli and S.aureus, on LB agar plates containing different amount of nanoparticles. Our results showed at all these concentrations, the nanoparticles caused a growth delay of E. coli, increasing the concentration of nanoparticles increased this growth delay. Our results showed that PLA method can be used for Ag nanoparticle formation for antibacterial applications.

9:51 Oral

Design of an Intelligent in situ Nanotechnology Sensor for Determining Bone Growth

Sirinrath Sirivisoot, Rajesh A. Pareta, Thomas J. Webster

Brown University, Providence, RI 02912, United States

e-mail: sirinrath@brown.edu

The objective of this research is ultimately to design a sensor based on nanotechnology to determine events (such as infection, inflammation, or bone growth) on the surface of an orthopedic implant and respond accordingly depending on what is happening. For example, long-term antimicrobial/antibacterial therapy leading to revision surgery can be avoided by incorporating antibiotics on a Ti implant surface, which releases when such a sensor recognizes bacteria functions. In this study, penicillin/streptomycin (P/S) and dexamethasone (Dex) were successfully immobilized by electropolymerization within polypyrrole thin films coated on the surface of Ti, which is widely used in orthopedic applications. Poly(D,L-lactic-co-glycolic acid) (PLGA) was further used to prolong Dex release. *In vitro* results showed that greater numbers of human osteoblasts adhered on these polymer-coated substrates than conventional Ti. X-ray photoelectron spectroscopy monitored and compared the reaction effectiveness and the yield of electropolymerization. Polypyrrole thin films with P/S and Dex, and even further coated with PLGA, all possessed nanometer scale roughness, as analyzed by atomic force microscopy. In summary, this study demonstrated that P/S or Dex drug incorporated within electroactive polypyrrole films, whose release could be controlled by the developed sensor, supported osteoblast adhesion and could potentially fight both bacterial infection and inflammation.

10:08 Oral

Plasma-engineered polymer thin films with embedded nanosilver for prevention of microbial adhesion

Claire Saulou[1], Muriel Mercier-Bonin[2], Sandrine Zanna[3], Phillipe Marcus[3], Patrice Raynaud[1], Bernard Despax[1]

1. *Laboratoire Plasma et Conversion d'Energie (LAPLACE), 118 Route de Narbonne, Toulouse 31062, France* **2.** *Laboratoire d'Ingénierie des Systèmes Biologiques et des Procédés (LISBP), 135 Avenue de Rangueil, Toulouse 31077, France* **3.** *Ecole Nationale Supérieure de chimie de Paris (ENSCP), 11 rue P. et M. Curie, Paris 75005, France*

e-mail: claire.saulou@insa-toulouse.fr

Recently, there has been a growing interest in the study of metallic nanoclusters surrounded by an insulating matrix, to prevent microbial adhesion. The present project is thus focused on the plasma deposition of thin films (~100 nm) containing Ag nanoparticles embedded in a polymeric matrix, on stainless steel. Silver has been chosen for its broad-spectrum antimicrobial properties. Stainless steel AISI 316 L was selected because of its extensive use in agro-food equipments and in biomedical devices. Nevertheless, a strong and specific microorganism adhesion was previously demonstrated on this surface. To avoid adhesion, stainless steel surfaces were coated with plasma-mediated nanocomposite films. The process originality relies on a dual strategy associating Ag target sputtering and plasma polymerization in argon-hexamethyldisiloxane plasma, using an asymmetrical RF discharge. The film properties can be controlled through changes of the operating conditions (precursor flow rate, applied power…). Polymeric matrix have been analysed by FTIR. The presence of Si-H, Si-O-Si, Si-$(CH)_n$-Si and C-H groups was established. The Ag atomic compositions, evaluated by XPS measurements, were in the range 0-20%. To determine the anti-adhesive efficiency, detachment experiments were performed in a shear stress flow chamber. The maximal detachment efficiency was achieved with the polymeric matrix, thus confirming its anti-adhesive properties, probably due to a surface energy modification. Ag antimicrobial effect is assumed to be related to Ag^+ ion progressive release from the embedded particles. The Ag^+ release kinetics was confirmed by ICP-MS measurements: a maximal release was reached after 2 day-contact time. In parallel, film toxicity was evaluated: a significant decrease in cell viability was observed for the maximal silver composition of 20%. From an engineering point of view, film properties have now to be optimized. The film stability will be also particularly investigated.

Coffee break

Thursday morning, 18 September, 10:30
Main Hall

Parallel Session

Nanoparticles I
Thursday morning, 18 September, 11:00
Room 219
Chair: Pilz, Monika

11:00 Invited oral

Evaluation of health risks of nanoparticles – a contribution to a sustainable development of nanotechnology

Volkmar Richter, Annegret Potthoff

Fraunhofer IKTS (IKTS), Winterbergstraße 28, Dresden 01277, Germany

e-mail: volkmar.richter@ikts.fraunhofer.de

Nanoparticles, which are much smaller than human cells, are being used already in many products: cosmetics, paints or tires. These tiny particles are even a selling point for car-care products. So far, little research has been done to evaluate their impact on the environment and humans. However, experience with other emerging technologies has shown that they are only accepted by society if possible health effects are analysed and published early on.

INOS, the "Identification and Assessment of the Effects of Engineered Nanoparticles on Human and Environmental Health" research project funded by the Federal Ministry of Education and Research (BMBF), now aims to shed light on these issues. The project involving five research partners aims to explore how ceramic and metallic nanoparticles and carbon nanotubes affect cells without performing tests on animals. The synthetic nanoparticles investigated are manufactured by project partners or already in use for engineering purposes. These nanoparticles are sheathed in oxide or organic films. The films are formed in practice during processing or are applied specifically to modify properties. These protective coatings can however influence how materials interact with water, cell culture media and cells. The nanoparticles are investigated – with and without protective sheaths, individually and as agglomerates – in cell cultures. This approach allows us to find out how the particles interact with cells of the skin, the lungs, intestine or nervous system. Do they cause DNA damage or have an effect on general cell functions and the immune system? The project aims to answer these questions. The findings will be made available to the public in a database. The project partners also intend to create an accredited laboratory, which will act as a point of contact for small and mid-sized enterprises in particular and carry out further analysis of nanoparticles.

11:35 Oral

Hierarchical 3D ZnO and their shape-preserving transformation into zinc spinel nanostructures

Yang Yang[1], Dong Sik Kim[1], Roland Scholz[1], Mato Knez[1], Seung Mo Lee[1], Ulrich Goesele[1], Margit Zacharias[2]

1. *Max Planck Institute of Microstructure Physics (MPI), Weinberg 2, Halle 06120, Germany* **2.** *Univ.Freiburg, Freiburg, Germany*

e-mail: yangyang@mpi-halle.de

We present novel hierarchical 3D ZnO and zinc spinel nanostructures produced by multi-transformation reactions using Zn as the starting material. In two representative instances selected for illustrating this strategy, various Zn precursors like Zn nanowires and polyhedral Zn microcrystals were first prepared by physical vapor deposition without any catalyst. Subsequently, we successfully synthesized branched ZnO nanowires and hollow ZnO polyhedrons with vertically aligned ZnO nanowires by oxidizing Zn nanowires and polyhedral Zn microcrystals, respectively, under optimal conditions. The growth of both ZnO nanobranches and vertically aligned nanowires was suggested as a self-supplying and self-catalytic process following the vapor transport solid condensation mechanism. Furthermore, the obtained ZnO nanostructures were homogeneously covered by a shell of amorphous Al_2O_3 or TiO_2 using atomic layer deposition. Through the solid–solid interfacial reaction of ZnO and Al_2O_3 (TiO_2), the 3D-nanostructures were transformed to hierarchical zinc spinel nanostructures conserving the shape of the corresponding ZnO nanostructures. This work demonstrates a simple and efficient pathway to design hierarchical ZnO and complex zinc spinel nanostructures, which are expected to have potential applications in nanotechnology.

11:55 Oral

Electrochemical preparation of magnetic nanowires

Beata Kalska-Szostko[1], Ewa Brancewicz[1], Józef Sveklo[2], Piotr Mazalski[2], Wojciech Olszewski[2], Krzysztof Szymański[2], Anna Sidor[1]

1. *University of Białystok, Institute of Chemistry, Hurtowa 1, Białystok 15-399, Poland* **2.** *University of Białystok, Institute of Experimental Physics, Lipowa 41, Białystok 15-424, Poland*

e-mail: kalska@uwb.edu.pl

Electrochemistry is a method, which can be used for the creation of nanomaterials. This method has big advantages concerning the reduced restrictions for shape and size of the samples. Furthermore it does not need expensive equipment for sample preparation.

In the paper the preparation of Ni, Co and Fe nanowires is presented. The diameter and length of the obtained nanowires can be tuned by the properties of the template porous material and the time of deposition, respectively. The quality of the nanowires depends also on the deposition mode (AC - alternating current or DC - constant current) and pH of the solution.

The anodization conducted in phosphoric acid allowed to obtain anodic alumina oxide (AAO) with the smallest pore diameter of about 40 nm. Usage of oxalic acid brings the largest pores of around 120 nm. The deposited material inside the pores has the diameter of the templates. The length can be as large as the thickness of the oxide and reaches up to 1 µm. The morphology of the wires was studied by atomic force microscopy (AFM) and electron scanning microscopy (SEM). The wires show a magnetization direction along the main axis. The magnetic characterization was done by magnetic force microscopy (MFM) and Mossbauer spectroscopy.

12:15 Oral

Luminescent silica nanotubes and -wires from cellulose whisker templates

Hanne Scheel, Cordt Zollfrank, Peter Greil

University of Erlangen-Nürnberg, Glass and Ceramics, Martenstr.5, Erlangen 91058, Germany

e-mail: hanne.scheel@ww.uni-erlangen.de

Luminescent silica nanotubes and -wires were fabricated by sol-gel coating of cellulose whisker templates. The cellulose templates were removed by calcination at 650 °C to generate silica nanotubes. At calcination temperatures of 900 °C the core region previously occupied by the cellulose whisker template was closed yielding silica nanowires. Transmission electron microscopy (TEM) revealed the formation of nanotubes and nanowires with diameters of 15 nm and lengths of 500 nm at both temperatures. Before and after calcination the nanotubes and -wires showed an intense blue photoluminescence (PL) excited by 270 nm photons which was dominated by two peaks at 450 nm (2.76 eV) and 470 nm (2.67 eV). Cathodoluminescence (CL) spectra were measured in TEM while the samples were irradiated with 150 keV electrons. The blue emission related to defects induced by electron irradiation was investigated *in-situ* as a function of irradiation dose. The as-prepared silica/cellulose composites and the silica nanotubes calcined at 650 °C showed a fast decay of the CL emission in contrast to the immense signal increase of the silica nanowires calcined at 900 °C . The observed irradiation induced changes in the CL spectra of the silica nanotubes and -wires will be discussed in terms of defect formation and transformation mechanisms.

Lunch break

Thursday afternoon, 18 September, 12:30
Inner Courtyards

Parallel Session

Nanoparticles II
Thursday afternoon, 18 September, 14:00
Room 219
Chair: Richter, Volkmar

14:00 Oral

Synthesis of nanoparticles using electrical discharges.

Matt Griffith, Andrzej Calka, David Wexler

University of Wollongong, Wollongong NSW, Australia

e-mail: andrzej_calka@uow.edu.au

Electric discharges were used to the synthesis of nanoparticles and nanofragments. We describe results of an experimental program underway to investigate phase transformations and/or particle fragmentation during electric discharges using a new pulsed power supply working at frequencies in the kHz range. The aims were to determine processing parameters required for the synthesis of potentially useful high surface area nanoparticles of VC and WC hardmetals.

Microstructural, morphological and phase changes induced by kHz discharges were characterised by X-ray diffractommetry and transmission electron microscopy. Results were found to depend on the often competing processes of fragmentation into nanoparticles, agglomeration of powder particles, particle melting and/or sintering and chemical reactions. Discharge synthesis of WC and VC resulted in products including: micron and submicron fracture products, nanostructural regions and nanorods.

14:17 Oral

Surface chemistry of non-oxidized, molecule-terminated silicon nanowires: monolayer formation, kinetic and oxidation resistance

Muhammad Bashouti

Technion, Technion, Haifa 32000, Israel

e-mail: M.Bashouti@gmail.com

The ability to manipulate the properties of Silicon nanowires (Si NWs) by controlling the chemistry of the Si surface is important for the realization of Si NW based devices for electronics and sensors. However, studies with 0D - 2D crystalline Si surfaces show that the presence of an insulating oxide overlayer is undesirable, because thick layers are electrically insulating and thin layers of the native oxide are electrically defective at the Si/Si-oxide interface. Since a large proportion of the Si atoms of a NW are located at the surface compared to a 2D Si sample, the surface properties of the NWs are of a far greater importance in controlling the electron transport properties than for bulk Si samples.

Here, a two step chlorination / alkylation process was used to connect C1-C11 alkyl functionality to Si NW surfaces without intervening oxide. The process functionalizes 50-100% of the Si sites on the Si NWs surface, most reasonably due to reduced steric effects. The alkylated Si NW surfaces show high chemical stability in ambient conditions, as compared to similar molecules adsorbed on 2D substrates. We attribute these observations to the lower steric hindrance effect on the Si NWs, as compared to 2D surfaces. The alkylated Si NW surfaces show high stability against oxidation for more than one month under ambient conditions. This fact is of practical importance when oxide free surfaces are required, e.g., for radial epitaxial on NWs to realize vertical P-N junctions for solar cells or radial Si/Ge super lattices for application in optoelectronics.

14:34 Oral

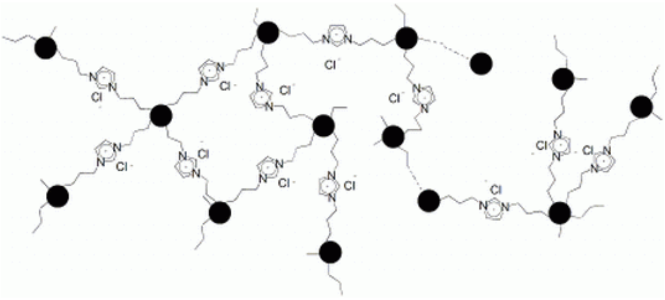
Nanoparticles connected through an ionic linker

Marie-Alexandra G. Neouze, Marco Litschauer

Vienna Technical University, 9, Getreidemarkt, Wien 1040, Austria

e-mail: mneouze@mail.zserv.tuwien.ac.at

The 2D or 3D linking of metal or metal oxide nanoparticles is still a challenge, as well as research concerning the association of ionic species with nanoparticles. The originality of the presented work lies in the combination of nanoparticles organization and concomitantly the introduction of ionic species. The two synthesis methods reported are related to the nucleophilic substitution taking place during the synthesis of imidazolium-based ionic liquids. The first approach utilized bis(trialkoxysilyl)-substituted imidazolium iodide to link the silica nanoparticles. In the second approach, the silica nanoparticles were first modified either by 3-chloropropyltrimethoxysilane or N-(3-trimethoxysilylpropyl)imidazol and then coupled through nucleophilic substitution. A comparison of both approaches shows that the second approach results in a more efficient linkage of nanoparticles. Furthermore, it is new and it is an original method for letting modified nanoparticles react with one another. This will result in covalently linking nanoparticles by means of an ionic linker and is characterized by using TGA, solid state NMR and



14:51 Oral

pHEMA-Silica Nanocomposites Through in Situ Sol-Gel Method

Francesco Branda, Aniello Costantini, Giuseppina Luciani, Antonio Pezzella, Brigida Silvestri, Fabiana Tescione

e-mail: branda@unina.it

Poly-2-hydroxyethilmethacrylate(pHEMA)-nanosilica composites were prepared by hydrolysis and polycondensation of ethoxysilanes (Stöber method) in the presence of HEMA monomers and successive hybrid polymer cure. Two procedures were followed.

Procedure A was used to prepare a nanocomposite with silica 30% weight content. The appropriate HEMA amount was dissolved into ethanol solution containing tetraethoxysilane (TEOS) (1.09 M), H_2O (12.8 M) and NH_3 (0.64 M). While stirring (50 min) the radical initiator (α, α'azoysobutyrronitrile (AIBN)) was added in concentration 0.1%. Water, ammonia and ethanol were removed at 60°C. The polymer was cured at 80°C (overnight) and 90°C (2h).

Procedure B differed mainly for the substitution of half TEOS amount with 3-aminopropyltriethoxysilane (APTS) that was preventively left to react (6d at 40°C) with an equimolar amount of HEMA. The coupling hybrid monomer formation was supported by ^{13}CNMR and mass analysis. The mole ratios H_2O/TEOS+APTS and NH_3/TEOS+APTS were taken constant to the values 11.8 and 0.59 when preparing pHEMA nanocomposite with silica weigh concentrations of 10, 20 and 30%.

The procedure strongly affected the nanocomposite structure: the silica nanoparticle mean diameter changed from 500 nm to about 10 nm when the coupling hybrid monomer was used. Transparent composites containing well dispersed silica nanoparticles were obtained by procedure B.

The silica content made the thermal stability to strongly increase and allowed surface hydroxyapatite formation during exposition to simulated body fluids (SBF) so as on bioactive ceramics. The changes in thermal stability, bioactivity and swelling behaviour were well correlated to the silica content and nanocomposite structure.

15:08 Oral

Synthesis, structural and magnetic properties of magnetic metal/semiconductor nanocrystals heterostructures

Sasanka Deka, Roberto Cingolani, Liberato Manna, Pantaleo Davide Cozzoli

National Nanotechnology Laboratory of CNR-INFM (NNL), via per Arnesano Km 5, Lecce 73100, Italy

e-mail: sasanka.deka@unile.it

Multicomponent nanostructures or hybrid nanocrystals were formed from different materials with distinctive properties. One particular material of such kind may combine photoluminescence, magnetic, or catalytic activity, in a single material.[1] Multifunctional nanocomposites based on magnetic metal and semiconductors would be useful in several predicted technological emerging fields, such as in nanomedicine, optoelectronics, magnetic bio-separation and detection, etc.[2,3] In the present report, we demonstrate the seeded growth strategy to grow semiconductor-magnetic metal hybrid nanostructures. Here we grew Co metal spheres preferentially on different faces of semiconductors nanorods (such as, CdS, CdSe, CdSe/CdS core/shell nanorods). The preferential growth of Co at the tip or on the side wall of the nanorods and their different structural and magnetic properties has been preliminarily investigated and will be discussed.

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Coffee break

Thursday afternoon, 18 September, 15:30
Main Hall

Parallel Session

Polymer Nanocomposites IV
Thursday afternoon, 18 September, 16:00
Room 219
Chair: Olaru, Mihaela

16:00 Oral

Fabrication of $BaTiO_3$-PMMA Polymer Nanocomposite Thin / Thick Films and their Dielectric Properties

Amir Habib[1], Nils Stelzer[1], Roland Haubner[2]

1. *Austrian Research Centers GmbH (ARC), Wien 2444, Austria*
2. *Institue of Analytical and Physical Chemistry Vienna University of Technology (CT), Getreidemarkt 9/164, Wien A-1060, Austria*

e-mail: amir.habib@arcs.ac.at

Thin and thick $BaTiO_3$-polymer nanocomposite dielectric films were prepared using $BaTiO_3$ nanoparticles and Poly methyl methacrylate (PMMA). The cubic BaTiO3 (~30-60nm) and tetragonal BaTiO3 (~120nm) synthesized via hydrothermal route were used as nanofillers. The high dielectric constant of 9 was achieved for the films of thickness in the range of 150-300nm, which corresponds to 30-40 nF/cm^2. The dissipation factor of the PMMA composite film was as low as 0.04 at 10^4 Hz. Thick films of 16.3 µm thickness were prepared via wet application method and tested for their capacitance and dielectric properties in the frequency range of 10-100 KHz for cubic and tetragonal $BaTiO_3$. The $BaTiO_3$ particles were dispersed homogeneously in the films at lower filler loading. The homogenous distribution of $BaTiO_3$ achieved by surface functionalization of $BaTiO_3$ nanoparticles and use of tetragonal $BaTiO_3$ resulted in the improvement of their electric properties in thick and thin films.

16:20 Oral

Characterization of PET nanocomposites with different nanofillers

Lyudmil V. Todorov, Carla I. Martins, Júlio C. Viana

University of Minho (UM), Campus of Azurém, Guimarães 4800-058, Portugal

e-mail: lvt@dep.uminho.pt

This study investigates the incorporation of different size and shape nanofillers on the properties of PET nanocomposites. PET was reinforced with 0.3 wt.% of four different shape/size nanoreinforcements, namely: 1D platelet-like shape organo-modified layered silicates (montmorillonite) with average particle sizes (i) 30 µm and other with (ii) 8 µm; (iii) 3D spherical shape titanium oxide with average particle size of 21 nm and (iv) 3D spherical shape silica with average particle size of 12 nm. PET nanocomposites were prepared by melt blending in an asymmetric batch minimixer followed by compression moulding process for sample preparation. The effect of nanofillers upon thermal, mechanical and structural properties in comparison to the neat PET is discussed.

Friday, 19 September

E-MRS & EPDIC Joint Plenary Session

Friday morning, 19 September, 9:00
Small Hall (237)

Coffee break

Friday morning, 19 September, 10:30

Parallel Session

Metal/Ceramic matrix I
Friday morning, 19 September, 11:00
Room 219
Chair: Kny, Erich

11:00 Invited oral

Nickel ceramic nanocomposite by electro-less coating - synthesis and properties

Thomas J. Graule, Yoram DeHazan

Empa, Swiss Federal Laboratories for Materials Testing and Research, High Performance Ceramics, Ueberlandstrasse 129, Dübendorf 8600, Switzerland

e-mail: thomas.graule@empa.ch

Present electro and electro-less nickel (EN) composite research seek new ways to produce protective coatings with improved wear resistance properties or coatings having internal lubrication properties. While co-deposition of micron size particles was extensively used in the past, recent research activities, especially in the electro-deposition arena, are focused on the incorporation of submicron and nano particles.
In order to realize nano or submicron composites, nano-particle dispersions need to be agglomeration-free and stable under the conditions of high ionic strength, multicomponent EN solutions at plating conditions (80-90°C). Recently we have reported on the successful stabilization of alumina colloids in EN solutions using commercial comb-polyelectrolytes [1,2].

The nanometer size alumina powders used in the current study were AluC and TM DAR, respectively. Commercial comb-polyelectrolyte surfactants, consisting of polyether side chains grafted onto a polycarboxylate backbone, and have molecular weights in the 20,000 g/mole range were applied to sterically stabilise the nanoparticle filler. Dispersion stability of colloidal alumina in EN solutions in the presence of comb-polyelectrolytes will be presented and correlated with the quality of deposited nickel nanocomposite layers. Dispersions having higher coverage of comb-polyelectrolytes show low zeta potential but high colloid stability. Initial hardness and POD wear rate tests show dependency on heat treatment and the type, size and concentration of the particles.

References

[1] Yoram de Hazan, Torben Reuter, Dennis Werner, Rolf Clasen, Thomas Graule, J. Colloid Interface Sci., accepted (2008).
[2] Yoram de Hazan, Dennis Werner, Jens Bock, Michael Groeteklas, Thomas Graule, in preparation

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11:35 Oral

“Mechanochemical” nanocomposite materials Me/X.

Andrey N. Streletskii, Igor V. Kolbanev

Institute of Chemical Physics RAS (ICP), Kosygin St., 4, Moscow 119991, Russian Federation

e-mail: str@center.chph.ras.ru

The work deals with possibilities of mechanical activation (MA) and mechanochemical methods for preparation of nanocomposite materials Me/X (Me=Al, Mg, Ti, etc; X= MoO_3, Teflon, C, BN, etc.) with high reactivity. Materials of such types are prospective as energetic and pyrotechnic materials, materials for hydrogen storage and generation of hydrogen, etc. Some methods of preparation have been developed, a defective structure, emerging upon mechanical treatment, and the stage mechanism of nanocomposite formation have been investigated. Considerable attention was paid to the structure and reactivity of “mechanochemical” nanocomposites. The structure of Nano Composites was investigated by TEM, SEM, AFM, XRD and other methods. The reactivity was checked in the three types of reactions: 1) The interaction of “external” gaseous and liquid reagents with nano dimension metals ($Al+O_2$, $Al+N_2$, $Ti+H_2$, $Al+H_2O$àH_2, etc.); 2) Shock wave initiated interaction in MA energetic composites (Al+Teflon, Mg+Teflon, $Al+MoO_3$, $Mg+MoO_3$); 3) The heating-initiated interaction between components of MA nanocomposites ($Al+MoO_3$, $Mg+MoO_3$, Al+C, Al+BN). The acceleration of transformations under the mechanical activation was observed. Thus, for example, mechanical activation results in decreasing the temperature of Al oxidation by 400°C, in-creasing the rate of combustion of energetic composites for more than two orders of magnitude, and the lowering of the temperature of aluminum carbide synthesis by 800 °C, etc. For systems involving Teflon it was possible to realize the detonation-like regime of chemical transformation. The contribution of different physical factors causing the acceleration of transformations after mechanical activation was analyzed.

11:55 Oral

Formation of germanium nanocrystals in SiO_2 matrix using RT magnetron sputtering

Uros V. Desnica[1], Maja Buljan[1], Krešimir Salamon[2], Nikola Radić[1], Pavo Dubček[1], Mile Ivanda[1], Zdravko Siketić[1], Iva Bogdanović-Radović[1], Sigrid Bernstorff[3]

1. *Rudjer Boskovic Institute, Bijenicka cesta 54, Zagreb HR-10000, Croatia* **2.** *Institute for Physics, Zagreb 10 000, Croatia* **3.** *Sincrotrone Trieste, Basovizza 34012, Italy*

e-mail: desnica@irb.hr

Germanium Quantum Dots (Ge QDs) were formed in SiO2 by magnetron sputtering co-deposition of Ge+SiO2, either in form of thick or multilayered films. Deposition temperature, Td, ranged from RT to 973 K. As-deposited samples were subsequently thermally annealed up to Ta = 1000 °C. Ge:SiO2 composition ranged from 40 - 60% mol Ge. The substrate was either SiO2 or ‹111› Si. In layered films (Ge+SiO2) these 'active layers', with Ge were separated by layers of pure SiO2, serving as 'spacer' between ‘active’ layers.

Grazing incidence small angle x-ray scattering (GISAXS) was applied for structural characterization of Ge QDs synthesized in SiO2 amorphous matrix. Chemical composition and phase of QDs were determined by Raman spectroscopy and the spatial distribution and concentration of Ge atoms by Rutherford Back Scattering.

The 2D GISAXS patterns were used to reveal the onset of synthesis of Ge QDs in SiO2, to determine their properties, and for QDs ordering, if occurs. The average size of QDs can be generally controlled by Ta and content of Ge. However, the introduction of spacers brings-in new, independent and better mean to control the size of Ge QDs. Up to Ta=1073 K Ge QDs are fully amorphous and at/above 973 K fully crystalline. Above Ta= 1073 K, and especially above 1173 K Ge atoms out-diffuse strongly from the sample. For RT deposited samples the best quality, spherical, crystalline, stable Ge QDs were obtained by post-deposition annealing in 973-1073 K range. The quality and possible ordering of Ge QDs was strongly affected by Td. Only for Td around 773 K, combined with proper thicknesses of 'active' and 'spacer' layers, the 3D ordering of Ge QDs into hexagonal superlattice was attainable. For either lower or higher Td only week, in-layer, 2D ordering could be achieved. Around Td = 973 K the deposition of Ge becomes inefficient, and deposited Ge atoms form non-spherical, faceted Ge nanocrystals.

12:15 Oral

Ti/C and Ti/B nanocomposites: comparison of hydrogen sorption-desorption properties

Olga Morozova[1], Tatiana Khomenko[1], Alexander Leonov[2], Christine Borchers[3], Ernst Kurmaev[4], Alexander Moewes[5]

1. *Institute of Chemical Physics RAS (ICP), Kosygin St., 4, Moscow 119991, Russian Federation* **2.** *Chemistry Department, Moscow State University, Leninskie Gory, 1-3, Moscow 119992, Russian Federation* **3.** *University of Goettingen, Institute of Material Physics, 1 Friedrich-Hund-Platz, Gottingen 37077, Germany* **4.** *Russian Academy of Sciences, Ural Division, Institute of Metal Physics, 18 S.Kovalevskaya str., GSP-170, Ekaterinburg 620219, Russian Federation* **5.** *University of Saskatchewan, 110 Science Pl., Saskatoon S7N5C9, Canada*

e-mail: om@polymer.chph.ras.ru

The effects of graphite and B on hydrogen absorption by Ti under the mechanical treatment in H2/He flow and on the thermal stability of Ti-hydride produced during milling were studied using kineticand spectroscopic techniques. The results obtained are compared with corresponding properties of pure Ti. Both additives stimulate the formation of occupation sites for hydrogen that are not present when pure Ti is milled in H_2/He flow. These sites are characterized by low H_2 desorption temperature: ~600 K instead of ~1000 K.

Lunch break

Friday afternoon, 19 September, 12:30
Inner Courtyards

Parallel Session

Metal/Ceramic matrix II
Friday afternoon, 19 September, 14:00
Room 219
Chair: Graule, Thomas

14:00 Oral

Defects in silicon nanocrystals embedded in amorphous silicon oxide

Simone Meloni, Mariella Ippolito, Luciano Colombo

Consorzio per le Applicazione del Supercalcolo Per Universita' e Ricerca (CASPUR), via dei Tizii 6, Roma 00185, Italy

e-mail: m.ippolito@caspur.it

Silicon nanocrystals (n-Si) in amorphous silicon oxide (n-Si)O2 is being intensively investigated as promising material for optoelectronics after the discovery of its photoluminescence at room temperature [1].

Two hypothesis have been raised to explain the photoluminescence of n-Si: i) the confinement of wavefunctions as due to the size of nanocrystals and, ii) the presence of defects that generate even more confined orbitals.

Recent photoluminescence experiments under intense magnetic fields [2] show that the emission from silicon nanocrystals grown in amorphous SiO2 (n-Si/a-SiO2) is due to the presence of very localized states rather than to quantum confinement. Experiments also shown than the presence of the defects depend on the size of the nanoparticles. Even though the presence and nature of defects in n-Si in vacuum have been already investigated [3, 4], a study of n-Si in a-SiO2 under experimental conditions, using realistic potentials, is still lacking. In this work, using state-of-the-art empirical force models [5] in combination with molecular dynamics, we have identified various defects in nanoparticle of different size and at various temperatures. These defects can be divided into two classes: i) coordination defects, ii) strain defects. Coordination defects consist in under or over-coordinated silicon atoms. Strain defects consist of stretched Si-Si bonds. In agreement with experiments, our simulations demonstrate that the number and the 'intensity' of these defects decrease with the increase of the of n-Si size. We also observed the diffusion of defects into the SiO2 matrix via a bond switching mechanism.

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14:20 Oral

Electronic band structures and surface states of ZnO finite well structures

Kuo-Feng Lin

Department of Photonics, Institute of Electro-Optical Engineering, National Chiao Tung Univ, Hsinchu 30050, Taiwan

e-mail: xia117.eo94g@nctu.edu.tw

Using tight binding representation of the layered systems grown along <0001> and <1-100> directions, we calculated the band structures (in Fig. 1) and wave functions (in the Fig. 2) for various ZnO slab layers with non-relaxed and non-reconstructed surfaces. We show that dangling bonds on the two end-surfaces cause surface bands for different direction grown slabs. Analyzing the wave functions across the layers, the surface states show a tendency toward surface localization. Particularly, the splitting of the degenerate surface bands increase due to increasing overlap between their wave functions, which are localized on two nonpolar [1-100] end-surfaces, while it is not present for the [0001] finite well with polar end-surfaces. Finally, we also found the extra electron-field due to the [0001] polar end-surfaces can effectively enhance the quantum confinement effect was shown in Fig. 3

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14:40 Oral

Enhanced high-temperature creep resistance of single-wall carbon-nanotubes-reinforced alumina polycrystals

Eugenio Zapata-Solvas[1], Rosalía Poyato[1], Diego Gómez-García[1], Arturo Domínguez-Rodríguez[1], Zonghon Lee[3], Velimir Radmilovic[3], Nitin P. Padture[2]

1. *Universidad de Sevilla (USE), Sevilla 41012, Spain* **2.** *Department of Materials Science and Engineering, the Ohio State University, Columbus 43210, United States* **3.** *Lawrence Berkeley National Laboratory, National Center for Electron Microscopy (LBNL), Berkeley, CA, United States*

e-mail: ezapata@us.es

This work outlines the remarkably enhanced creep resistance of single-walled carbon-nanotubes-reinforced alumina polycrystals. When tested at similar conditions of stress and temperature, the strain rate of such material is two orders of magnitude lower than that reported in non-reinforced alumina polycrystals. The sample processing technique is carefully described as well as the microstructural characterization of the sintered specimens. Particular emphasis is focused on the homogeneity of the nanotubes distribution onto the ceramic grain boundaries. Furthermore, it was verified that nanotubes have not lost their single-walled character either during sintering or during mechanical testing.

The results are compared with those found in literature for rare earth-doped alumina solid solutions. The role of a non-homogeneous distribution of nanotubes is also discussed.

Coffee break
Friday afternoon, 19 September, 15:30
Main Hall

Posters

Monday, 15 September

Joint Poster Session 1

Polymer matrix nanocomposites
Monday afternoon, 15 September, 16:00
Main Hall

16:00 Poster F01

Characterisation of the Chitosan/layered silicate nanocomposites

Catalina Natalia Cheaburu, Cornelia A. Vasile

Petru Poni Institute of Macromolecular Chemistry of the Romanian Academy, Aleea Grigore Ghica Voda 41A, Iasi, Romania

e-mail: duncaty@icmpp.ro

Recently, the description and the synthesis of hybrids, organic or anorganic nanostructured materials had gained much attention due to the particular characteristics and potential applications of new synthesized nanocomposites. Several scientists showed that the addition of chitosan to layered silicates e.g. modified and unmodified montmorilonite (MMT) may improve its thermal stability due to the interactions which occur between the clay particles and chitosan. Chitosan/layered silicate nanocomposites with different ratios via solution-mixing technique showed also that chitosan chains were inserted into silicate layers to form the intercalated nanocomposites. The interlayer distance of the silicates in the nanocomposites enlarged as their amount increased.

This study deals with characterization of chitosan / layered silicate nanocomposites obtained by solution-mixing technique, having different compositions including treated and untreated montmorilonite (MMT). To establish an optimum amount of MMT and also the effect of nanoparticles on nanocomposite properties, DSC, X-ray diffraction and TG measurements were performed.

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16:00 Poster F02

Nanocomposites based on montmorillonite/acrylic copolymers for aqueous coating of soft surfaces

Onur Yilmaz[1], Aurica P. Chiriac[2], Catalina Natalia Cheaburu[2], Loredana E. Nita[2], Gurbuz Gulumser[1], Donatella Duraccio, Sossio Cimmino, Cornelia A. Vasile[2]

1. *Ege University, Leather Engineering Department, Ege University Campus, İzmir 35100, Turkey* **2.** *Petru Poni Institute of Macromolecular Chemistry of the Romanian Academy, Aleea Grigore Ghica Voda 41A, Iasi, Romania*

e-mail: onuryilma@gmail.com

The importance of waterborne coatings has been increased because they are more environmental friendly, have less toxicity and improved flame retardant properties. Beside these advantages it was faced with some disadvantages as decreased mechanical properties, poor water resistance etc., due to the usage of emulsifiers. Consequently, water-based polymer nanocomposites have been increased its importance and have started to be studied by various research groups [1-3] to overcome some of these problems and to improve desired properties. Some recent studies on clay/polymer nanocomposite emulsion coatings have been mostly focused on thermoset or hard thermoplastic polymers in order to obtain better mechanical properties especially for coating of though surfaces. But there are limited works focused on the improvement of the coatings properties for soft surfaces such as textile and leather. The aim of this work is synthesis of the nanocomposites based on montmorillonite and acrylic comonomers e.g. butyl acrylate, methyl methacrylate. Batch emulsion polymerization method was applied. The obtained emulsions and their films were characterized by means of FTIR, XRD, DSC and also mechanical tests were performed.
The DMA analysis of the nanocomposites showed that some mechanical properties are improved significantly especially at the temperatures above Tg. The ultrasonication process was found to be useful to increase the homogeneity of the emulsions containing montmorillonite and to achieve the intercalation. The obtained nanocomposite emulsions were considered to be suitable to apply on garment leathers in finishing formulations as base-coat binders due to their good film forming ability and elasticity.

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16:00 Poster F03

Synthesis and Characterization of Hybrid Silica/poly-Thiophene Nanocomposites of a Core-Shell Morphology

Shirly Partouche, Vadim Kotlyar, Anna Peled, Vladislav Sapozhnikov, Jean-Paul Lellouche

Bar Ilan Universiry, Ramet-Gan 52900, Israel

e-mail: ch204@mail.biu.ac.il

Nanocomposites of inorganic nanomaterials and conductive polymers (CPs) have received special attention due to the expected synergistic contributions of both organic and inorganic components. Some practical applications of nanocomposites containing silica and conducting polymers were extensively studied by Armes et al. (M. Gill, S. P.

Armes, *Langmuir.*, 1992, 8, 2178; S. Maeda, S. P. Armes, *J. Mater.Chem.*, 1994, 4, 935). Nanocomposites of functional polythiophene are relatively unexplored. For example, nanometre-sized PEDOT-silica core-shell particles were already synthesized using an oxidative dispersion approach, i.e. precipitation of the insoluble PEDOT polymer onto a silica particle surface.

To the best of our knowledge, no extensive studies dealing with the fabrication of silica/polythiophene nanoparticles of a core-shell morphology prepared using an approach based on *hybrid* silica particles were ever undertaken in this field. Herein, we report the synthesis of hybrid silica/polyThiophene nanocomposite particles using a multistep synthetic procedure. First, a hydrolytically unstable triethoxysilane-*N*-thiophenyl anchoring species was prepared (amide chemistry). Second, a Water in Oil (W/O) micro-emulsion method using TEOS and the former *N*-thiophenyl-Si(EtO)$_3$-silane afforded corresponding hybrid silica nanoparticles (190-280 nm average diameter). These hybrid silica nanoparticles possessed surface-localized *N*-thiophenyl anchoring groups that were used for the preparation of the corresponding core-shell nanocomposite particles using the FeCl$_3$-mediated chemical oxidative polymerization of various thiophenyl derivatives such as polyThp and poly(3-Thp-acetic acid).

16:00 Poster F04

Electrical properties of composite nanomaterials, containing metal nanoparticles.

Umarbek Abdurakhmanov[1], Fakhriddin Boymuratov[1], Andreas A. Arshakuni[2], Gleb Yurkov[2]

1. *National University of Uzbekistan, Tashkent 100174, Uzbekistan* **2.** *Kurnakov Institute of General and Inorganic Chemistry RAS (IGIC), Leninsky prospect, 31, Moscow 119991, Russian Federation*

e-mail: iourkov@rambler.ru

Two types of composites were prepared. One of them was a metal-polymer composite comprised of nanoscale nickel particles, and the other one was comprised of high-dispersed nickel particles. In both cases, phenilon was used as the polymer matrix. One of the composites was prepared by means of the thermal decomposition of nickel formate in phenilon. The other was made via mixing a nickel powder with phenilon in a mill. For these samples, the resistance and the frequency dependence of permittivity in the range from 20 to 200 Hz were measured, and their conductivity and static permittivity values were determined. It was found that the percolation-like behaviour of conductivity (σ) and static permittivity (ε) which was observed for the Ni particles of 1-3 μm in size(high-dispersed particles) gave way to another behaviour characterized by an additional contribution to σ and ε below the percolation threshold for the Ni particles of ≤ 30 nm in size (nanoparticles). It was shown that this peculiarity of the behaviour of σ and ε of the composites was in agreement with the network hierarchy model of composites which had been proposed recently by Balberg et al. Thus, the behaviour of σ and ε of the metal-polymer composites under study can be understood in the frame of the model of composites which assumes the existence of a "hierarchy" of electrically connected networks in composites and the dependence of the conductivity of these composites from the sizes of filler particles (from the ratio of values of the radius of filler particles and the tunneling range parameter). This work was partial financally supported by the Russian Foundation for Basic Research (grant nos.06-03-72031-MSTI,07-03-00885,07-08-00523,08-08-90250),INTAS-05-1000008-7834, the grant of the President of the Russian Federation MK-253.2007.3, Russian Science Support Foundation, ISTC nos.3457, the Russian Academy of Sciences of the research programs.

16:00 Poster F05

Electrical conductivity of nanocomposite materials

Vitaly V. Novikov, Katherine A. Nezhevenko

Odessa National Polytechnical University (NVV), Shevchenko Prospekt, 1, Odessa 65044, Ukraine

e-mail: nejevenko@ukr.net

The metal-filled polymer nanocomposites are being widely used as conducting materials over last years. As a result there exists a problem to forecast the effective properties of such composites. Nowadays, there is no model adequate to describe real nanocomposites, and there are no methods for the calculation of the effective electrical conductivity of nanocomposite polymers filled with metal powders that take into account the clusterization (aggregation) of the filler particles and the contact electrical conductivity between the metal filler particles.

The effective electrical conductivity of the metal-filled polymers depends on the conductivity of filler particles chains. In order to define the contact conductivity between the filler particles we consider the electron passage in the contact zone between the particles and the existing in this region image forces. The average contact conductivity in the aggregate (cluster) consisting of the filler particles was defined as:

$\sigma_k=2e^2\sigma_f/\pi R\varepsilon\varepsilon_0\varphi_M$

where φ_M- the work function of the electron from metal; e – the charge of the electron; ε -the relative permittivity of the contact, ε_0 – the dielectric constant, R – the radius of the filler particle, σ_f- the electrical conductivity of the filler.

The fractal model was introduced in order to describe the chaotic structure of the nanocomposite. The filled polymeric composite is presented as a chaotic mix of two sorts of polyhedrons: the polyhedrons with the conductivity and the polyhedrons with the conductivity of the polymer. The effective conductivity of a composite with chaotic structure was determined using an iterative averaging method. The comparison between the calculation of the effective conductivity of the nanocomposites and experimental data demonstrates their close agreement.

The above fractal model of the chaotic structure and the calculation method allow us to determine the effective conductivity of nanocomposites, without resort to insertion of fitting parameters.

16:00 Poster F06

Electrical signals in polytetrafluoroethylene matrix nanocomposites under the action of weak laser shock waves

Yurij Nikiforov[1], Bogdan Kovalyuk[1], Mihajlo Nischenko[2], Olga Rzheshevska[1], Volodymyr Hlado[1]

1. *Ternopil Ivan Pul'uj State Technical University, Ruska, 56, Ternopil 46000, Ukraine* **2.** *G.V. Kurdyumov Institute for Metal Physics National Academy of Sciences (IMP), Vernadsky Blvd. 36, Kyiv UA03680, Ukraine*

e-mail: Kovalyukdan@Yahoo.com

The process of the formation of electrical signals in polymer composite materials subjected to shock waves generated by a laser were investigated. The laser shock waves (LSW) were formed by using a Q-switched GOS-1001 neodymium-glass laser.

Electrical contacts withstanding fast the mechanical loads caused by the LSW action, were applied. For making the contacts a method of chemical metallization was used. Taking advantage of a scanning electronic microscopy SEM-106 the morphological structure of the metallic coating of polytetrafluoroethylene and polytetrafluoroethylene specimens with different weight fillings of carbon nanotubes was investigated as well as the metal-polymer border cut off. Numerous micro-pits, nano- and micro-pores were found. The adhesion properties of surfaces of polytetrafluoroethylene reinforced with nanotubes are stronger than those without nanotubes. Factors which affect the adhesion strength have been analysed.

Electrical signals which achieve more than hundreds millivolts in magnitude after LSW - treatment of the specimens were found experimentally in the polytetrafluorethylene matrix filled with carbon nanotubes. A comparison of the obtained signals in different materials was carried out. The investigation of the resistance and the capacity which were measured at 1 MHz proved that the capacity of a polytetrafluorethylene matrix containing carbon nanotubes is 3-4 times higher than a polytetrafluoroethylene matrix without nanotubes, when geometry and dimensions of the specimens are kept the same. The nature of the appearing signals, which is likely to be caused by the behavior characteristics of the quantum-mechanical bonds of carbon nanotubes under LSW action, has been analysed.

16:00 Poster F08

Ultrasound-assisted synthesis of Co-containing nanoparticles

Pavel Elkin, Gleb Yurkov

Kurnakov Institute of General and Inorganic Chemistry RAS (IGIC), Leninsky prospect, 31, Moscow 119991, Russian Federation

e-mail: ter_mine@mail.ru

In this work, we have prepared nanosize-needles of mixed content (Co / Co oxide) using the sonochemical method for decomposition of metal complexes. In our research, we used cobalt carbonyl (Co2(CO)8) as the metal precursor. In the experiments, 2 g of carbonyl (5.8 mmol) were dissolved in 100 ml of deionized distilled water (sample 1) or in a water-alcohol (1:1 volume) mixture (sample 2). After this, 0.5 g of Poly-ethyleneglycole was added to the mixture. The resulting solution was treated with ultrasonic (Bandelin Sonopuls 3200, Ti-probe KE-76, amplitude 50%) for 40 min. The reaction mass was then centrifuged, and the resulting powders were studied. According to the TEM images, sample 1 contains nanosize-needles of about 19 nm in length and 5 nm in diameter which are congregated with each other into more complex web-like structures. Sample 2 also contains nanosize-needles (28 nm in length, 4 nm in diameter), however, along with spherical nanoparticles (7 nm in diameter). According to the XRD patterns, both the samples consist of polyethylene glycol, Co, and Co3O4. Magnetic measurements of the samples revealed their low blocking temperature (near 25 K°), which indicates that the samples have compound composition. ESR measurements displayed no signals from ions for sample 2 and a weak paramagnetic signal for sample 1. That indicates that both the samples are paramagnetic but display strong spin-lattice relaxation. Acknowledgements: this work has received partial financial support from the Russian Foundation for Basic Research (grant nos. 06-03-72031-MSTI, 07-03-00885, 07-08-00523, 08-03-00681, 08-08-90250), INTAS-05-1000008-7834, the grant of the President of the Russian Federation MK- 253.2007.3, Russian Science Support Foundation, ISTC nos. 3457, the Russian Academy of Sciences of the research programs.

16:00 Poster F09

The influence of nanosilica on wear resistance of ceramic-polymer composites intended for dental fillings

Joanna Siejka-Kulczyk[1], Joanna Mystkowska, Malgorzata Lewandowska[1], Eugeniusz Sajewicz, Jan R. Dąbrowski[2]

1. *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland*
2. *Bialystok Technical University, Faculty of Mechanical Engieering, Wiejska 45C, Białystok 15-351, Poland*

e-mail: malew@inmat.pw.edu.pl

Good wear resistance is one of the major requirements for ceramic – polymer composites intended for dental fillings. It is strongly affected by the size and amount of fillers. The main goal of this study was to evaluate the influence of nanofiller (nanosilica) addition on tribological properties of such composites.

Ceramic – polymer composites based on acrylic resins (bis – GMA + TEGDMA) and urethane – methacrylate resin (UM) with 60 % total volume fraction of filler were fabricated. Nanosilica contents were: 0, 10, 20 vol. %. Next, the materials were subjected to wear tests using occlusion simulator tester. The apparatus provides reciprocating movement and cyclic loading of the testing sample. In this way, some similarity to the masticatory pattern occurring in the mouth has been reached. Human enamel was used as a countersample. Wear resistance of both composites and enamel was estimated. Friction coefficient was also measured.

The results of the study indicate that nanosilica addition significantly improves the wear resistance of ceramic – polymer composites and reduces the wear of enamel. It was found that nanosilica addition does not influence on friction coefficient value. It was also revealed that the kind of resin does not significantly influence the wear behaviour of the composites.

16:00 Poster F10

Preparation and characterization of organic-inorganic nanocomposites based on dithiophosphate acids/TiO_2 systems

Aneta Kisielewska, Ireneusz Piwoński

University of Łódź, Department of Chemical Technology and Environmental Protection, Pomorska 163, Łódź 90-236, Poland

e-mail: anetailik@uni.lodz.pl

Because of long life, reliability and durability many kinds of titania coatings are used as part of bone implants [1]; intelligent protective coatings require low friction and wear [2]. Application of nanocomposites consisting of organic lubricant molecules in the form of thin film onto inorganic surface considerably lowers friction and wears [3].

In this approach, the organic-inorganic nanocomposites were created by deposition of di(*n*-alkyl)ditiophosphate acids (HDDP) on TiO_2 substrates with the use of dip-coating (DC), self-assembled (SA) and Langmuir-Blodgett (LB) methods. Ultra thin TiO_2 films prepared by dip-coating sol-gel method on Si (100) wafers were used as amorphous, anatase and rutile substrates.

The surface morphology, hydrophobicity and tribological behaviour, including the influence of alkyl chains length of HDDP (C12, C14 and C16), titania substrate phase and modification method, were characterized by surface probe microscopy (AFM/FFM), wetting contact angle and microtribometer measurements.

The surface morphology of modified TiO_2 substrates exhibit various morphologies from thin and smooth to closely-packed agglomerates of HDDP depending on the type of modifier and the deposition method. Smooth surfaces were obtained in LB method while thick agglomerates were observed for DC deposition.

Of amorphous and crystalline phases of TiO_2 (anatase and rutile) the lowest friction coefficient and wear is exhibited by rutile. However, HDDP/TiO_2 nanocomposite layers exhibit better antifrictional properties than unmodified titania surfaces. The best antiwear behavior and the lowest friction coefficient present C14 HDDP layers deposited by DC on rutile phase due to the formation of dense protective layer on hard substrate.

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16:00 Poster F11

Thermal and mechanical properties of polyurethane nanocomposites with modified nanosilica

Joanna Ryszkowska[1], Maria Zielecka[2], Anna Pytel[2], Bartlomiej J. Wasniewski[1]

1. *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland* **2.** *Industrial Chemistry Research Institute (ICRI), Rydygiera 8, Warszawa 01-793, Poland*

e-mail: barva@poczta.onet.pl

Polyurethanes (PUR) are commonly used materials in the medicine, automotive and mining industry. Fumed silica nanoparticles (nanosilicas) are fillers commonly added to improve the thermal, rheological and mechanical properties of polyurethane.

In this study, nanocomposites with nanosilica and modified nanosilica with a –NCO group were obtained. The aim of these studies was to develop and compare polyurethane nanocomposites containing from 0.5% to 4% wt of nano SiO_2 and modified nanosilica. Polyurethane (PU)/nanosilica composites were obtained from "in situ" polymerization using polyester polyols of molecular weight ~1940 Da, 4,4 diphenyl methane diisocyanate (MDI), dicyandiamide as a chain extender and silica dioxide as a nanofiller. According to the amount of nanofiller, density, abrasive wear and wet angle of nanocomposites were investigated. Thermal properties such as degradation processes with thermo gravimetric analysis (TGA) and glass transition with differential scanning calorymetry (DSC) were determined. Glass transition, is one of the most important properties in determining the suitability of a polymer in an engineering application. Shifting of the glass transition after using nanofiller has been reported by many authors. In our case no significant difference was observed. The comparison of the FTIR spectra of composites with PU matrix, allows us to detect differences in characteristic bonds area.

16:00 Poster F12

Microstructural analysis of the polyvinyl alcohol template on the porosity of nanocrystalline alumina prepared by sol-gel method

Zoltán Ecsedi[1], Ioan Lazău, Cornelia Păcurariu, Paul C. Barvinschi[2]

1. *Politehnica University of Timişoara, P-ţa Victoriei no. 2, Timisoara 300006, Romania* **2.** *West University of Timisoara (UVT), Bd.V. Parvan nr.4, Timisoara 300223, Romania*

e-mail: zoltan.ecsedi@chim.upt.ro

The effects of polyvinyl alcohol (PVA) template and calcinations temperatures on the characteristics of the alumina films were investigated. The samples were prepared by sol-gel method using aluminium triisopropylate precursor. The variation of microstructure, pore size and pore volume, were determined by nitrogen adsorption/desorption analysis, the polymorphic transformations and the crystallite sizes of alumina during the heating were studied using X-ray diffraction. The burning out process of the organic compounds and the polymorphic transformations combined with the shrinkage of the film during the thermal treatment leads to changes in the porosity and in the nanosized pores diameter. Nanocrystalline alumina with tailored surface area in range of 10-2631 m^2/g and narrow distribution of pore sizes in range of 0.4-28 nm were obtained.

16:00 Poster F13

Nanocomposites based on acrylic copolymers and ZnO nanoparticles

Lucia Dumitrescu, Dana Perniu, Ileana Manciulea

Transilvania University of Brasov, Centre Product Design for Sustainable Development, Eroilor 29, Brasov 500036, Romania

e-mail: lucia.dumitrescu@gmail.com

Organic–inorganic hybrid nanocomposites are materials whose chemical and physical properties are tailored by association of organic and inorganic moieties at the nanometer scale. The organic–inorganic nanocomposites exhibit additional characteristics over those of conventional single-phase polymer materials, and therefore have a wide range of applications in fields such as: optics, electrics, biology, catalysis etc.

The paper presents research concerning the obtaining of composite coating nanomaterials for wood finishing and bio-protection. The new nanocomposites, consisting of a hybrid of organic and inorganic nanomaterials, are based on functionalized acrylic copolymers in water dispersion with ZnO nanoparticles obtained by sol-gel process.

The presence of acrylic copolymers in water emulsion (based on monomers ethyl acrylate, butyl acrylate, acrylonitrile) and ZnO nanoparticles enables the formation of a crosslinked nanometric network of inorganic and organic domains, put into evidence by AFM analysis. The interphase characterization of the nanostructured materials synthesised was performed using FT-IR.

The obtained nanocomposites can be used as coating materials with improved properties of wood coating systems such as scratch resistance (scrub tester) and specific wood finishing characteristics.

Considering the biocide activity, both for acrylic copolymers and ZnO nanoparticles, the obtained nanocomposites were biologically investigated and proposed as wood preservation agents.

16:00 Poster F14

Nanostructured coating materials based on acrylic copolymers and TiO_2 nanoparticles

Dana Perniu[1], Lucia Dumitrescu[1], Ileana Manciulea[1], Daniela Mihalevschi[2]

1. *Transilvania University of Brasov, Centre Product Design for Sustainable Development, Eroilor 29, Brasov 500036, Romania* **2.** *National Institute of Wood, Bucharest 0021, Romania*

e-mail: lucia.dumitrescu@gmail.com

Organic-inorganic hybrid materials are very interesting for several applications thanks to their properties based on the synergistic combination of different components. The paper presents research concerning a new class of nanomaterials for wood finishing. Designed to exhibit bio-protective and aesthetic characteristics, these new nanomaterials, consisting of a hybrid of organic and inorganic nanomaterials, are based on composites of functionalized acrylic copolymers, in water dispersion, with TiO_2 nanoparticles, enabling a superior combination of properties that cannot be achieved by using any single material.

The presence of acrylic copolymers in water emulsion, bearing suitable reactive functional groups, leads to the formation of a crosslinked network composed of inorganic and organic domains on nanometric scale. AFM analysis was employed to evaluate the particle dispersion - critical parameter to enable the most interaction with the polymer matrix and achieve the desired properties of the material. The interphase characterization of the nanostructured materials synthesised was performed using FT-IR.

The obtained nanostructured coating materials based on acrylic copolymers and TiO_2 nanoparticles showed improved properties for wood coating systems and biocide activity.

16:00 Poster F15

Dielectric spectroscopy studies of sonochemically prepared CdS-PVA nanocomposites

Yashar Azizian[1,3], Mustafa B. Muradov[1], Rasim K. Mamedov[1], Ali Khodayari[2]

1. *Baku State University, Department of Physics (BSU), Z.Khalilov str. 23, Baku, Azerbaijan* **2.** *Islamic Azad University Ardabil Branch young research club, Ardabil 01700, Iran* **3.** *Mohaghegh Ardabili University, Department of Physics, Ardabil 0179, Iran*

e-mail: yashar.a.k@gmail.com

CdS nanocrystals in the powder form were successfully prepared using sonochemistry method. Structural and morphological characterizations of as prepared samples were done by means of X-ray powder diffractometer (XRD) and Scanning electron microscopy (SEM). The results show that spherical nanocrystallites were formed with a mean size of about 5nm in cubic structure. The nanopowders were embedded into PVA matrix and some dielectric properties of CdS-PVA nanocomposites were characterized using Impedance spectroscopy technique. Detailed studies of dielectric and impedance spectroscopy studies of CdS-PVA nanocomposites in a wide range of frequency (1kHz-1MHz) and temperatures (298K- 423K) show that these properties are strongly temperature and frequency dependent. The change of dipole orientation and charge migration, porosity of polymer structure and space charge carriers plays an important role in relaxation mechanisms and conduction process.

16:00 Poster F16

Mechanical properties of PET- rubber composites with TiO_2 additives

Cristina Vladuta

Transilvania University of Brasov, Centre Product Design for Sustainable Development, Eroilor 29, Brasov 500036, Romania

e-mail: crisvladuta@yahoo.com

Poly-ethylene terephthalate (PET) and rubber interactions lead to unstable morphology and poor interfacial adhesion, resulting in inferior mechanical properties of the PET-rubber composites. The mechanical behaviour of PET-rubber composites with additives like TiO_2 nanoparticles as compatibilizer (<5% wt) are been studied in the present work.

PET-rubber composites were kept under visible light and UV irradiation. The interface properties of the composites with TiO_2 nanoparticles were explained by mechanical tests. The measurements of the tensile strain, shear and compression were performed on a Zwick test System and the impact tests (Charpy tests) were made using an Impact Plast instrument. The Finite Element Method (FEM) was applied using patran/nastran software, and the experimental results were used as input data.

Mechanical properties were found to be affected by the conditioning temperatures of the composites as well as the type of the additives.

16:00 Poster F17

Nanostructured polymer matrices for a magnetic composite

Aurica P. Chiriac, Loredana E. Nita, Iordana Neamtu

Petru Poni Institute of Macromolecular Chemistry of the Romanian Academy, Aleea Grigore Ghica Voda 41A, Iasi, Romania

e-mail: achiriac1@yahoo.com

One of the most important goals in the research concerning nanostructured polymers is the development of new materials with increased functional properties such as magnetic, electrical and optical, biocompatibility, thermal resistance, etc. The value of the polymer matrix can be improved with organic or inorganic additives, the development and tailoring of new nanostructured materials offering the possibility to increase their functional properties and to promote their use in automotive, aerospace, building, electrical, optoelectronic and biomedical applications. Poly(aspartic acid) based materials are attractive due to their biocompatibility and biodegradability. They have applications in medicines, cosmetics, and food. At the same time, no toxic or mutagenic effects have been reported for poly(aspartic acid). Poly(ethylene glycol) is a hydrophilic nonionic polymer used in many biochemical and industrial applications (cosmetics, food, pharmaceutical products) due to its exceptional solubility in water and in many organic solvents, lack of toxicity and biocompatibility. In this paper, a new type of biocompatible block copolymer based on poly(ethylene glycol)(M_w - 4000)-b-poly(succinimide) was synthesised through a condensation process in DMF. Poly(succinimide) was prepared by thermal polycondensation of D,L - aspartic acid. The synthesised block copolymer is a matrix able to encapsulate inorganic magnetic material or bioactive substances, with the aim of biomedical application. The properties of the prepared macromolecular compound including chemical composition, hydrodynamic diameter of the particles, zeta potential and the morphology are studied by FTIR spectroscopy, laser light scattering and SEM.

16:00 Poster F18

Preparation and characterization of polysulfone membranes containing Ag nanoparticles by a convenient ultraviolet irradiation technique

Viorica Gaina, Constantin Gaina, Mihaela A. Olaru

Petru Poni Institute of Macromolecular Chemistry of the Romanian Academy, Aleea Grigore Ghica Voda 41A, Iasi, Romania

e-mail: vgaina@icmpp.ro

A novel silver/polysulfone nanocomposite membrane was prepared by a convenient ultraviolet irradiation technique, through *in situ* reduction of silver salt ($AgNO_3$) added to a solution of commercial UDEL polyethersulfone dissolved in *N*-methyl-2-pyrrolidinone (NMP). The UV-reduction of Ag^+ to Ag^0 nanoparticles was confirmed by means of UV-vis spectroscopy, from aggregation phenomena. The effects of dispersion of silver nanoparticles within polysulfone matrix were investigated by means of ATR-FTIR, dynamic mechanical thermal analysis and differential scanning calorimetry. Using X-ray diffraction, it was shown that annealing produced silver crystallites of 70-90 nm across, which are partially textured in “sheetlike” {110} planes.

16:00 Poster F19

Starch based biodegradable nanocomposites: structure and properties

Tatjana Ivanova, Nadezda Lilichenko, Robert Maksimov, Janis Zicans

Riga Technical University (RTU), Azenes St. 14/24, Riga LV-1048, Latvia

e-mail: zicans@ktf.rtu.lv

In this research plasticized starch (PS) based nanocomposites with varying *Vadakste* clay (V) clay content (1 to 6 wt. %) are investigated. Fabrication technology of the nanocomposites by using solution intercalation method is worked out. Structure, tensile mechanical properties and moisture sorption-desorption kinetics of the PS/V nanocomposites are investigated. A mathematical model for characterization of the elastic properties of the PS/V nanocomposite is developed.

Manufacturing procedure of the PS/V nanocomposites included following technological steps: (1) preparation of the V dispersion in the distilled water; (2) treatment of the V dispersion with ultrasound (US); (3) fabrication of the PS/V dispersion with defined amounts of water, glycerol, starch and V. During the manufacturing procedure it was determined that 45 minute US treatment time is optimal for fabrication of the nanocomposites with a glycerol: starch ratio 3:5. Tensile stress-strain behaviour of PS/V nanocomposites, obtained according to such a technological procedure, substantially improved with addition of considerable small amounts of the clay nanofiller. Tensile strength and Young‘s modulus of the PS/V nanocomposites with V content of 6 wt. % increase 1,9 and 2,6 times respectively, while ultimate elongation decrease to some extent. Such a clay content, however, does not cause brittlening of the nanocomposite. By increasing absorbed moisture level, stress-strain behaviour of the nanocpomposites worsen, however, clay particles still show it reinforcing effect. Found mathematical model that can be used for the nanocomposite elasticity constant prediction considers most important structural aspects of the multilayered clay mineral, including amount of the elementar layers in the packet, interlayer space, density, shape, dimensions and aspect ratio of the clay particles. Coefficient of the moisture transmission rate of the nanocomposites at this clay content decreases 2,1 times.

16:00 Poster F20

A study of the effect of nano-magnesium hydroxide on the flammability of epoxy resin

Marta Martins, Celeste M. Pereira

Instituto de Engenharia Mecânica e Gestão Industrial (INEGI), Rua Doutor Roberto Frias, 378, Porto 4200Porto, Portugal

e-mail: cpereira@inegi.up.pt

An increasing number of structures are being made from fibre reinforced composites. For example, on aircraft, some crucial components are generally made from carbon fibre reinforced composites using an insulating epoxy matrix. Furthermore, standard epoxy resins are highly flammable and produce large quantities of smoke and toxic gases. Their increasing commercial utilization may bring these polymers into fire situations at any time, adding urgency to the development of effective and environmental friendly flame retardant systems to reduce fire hazards. Commercially available flame retardants can be highly effective but they have some important disadvantages, like, negatively affecting the resin workability, the quality (physical and mechanical properties) of the final product, in addition to being harmful. The concept of nanoscale flame retardants provides opportunity for synthesis of new polymer materials with unique properties. Nano-magnesium hydroxide, nano-$Mg(OH)_2$, could also represent a rational alternative to the conventionally filled epoxy because they have distinct advantages over traditional flame retardants on its related problem areas.

The purpose of this work is to study the effect of nano-$Mg(OH)_2$ and carbon fibers on flammability properties, such as the time-to-ignition, heat release rate, smoke production, and CO_2 yield. For that, several samples were prepared by an ultrasonic mixing method and fire reaction tests were performed in Cone Calorimeter.

16:00 Poster F21

Metallic filler containing polymer nanocomposites

Remo Merijs Meri[1], Andris Shutka, Ilmars Zalite[2], Martins Kalnins[1]

1. *Riga Technical University (RTU), Azenes St. 14/24, Riga LV-1048, Latvia* **2.** *Institute of Inorganic Chemistry, Riga Technical University, Riga LV-2169, Latvia*

e-mail: zicans@ktf.rtu.lv

Inorganic filler modified polymer nanocomposites extensively enter in our everyday lives. Depending on the chemical nature, structural arrangement, dimensions, aspect ratio as well as other architectural parameters of the filler particles corresponding polymer nanocomposites can possess certain specific, unconvential properties, i.e., enhanced barrier performance, conductivity, magnetic and electromagnetic shielding effect. One of the most interesting ways in this research area is a polymer nanocomposite modified with a metallic nanofiller which could be viewed as a logical continuation for the scientific investigations started already long ago. In spite of much work already done in this field, many aspects of the metallic nanofiller modified polymer matrix nanocomposites still remain uncovered. Consequently this research is devoted to the investigation of the ferrite filled polymer nanocomposites. Fe-Si-O ferrite powder was obtained by plasma technology in cooperation with the institute of Inorganic Chemistry of Riga Technical University. Two fabrication methods, i.e., melt blending and solution casting, are used for preparation of polycarbonate and polyvinylalcohol based nanocomposites respectively. The amount of the magnetic filler in the nanocomposites was changed up to 10 vol. percent. Most important technological parameters of the nanocomposite manufacturing methods are defined. Tensile stress-strain characteristics (modulus of elasticity), calorimetric qualities (glass transition, melting temperature, crystallinity degree) as well as physical (density, melt flow rate), electrical (volume and surface resistivity) and magnetic (coercivity) properties of the nanocomposites are investigated and interesting results are obtained. Some possible application examples of such nanocomposites are materials used in electronics housings for electromagnetic charge suppression and EMI shielding, motor and actuator devices, etc.

16:00 Poster F22

Effect of Freezing and Thawing Process on Betamethasone Release from Polyvinyl alcohol Nanospheres

Shahin Bonakdar[1], Seyed Ali Poursamar[1], Mohammad Rafienia[2], Motahareh Hosseini[1], Mohammad Ali Shokrgozar[3]

1. *Amirkabir University of Technology (AUT), Hafez, Tehran 15914, Iran* **2.** *Isfahan University of Medical Science, Isfahan 88764456, Iran* **3.** *Pasteur Institute of Iran, Pasteur Institute of Iran NO. 69 Pasteur Ave Tehran Iran, Tehran 13164, Iran*

e-mail: shahinbonakdar@yahoo.com

Betamethasone is a glucocorticoidsteroid with anti-inflammatory and immunosuppressive properties which can be used in treatment of asthma and itching. It may have some influence on chondrocyte proliferation. In this research, Polyvinyl alcohol nanosphere were prepared by oil in water emulsion method and the nanospheres were exposed on 1, 2 and 4 Freeze-Thawing (F-T) process including 24 hours freezing cycle at -25°C and 24 hours thawing at ambient temperature. Nanosphere production was confirmed by transmission electron microscopy and betamethasone release was analyzed by UV spectrophotometer at 245 nm. These data revealed the effect of the Freeze-Thawing process on drug delivery in which increasing the F-T cycles can decrease the rate of drug releasing. The effect of betamethasone concentration was also conducted on isolated human chondrocyte and MTT assay was utilized to assess the cell viability. The results showed that these biocompatible nanospheres can be used in sustained release of such drugs more than four month and it may be controlled by F-T cycles.

16:00 Poster F23

Nanocomposite Ag nanoparticles-containing polyurethane/collagen nanofibrous membranes as wound dressings

Jyh-Ping Chen, Yuin Chiang

Chang Gung University, Taoyuan 3330, Taiwan

e-mail: jpchen@mail.cgu.edu.tw

Nanofibrous membrane (NFM) intended as wound dressing was prepared by electrospinning a polyurethane (PU) solution containing Ag ions and followed by reduction of Ag ions to Ag nanoparticles. The electrospun PU membrane has unique properties, such as high surface area-to-volume ratio and porosity, controlled evaporative water loss rate, good mechanical properties, good fluid drainage ability, and excellent antimicrobial activity. With an aim to promote scarless wound healing, a bioactive collagen layer was generated on the fiber surface by low temperature oxygen plasma treatment to improve the hydrophilicity property of PU and facilitate covalent binding of collagen molecules to the plasma-treated PU surface. The effects of different operation parameters during electrospinning were studied for their effects on fiber morphology and diameter, which include solvent type, polymer concentration, flow rate, voltage, tip-to-collector distance, and silver ion concentration. The NFM was subject to detailed analysis by SEM/EDS, FE-SEM, TEM, SPM, confocal laser scanning microscopy, ESCA, XRD, FT-IR, and tensile testing. A NFM with no bead formation could be obtained with fibre diameters around 100 nm. The presence of embedded silver nanoparticles and surface-grafted collagen could also be confirmed both qualitatively and quantitatively. After plasma treatment, the NFM's antimicrobial activity also improved substantially to nearly 100% inhibition of bacterial growth with concomitant increase of membrane hydrophilicity, which facilitates its use as a functional wound dressing. From animal studies, the NFM was better than gauze and commercial collagen sponge wound dressing in wound healing rate. This novel electrospun matrix will have potential as a wound dressing for skin regeneration.

16:00 Poster F24

Silver nanoparticles for antimicrobial applications

Andrea Travan

Università di Trieste, Trieste, Italy

e-mail: andrea.travan@iol.it

Infections associated with orthopaedic implants are life-threatening complications that often occur in medical device insertions. Presently, bacteria are becoming remarkably resistant to antibiotics so there is a new interest on silver as a promising antimicrobial material mainly in the form of nanoparticles. It is known that silver particles must be nanosized because their aggregation leads to the loss of properties; an efficient way to prevent their aggregation is by using polymers. In this work solutions and gels containing silver nanoparticles were prepared by reducing silver ions in the presence of polysaccharides and their antibacterial activity was assessed. Nanoparticles were produced by reducing silver ions with ascorbic acid in a chitosan(-derivative) solution. Biological tests were performed with four strains of bacteria. Bacterial growth kinetics tests and colony count tests were performed using solutions with various concentrations of polymer and silver. A mixed polysaccharide gel was prepared and the antimicrobial properties of this gel were studied by bacterial adhesion tests. Cytotoxicity assays (LDH) of the gels were performed with osteoblasts (MG63), fibroblast-like (NIH3T3) and hepatocyte-like cell lines (HepG2). Bacterial growth kinetics of the system proved that the silver nanoparticles solutions do possess antimicrobial effect. Colony Count Tests revealed the system to be bactericidal. A 3D hydrogel was prepared and it displayed as well a powerful antimicrobial activity, as shown by bacterial adhesion tests. No bacteria could grow on the surface of the gel because of the presence of the nanoparticles. Cytotoxicity assays proved that this gel was not toxic to the cell lines used. Silver nanoparticles-polysaccharide systems are easy to prepare, reproducible and stable in time. They display a powerful bactericidal activity either in solutions or as gels which are not toxic to cells.

16:00 Poster F25

Adsorption and acoustic properties of ordered carbon nanotube arrays.

Aleksandr S. Chashynsky, Viatcheslav V. Barkaline

Belarussian National Technical University (BNTU), F. Skariny, 65, Minsk 220027, Belarus

e-mail: smart1@rambler.ru

Results of molecular dynamics simulation of adsorption properties of nanostructured carbon material are presented. Selective permittivity both of single tube and tubes' bundles depending on their

structures is demonstrated. Role of rings in adsorbate chemical structures is studied from the viewpoint of adsorption energy. Effect of chain DNA immobilization on carbon nanotube arrays is discussed. Oxygen adsorption effect on the Van der Waals interaction contribution to the elastic moduli of ordered carbon nanotube arrays was estimated. Mechanical instability of square lattice of nanotubes with respect to the transition to a triangular one was demonstrated. Variation of the elastic moduli due to the adsorption was shown to be of the same order of magnitude as the moduli themselves. This leads to variation of phase velocities of acoustic waves propagating across the array which proved to be dozens of times greater then mass loading by adsorbate for the acoustic wave.

16:00 Poster F26

Synthesis and characterization of hybrid sol-gel composites containing carbon nanostructures

Luís M. Gonçalves[1], Rui A. Araújo[1], Maria F. Proença[1], Maria Conceição Paiva[3], Carlos J. Silva[1], Maria J. Gomes[2]

1. *Department of Chemistry, University of Minho, Campus Gualtar, Braga 4710-057, Portugal* **2.** *University of Minho (UM), Campus de Gualtar, Braga 4710057, Portugal* **3.** *Institute of Polymers and Composites, University of Minho, Campus de Azurém, Guimarães, Braga 4800-058, Portugal*

e-mail: mjesus@fisica.uminho.pt

The sol-gel procedure gives an opportunity to obtain solid-state large size monoliths with a high purity grade and at room temperature conditions. The production of optically clear and elastic hybrid organic-inorganic materials via this synthetic route could be used to prepare composite materials where a large diversity of species could be hosted. Interaction between the hosted species and matrix has a strong influence on the physical and chemical properties of the final material and new functionalities could be envisaged.

Carbon nanofibres (CNF) and carbon nanotubes (CNT) are a class of materials with unique thermal, electrical and mechanical properties. Moreover their application in the preparation of new composites requires modification of the surface properties to improve reactivity and to reduce de hydrophobic characteristics and surface energy.
This work will report studies involving the preparation of hybrid elastic materials: the lowest value of the Young's modulus (9 MPa) is comparable to that of the caoutchouc (about 8 MPa). The high flexibility can extend the range of applications of urealilicates allowing them to be positioned on non-planar or curved surfaces. Composites, doped with CNT and CNF, obtained by the sol-gel method and the characterization of their chemical and physical properties is also reported.

16:00 Poster F27

Fluorination of Carbon Nanotubes in CF_4 Plasma

Alexandre Felten[1], Jean-Jacques Pireaux[1], Jacques Ghijsen[1], Robert L. Johnson[2], Caroline M. Whelan[3], Xiaoxing Ke[4], Gustaaf Van Tendeloo[4], Carla Bittencourt[5]

1. *University of Namur, Laboratoire Interdisciplinaire de Spectroscopie Electronique (LISE), 61 rue de Bruxelles, Namur 5000, Belgium* **2.** *University of Hamburg, Institute for Experimental Physics, Luruper Chausse 149, Hamburg D-22761, Germany* **3.** *IMEC, Kapeldreef 75, Leuven B-3001, Belgium* **4.** *University of Antwerp, EMAT, Groenenborgerlaan 171, Antwerp B-2020, Belgium* **5.** *University of Mons-Hainaut, LCIA (UMH), Mons 7000, Belgium*

e-mail: jacques.ghijsen@fundp.ac.be

CNTs have been proposed as building blocks for advanced materials such as reinforced polymer and metal matrices, because they exhibit either metallic or semiconducting properties and are quite unique in terms of their chemical and thermal stability, strength and elasticity. However, the relatively low reactivity of the CNT-surface presents a challenge for their integration into complex material assemblies. Our approach is to activate their surface by grafting functional groups that improve their interaction with other materials including polymers and metals.
Fluorination of CNTs has proved to yield high utility products that can be used directly or as precursor for other derivatives. Typically, this is accomplished by immersing the nanotubes in appropriate chemical solutions or exposing them to vapours at high temperatures. Fluorine gas generally results in high reaction rates and deep penetration into carbon related materials. The imprecise control of the fluorination depth makes it difficult to accomplish treatment limited to sidewall functionalization. Conversely, plasma treatment has the potential to limit fluorination to the CNT surface.
In this study MWCNTs were exposed to CF_4 rf-plasma and the resulting impact on CNT electronic structure investigated using X-ray and UV photoelectron spectroscopy. XPS showed that plasma treatment effectively grafts fluorine atoms at the CNT surface. The fluorine atomic concentration and the nature of the C-F bond (semi-ionic or covalent) can be tuned by varying the plasma conditions. UPS confirms that the valence electronic states are altered by the grafting of fluorine atoms. Characterization with high resolution-TEM reveals that while the plasma treatment does not induce significant etching impact on the CNT surface, it increases the number of active sites for gold cluster formation. Dispersion characteristics found for CF_4-functionalized-MWCNTs will be discussed in terms of fluorine concentration at the CNT surface.

16:00 Poster F28

FePt-filled Carbon Nanotubes by Wet Synthesis

Aldo Capobianchi[4], Sabrina Foglia[5], Elia Palange[1], Lorenzo Arrizza[2], Claudio Veroli[3], Marcelo Vasquez Mansilla[6], Dino Fiorani[4]

1. *Università degli Studi dell'Aquila, Dipartimento di Ingegneria Elettrica, L'Aquila 67100, Italy* **2.** *Università degli Studi dell'Aquila, Centro di Microscopia Elettronica, L'Aquila 67100, Italy* **3.** *Istituto per lo Studio dei Materiali Nanostrutturati (ISMN-CNR), Monterotondo, Roma I-00016, Italy* **4.** *Istituto di Struttura della Materia, ISM-CNR, Monterotondo (RM) 00016, Italy* **5.** *CNR-IFN, Roma 00156, Italy* **6.** *Centro Atómico Bariloche (CAB), Av. Bustillo 9500, San Carlos de Bariloche, Río Negro R8402AGP, Argentina*

e-mail: aldo.capobianchi@ism.cnr.it

Since their discovery [1], carbon Nanotubes (CNTs) has been attracting great interest from both fundamental and technological point of view. Some unique properties of CNTs, such as the possibility of tailoring the electrical conductivity, the mechanical resistance combined with the small dimensions and high aspect ratio, enable the development of nanotechnology in various fields. The encapsulation of materials inside the CNTs cavity has attracted great interest for fine tailoring of the physical properties at nanometric scale. In this paper, FePt clusters are inserted in CNTs using a new wet chemical method [2], [3]. The procedure allows the filling of CNTs with nanoclusters of various materials, without causing any external material growth. To transform the magnetically soft face-centred cubic crystallographic phase, obtained at T_{room}, into the magnetically hard face-centred tetragonal one ($L1_0$), heat treatment at high temperatures (700°C) is necessary. After annealing at 700 °C, regularly spacing of FePt nanoparticles within the CNTs were observed in high resolution transmission electron microscopy images. Moreover, X-ray diffraction measurements indicate the presence of $L1_0$, confirmed by magnetization cycles.

Reference:

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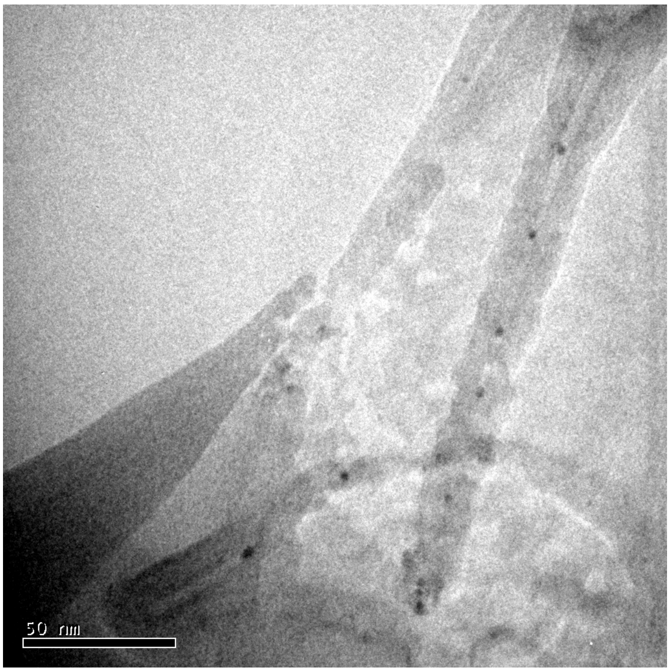
3. Aldo Capobianchi, Sabrina Foglia, Patrizia Imperatori, Andrea Notargiacomo, Maria Giammatteo, Tiziana Del Buono and Elia Palange, Carbon, 45 (2007) 2205–2208



16:00	Poster	F29

The determination of glass transition temperature of nanocomposites PVC/CNT

Jolanta Tomaszewska[1], Georg Broza[2], Kazimierz Piszczek[1], Malgorzata Głuszczenko[1], Przemysław Postawa[3], Karl Schulte[2], Tomasz Sterzyński[4]

1. *University of Technology and Life Sciences, Faculty of Chemical Technology and Engineering (UTP), Seminaryjna 3, Bydgoszcz 85-326, Poland* **2.** *Technical University Hamburg-Harburg, Institute of Polymers and Composites (TUHH), Hamburg 21073, Germany* **3.** *Częstochowa University of Technology, Armii Krajowej St., Częstochowa 42-200, Poland* **4.** *Poznań Technical University, pl. Marii Skłodowskiej-Curie 5, Poznań 60-965, Poland*

e-mail: jolanta.tomaszewska@utp.edu.pl

The investigation of the glass transition temperature was realized by DMTA and dielectric losses measurements, for the nanocomposites of PVC with CNT. The matrix of the nanocomposites was prepared by the dry blend procedure, of PVC S 70 Polanwil (Anwil Poland) 100 wt.%, plasticizer DINP (Exxon, Germany) 10 wt. % and tin stabilizer MOK 17 (Accros, Belgium) 4 wt.%.

The CNT (Nanocyl, Belgium) in a concentration of 0.01 wt. % to 0.05 wt.% were homogenized by use of a sonificator, and introduced to the PVC composition. The gelification of the PVC/CNT composites was performed by means of a Brabender kneader operating by 160°C, during 10 minutes. The final samples were produced by milling, followed by pressure moulding, in a form of plates with a thickness of 3 mm for the DMTA measurements, and as a film with a thickness of 0.5 mm for the dielectric investigations.

The measurements were realized by two DMTA bending frequencies (1 and 10 Hz) and by dielectric field frequency of 1000 Hz. The position of the tg d maximum was taken as the glass transition temperature.

We have observed the dependence of the loss factor (tg d) on the applied measurement frequency. With increasing frequency an increase of T_g in the range from 67°C (for the DMTA measurements by 1 Hz) to 96°C (dielectric investigation by 1000 Hz) was noted. In all cases the PVC matrix revealed lower T_g comparing with corresponding composites with CNTs. These phenomena may be explained by the composition dependent changes of chain mobility, and particularly to certain intermolecular interaction between the PVC matrix and the carbon nanotubes.

16:00	Poster	F30

Manufacturing and investigation of CNT/polymer nanocomposites

Ilze Elksnite[1], Juris Bitenieks, Valdis Kalkis[2], Janis Zicans[1]

1. *Riga Technical University (RTU), Azenes St. 14/24, Riga LV-1048, Latvia* **2.** *University of Latvia, Kr. Valdemara Str. 48, Riga LV-1013, Latvia*

e-mail: zicans@ktf.rtu.lv

In the last years scientific research on nanoscale materials has gained considerable success and at present some developments have efficiently entered into the automative, building and packaging commercial sector. Due to its small dimensions, high aspect ratio, inherently high stiffness and strength, considerably small specific weight, unique electrical, magnetic and thermal characteristics, probably the most promising nanomaterials are carbon nanotubes (CNT). CNT-polymer nanocomposites have found some uses in applications such as anti-static layers, chemical vapor sensors, thermal resistors and others. To ensure reliable exploitable properties of the CNT-polymer nanocomposites, a high dispersion of CNTs in the polymer matrix without agglomeration is required. In contrary, CNTs with their high van der Waals interactions, high surface area, and high aspect ratio cause the self-aggregation that disturbs the improved properties of CNT/polymer nanocomposites.

CNT modified polymer nanocomposites have been investigated in this research. Bayer Baytubes – agglomerates of multiwall CNT with low outer dimeter, narrow diameter distribution and an ultra high aspect ratio – are used as a filler (up to concentrations of 10 vol. %) for preparation of either polyvinlylacetate (PVAc) or styrene-acrylic copolymer (SAC) nanocomposites. Most important technological parameters for manufacturing of the nanocomposites by solution casting are defined. Specific attention is paid to the method of dispersing the CNT in the corresponding solvent. Physical (density) properties, calorimetric and thermo gravimetric parameters, electric (conductivity, surface and volume resistivity) properties, as well as tensile stress-strain characteristics of the PVAc/CNT and SAC/CNT nanocomposites are investigated. Some possible application examples of such nanocomposites are for electro conductive adhesives and paints.

16:00 Poster F31

Enhanced dispersion of MWCNTs and synergistic properties in multiphase epoxy nanocomposites by incorporation of inorganic nanoparticles

Jan Sumfleth, Luis Antonio S. De Almeida Prado, Sergej Richau, Montira Sriyai, Karl Schulte

Technical University Hamburg-Harburg (TUHH), Denickestr. 15, Hamburg 21073, Germany

e-mail: jan.sumfleth@tuhh.de

Multiphase epoxy-nanocomposites based on multi-wall carbon nanotubes (MWCNT) and inorganic nanoparticles (TiO2 and SiO2) were produced using a highly effective shear mixing process including a three roll mill. Using electron and optical microscopy, the formation of hybrid structures could be found. Titania nanoparticles are attached at the surface of carbon nanotubes. Due to intrinsic chemical interactions between carbon nanotubes and TiO2 no additional surface functionalisation was necessary to obtain this hybrid structure. Thus, an enhanced dispersion of carbon nanotubes was realised. The hydrophilic surface of SiO2 nanoparticles causes the formation of independent networks of both SiO2 and MWCNTs. Therefore, the change of the state of dispersion is less pronounced compared to the MWCNT/TiO2 structures. Changes in the state of dispersion lead to a decrease in electrical conductivity. If the TiO2 content exceeds a critical value, the conductivity decreases some orders of magnitude since the formation of a percolated network is facilitated. Similar results were found for the combination of MWCNTs and SiO2. Although SiO2 networks can stimulate the MWCNT-network formation, conductive pathways of MWCNTs can be disrupted if the SiO2 content is increased. Besides an altered state of dispersion, the hybrid structure leads to several synergistic effects, e.g., the glass transition of the nanocomposites. Although a decrease of the glass transition temperature (Tg) is observed for the nanocomposites containing only one kind of filler, the combination of TiO2 (or SiO2) and carbon nanotubes into a hybrid structure suppresses the decrease of Tg, thus demonstrating the potential of such hybrid structures as fillers for multi-functional epoxy systems. Additional thermo-mechanical and mechanical tests were conducted to emphasize the strengthening effect of a third phase based on inorganic nanoparticles in carbon nanotube epoxy composites.

16:00 Poster F32

Polyester elastomer nanocomposites with carbon nanotubes

Magdalena Kwiatkowska[1], Georg Broza[2], Karl Schulte[2], Zbigniew Roslaniec[1]

1. *Szczecin University of Technology, Institute of Materials Science and Engineering, Piastow 19, Szczecin 70-310, Poland* **2.** *Technical University Hamburg-Harburg, Institute of Polymers and Composites (TUHH), Hamburg 21073, Germany*

e-mail: magdalena.kwiatkowska@ps.pl

Carbon nanotubes as a filler of polymer nanocomposites may exhibit good tensile strength depending on their nanostructure and aspect ratio. The nanotubes show superior strength properties over all known fillers used in the production of polymer composites. The deciding factors are: interaction interface and good dispersion of nanofiller [1].

Investigation of structure and physical properties of polymer nanocomposites containing single and double-wall carbon nanotubes has been made. As a polymer matrix poly (ether-ester) multiblock elastomer was used. A weight ratio of hard to soft segments of obtained polyester nanocomposites PBT/PTMO was 45:55. The concentration of carbon nanotubes to polymer spread from 0,05 to 0,5 wt.% (for both single and double-wall CNT's).
The nanocomposites were synthesized *in situ* during the synthesis of polymer. Polymer matrix and nanocomposites were prepared in a two stage process involving transesterification and polycondensation in melting state.

This research work was supported by the Polish Ministry of Science and Higher Education under project number DFG/83/2006.

Lierature:

1. May Y., Yu Z., Polymer nanocomposites, CRC Press LLC, 2006.

16:00 Poster F33

An experimental study of the effect of charge density on the Taylor cone

Jon J. Stanger[1], Nick Tucker[1], Mark Staiger[2], Kerry Kirwan[3], Nigel G. Larsen[1], Roger J. Reeves[4]

1. *The New Zealand Institute for Crop and Food Research Ltd (CFR), Private Bag 4704, Christchurch 8140, New Zealand* **2.** *Dept. mechanical Engineering, University Canterbury (ME-UOC), Private Bag 4800, Christchurch 8140, New Zealand* **3.** *University of Warwick, Gibbet Hill Road, Coventry CV4 7AL, United Kingdom* **4.** *Department of Physics and Astronomy, The MacDiarmid Institute for Advanced Materials and Nanotechnology, University of Canterbury, Christchurch, New Zealand, Christchurch, New Zealand*

e-mail: tuckern@crop.cri.nz

The importance of charge density in electrospinning can be demonstrated by its presence in all mathematical models of the process either as charge density or as quantities derived from it. A good understanding of the effects of charge density on the electrospinning process is vital in diagnosing problems with new polymer-solvent systems, aiding development of specified nanofibres for industry and ensuring mathematical models are accurate. Using two different experimental approaches to increasing the charge density the effects on the Taylor cone and hence the mass deposition rate and initial jet diameter were examined. It was found that an increase in charge density results in a decrease in the mass deposition rate and initial jet diameter. A theory is proposed for this behaviour in that an increase in charge density leads to the tip of the Taylor cone forming a smaller radius of curvature resulting in the concentration of electric stresses at the tip. This leads to the electrostatic forces drawing the initial jet from a smaller effective area or "virtual orifice".

16:00 Poster F34

Development of research electrospinning machines

Nick Tucker[1], Jon J. Stanger[1], Neil Buunk[2], Mark Staiger[3], Roger J. Reeves[4], Nigel G. Larsen[1]

1. *The New Zealand Institute for Crop and Food Research Ltd (CFR), Private Bag 4704, Christchurch 8140, New Zealand* **2.** *Electrospinz Ltd (ESP), 44 Lee St, Blenheim 8140, New Zealand* **3.** *Dept. mechanical Engineering, University Canterbury (ME-UOC), Private Bag 4800, Christchurch 8140, New Zealand* **4.** *Department of Physics and Astronomy, The MacDiarmid Institute for Advanced Materials and Nanotechnology, University of Canterbury, Christchurch, New Zealand, Christchurch, New Zealand*

e-mail: tuckern@crop.cri.nz

Electrostatic attraction of liquids was first observed by William Gilbert in 1628, and attempts were made to commercialise the process in the 1900s and 1930s. In the late 1960s the physics of thread formation were described. More recently electrospinning has emerged as a ready way to produce nanoscale polymer fibres. This poster describes the development of a laboratory scale electrospinning machine and some preliminary results concerning the manufacture of composites from biodegradable and bio-origin materials.

At the laboratory scale the typical machine uses a syringe pump to provide a constant volume flow rate feed with the whole apparatus housed inside a protective enclosure, whilst this setup is certainly effective, it only allows limited access to the apparatus during operation and is intrinsically a batch process. To produce significant quantities of material, it is necessary to devise a continuous process. If the machine is to be used in a research laboratory it is necessary to allow provision for modification to the machine. The machine described uses a constant head device to feed the spinning tip (a standard micropipette tip). The use of this type of constant pressure device allows the user to establish a stable meniscus for the formation of the Taylor cone, and the consequent drawing of fibre, the rate of meniscus replenishment is automatically matched to rate of fibre removal. The machine operates with dual polarity. This allows the user to explore the charge carrying ability of subject materials, and to charge the target rather than the spinning tip; a charged target may be required if spinning from a melt rather than a solution.

A passive method for producing orientated fibres is also described.

16:00	Poster	F35

In-flight charge loss from electrospinning jets

Nick Tucker[1], Jon J. Stanger[1], Nigel G. Larsen[1], Mark Staiger[2], Roger J. Reeves[3], Kerry Kirwan[4]

1. *The New Zealand Institute for Crop and Food Research Ltd (CFR), Private Bag 4704, Christchurch 8140, New Zealand* **2.** *Dept. mechanical Engineering, University Canterbury (ME-UOC), Private Bag 4800, Christchurch 8140, New Zealand* **3.** *Department of Physics and Astronomy, The MacDiarmid Institute for Advanced Materials and Nanotechnology, University of Canterbury, Christchurch, New Zealand, Christchurch, New Zealand* **4.** *University of Warwick, Gibbet Hill Road, Coventry CV4 7AL, United Kingdom*

e-mail: tuckern@crop.cri.nz

Due to the difficulty of measuring the electric current being drawn from the high voltage power supply to the high voltage electrode in the electrospinning process the electric current typically observed is the current flowing from the opposite electrode to ground. This current can then be used to infer details about the electrostatic environment such as the charge density on the fluid jet. It has been shown in literature that assuming initially the current is conducted in an ohmic mode and a reasonable conductivity for the polymer solution an electric current with the same order of magnitude to that observed. As conductivity is directly related to ionic concentration it was possible to add a known amount of ionic salt and measure the electric current while electrospinning fibre. This measured current was then compared to the expected electric current calculated from the ionic concentration. It was found that as the ionic concentration increased the observed electric current increased but at a slower rate than the calculated electric current increased. This suggests that a significant portion of the charge on the jet may be lost during flight. This further implies that in order to increase the charge density where the bending instability occurs (driving force proportional to charge density) the initial charge density must be drastically increased to compensate for the losses in flight. This may be limited as the effects of increased charge density may be detrimental to the formation of the Taylor cone.

Wednesday, 17 September

Joint Poster Session 2

Metal/ceramic matrix nanocomposites
Wednesday afternoon, 17 September, 16:00
Main Hall

16:00	Poster	F36

Luminescense and mechanical properties of Al_2O_3 nanopowder basis nanoceramics

Andrey Nomoev

Buryat State University, Physics Department (BSU), Smolina 24 A, Ulan-Ude 02-936, Russian Federation

e-mail: nomoevav@mail.ru

The investigation of the preparation of submicrograin (of several micrometers) dense strong ceramics of alumina (Al_2O_3) nanopowder has been carried out. The obtained ceramic properties were investigated with the use of SEM, TEM, XRD, luminescence spectroscopy. It was shown that the ceramics of different composition irradiate visible light at different wavelength ranges being excited by ultraviolet lasers. The intensive well separated luminescense red peak at 2.0 eV o was observed in ceramics Al_2O_3 nanopowder basis at all ceramics sintering temperature. The range of ceramics sintering temperature is 1200-1600 ^{0}C. The decay time of this red band is exponential at room temperature. The sintering process of the different produced above-mentioned nanopowders and the resulting ceramics strongly depend on size and shape of particles of the used powders. The data about the shape-formation and coagulation of ceramic samples at different powders combination were received. At moderate density, the microhardness 16-35 GPa for some of sintered strong samples of submicrograin (of several micrometers) structure had been achieved. Using different schemes of pressing and sintering temperature we can change pores size and grains of ceramics.

16:00	Poster	F37

Formation of nano-cluster structure of γ-Fe_2O_3 in an amorphous SiO_2 matrix

Dzmitry A. Kotsikau[1], Maria I. Ivanovskaya[1], Vladimir V. Pankov[2], Julia Lyubina[3]

1. *Research Institute of physical-chemical problems (FHP), Leningradskaja 14, Minsk 220050, Belarus* **2.** *Belarusian State University (BSU), F. Skaryna av. 4, Minsk 220050, Belarus* **3.** *Leibniz-Institute for Solid State and Materials Research, P.O.Box 270116, Dresden D-01171, Germany*

e-mail: kotsikau@bsu.by

Structural features of magnetic materials containing γ-Fe_2O_3 particles (2-5 nm) dispersed over amorphous porous SiO_2 matrix have been studied by TEM, EPR, XRD, IR- and Moessbauer spectroscopy. γ-Fe_2O_3-SiO_2 nanocomposites were prepared by mixing Fe_3O_4 nH_2O and SiO_2 nH_2O sols. Thermo-stimulated structural transformations in the nanocomposites were studied in the temperature range of 100-1100°C depending on Fe_2O_3 content (1-8 wt. %). High thermal stability of γ-Fe_2O_3 clusters in the pores of SiO_2 matrix was revealed. Partial transformation of γ-Fe_2O_3 into α-Fe_2O_3 and the particle growth to 20 nm occur only under high-temperature (1100°C) treatment. High thermal stability of small γ-Fe_2O_3 grains in the γ-Fe_2O_3-SiO_2 nanocomposites can be explained by the tendency of Fe^{3+} ions to have high-symmetric cubic coordination of ions like in Fe_3O_4 nH_2O particles in the corresponding sol. Additional stabilization of cubic symmetry is connected with OH-groups occurring in Fe^{3+} coordination environment. These groups are difficult to remove from the mesa-porous SiO_2 structure. Magnetically active nanoclusters dispersed over various matrixes can be potentially used to obtain materials demonstrating magnetoresistive effect

16:00 Poster F38

Hydrogen absorption and desorption kinetics of magnesium hydride nanocomposite with nanosized metal oxides as catalysts

Marek Polański, Iwona E. Malka, Jerzy Bystrzycki

Military University of Technology, Faculty of Advanced Technology and Chemistry, Kaliskiego 2, Warszawa 00-908, Poland

e-mail: imalka@wat.edu.pl

Magnesium hydride (MgH_2) is one of the most attractive hydrogen storage materials because of its high hydrogen storage capacity (7.6 wt %), light weight and low cost. However, the high desorption temperature (above 300ºC) and the slow hydrogen absorption and desorption kinetics limit the practical application of this hydride.

In our work, we have shown that hydrogen sorption kinetics of nanocrystalline MgH_2 powders can be significantly improved by adding nanosized metal oxides as catalysts. Recently, we have found [1], that introduction of Cr_2O_3 nanoparticles in the course of the MgH_2 milling process results in the synthesis of nanocrystalline/nanoparticle composite, which shows very fast hydrogen sorption properties. Therefore, following this approach, we have used high energy (ball) milling to fabrication of MgH_2-Me_xO_y nanocomposites (Me_xO_y=Cr_2O_3, TiO_2, Fe_2O_3, Fe_3O_4, In_2O_3, ZnO). The hydrogen sorption kinetics of investigated nanocomposites was evaluated using a volumetric Sievert apparatus. The phase structure, morphology and chemical composition were investigated by XRD, SEM, EDS and DSC-TG.

Microstructural investigations of mechanical (ball) milled MgH_2 powders without and with nano-catalysts showed a MgH_2 particle size of 0.5-10µm. The milled MgH_2 exhibited a homogeneous crystallite size distribution with average crystallite size smaller than 100 nm. The brittle nano-catalyst particles were embedded by the MgH_2 matrix, forming a nanocomposite structure. The particle size of catalysts was found to be 10-300 nm. Our results indicate that in both absorption and desorption reactions, the superior catalytic effect of Cr_2O_3 and TiO_2 was observed. The catalytic effect of investigated metal oxides is also expressed in lowering activation energy of dehydriding reaction. The mechanism of catalysis is not clear so far and some proposals will be presented and discussed.

1. M. Polanski, J. Bystrzycki, T. Plocinski, IJHE, 33 (2008) 1859-1867

16:00 Poster F39

Mechanical and corrosion properties of Ni-free austenitic stainless steel/hydroxyapatite nanocomposites

Maciej Tuliński, Mieczysław Jurczyk

Poznań Technical University, pl. Marii Skłodowskiej-Curie 5, Poznań 60-965, Poland

e-mail: maciej.tulinski@doctorate.put.poznan.pl

Recently, a new manufacturing process of nickel-free austenitic stainless steels with nitrogen absorption treatment has been developed. In this method, small devices can be precisely machined in a ferritic phase and than during nitrogenization of their surfaces in nitrogen gas at temperature approx. 1200oC they become nickel-free austenitic stainles steels with better mechanical and corrosion resistance properties.

In the present work, a nanocrystalline nickel-free stainless steels as well as nickel-free stainless steel/hydroxyapatite nanocomposites has been synthesized by the combination of mechanical alloying (MA), heat treatment and nitrogenation of elemental microcrystalline Fe, Cr, Mn and Mo powders. Phase transformation from ferritic to austenitic was confirmed by XRD analysis.

The microhardness of the final bulk material was studied using Vickers method. The result is almost two times greater than in austenitic steel obtained by conventional methods. This effect is directly connected with structure refinement and obtaining of nanostructure.

Mechanical alloying is a very effective technology to improve also the corrosion resistance of stainless steel. Decreasing the corrosion current density is a distinct advantage for prevention of ion release and it leads to better cytocompatibility. Corrosion tests were performed in Ringer's solution.

According to existing conceptions, decreasing of material's crystallites size to nanometric scale allows to achieve much better mechanical properties (e.g. microhardness) compared to conventional materials. With regard to austenitic stainless steels it could help to obtain better biomedical implants (e.g. stents) with better mechanical properties, corrosion resistance and biocompatibility.

The results show that nickel-free stainless steel/hydroxyapatite nanocomposites could be promising bionanomaterials for use as a hard tissue replacement implants from mechanical and corrosion properties point of view.

16:00 Poster F40

Ionic liquid entrapped in metallic silver

Marie-Alexandra G. Neouze, Marco Litschauer

Vienna Technical University, 9, Getreidemarkt, Wien 1040, Austria

e-mail: mneouze@mail.zserv.tuwien.ac.at

One of the numerous features of ionic liqids (ILs) is their suitability for electrochemical deposition; they are an environmentally friendly alternative for silver electrodeposition. This is directly linked to the synergetic effect of ionic liquids and metals.

Consequently a challenge concerns the study of the possible formation of metal - ionic liquid composite adapting the method developed by Avnir and co-workers for organic molecules entrapment within metal matrixes. This could be a unique way to investigate further the formation mechanism of the metal - organic compounds and could open new applications linked to the ionic liquids.

Moreover the physico-chemical properties of entrapped ionic liquids were already revealed as being original and depending on the entrapment parameters, namely pore diameter etc.

We will present the characterization of the synthesized metal - ionic liquid composite material, by determining the ionic liquid entrapment percentage within the matrix and the thermal stability of the compound. Dynamic scanning calorimetric experiments are comparing physico-chemical values of genuine ionic liquid and the composite compound.

16:00 Poster F41

Mechanical and corrosion properties of titanium – hydroxyapatite nanocomposites

Katarzyna Niespodziana[1], Karolina Jurczyk[2], Mieczysław Jurczyk[1]

1. *Poznań Technical University, pl. Marii Skłodowskiej-Curie 5, Poznań 60-965, Poland* **2.** *Univ. of Medical Sciences in Poznań, Dept. of Conservative Dentistry, Poznań, Poland*

e-mail: katarzyna.niespodziana@put.poznan.pl

Titanium and its alloys are preferred metal materials for bone replacement, as they have proven a better biocompatibility and good mechanical properties in comparison to other metals and alloys used in medicine. However, they have poor tribological properties and are bio-inert biomaterials which means that they cannot directly bond to the bone. Some of those poor mechanical and biological properties of titanium can be improved by making composite materials using titanium to reinforce ceramic particles for example hydroxyapatite. Hydroxyapatite (HA, $Ca_{10}(PO_4)_6(OH)_2$) is bio-active material and after some time it is partially resorbed and replaced by natural bone. Unfortunately, hydroxyapatite had poor mechanical properties and cannot be used for hard tissue replacement implants. For this reason, fabrication of Ti – based composites reinforced with ceramics particles seems to be a promising candidate way to create more perfect implants.

In the present work Ti-HA (3, 10, 20, 50 vol%) nanocomposites were produced by the combination of mechanical alloying (MA) and powder metallurgical process. The resulting microstructures were characterized using X-ray diffraction, scanning electron microscope and transmission electron microscopy. The properties of the nanocomposites were investigated by mechanical and in vitro studies. The experimental results show, that Ti-HA nanocomposites have better mechanical and corrosion properties in comparison with microcrystalline titanium. Foe example: Vickers microhardness of Ti-10 vol% HA nanocomposite is 1500 HV0.2 (pure Ti metal – 250 HV0.2) and corrosion resistance in Ringer solution is $I_c = 1.19 \cdot 10^{-7}$ A/cm², $E_c = -0.41$ V for Ti-10 vol% HA and $I_c = 1.31 \cdot 10^{-5}$ A/cm², $E_c = -0.36$ V for Ti. In conclusion, titanium – ceramics nanocomposite are suitable for hard tissue replacement from the point of view of both mechanical and corrosion properties.

16:00 Poster F42

Application of the spectroscopic ellipsometry for studying of the $TiSi_2$ silicide formation induced by thermal annealing of the Ti/Si multilayered films

Yuri Kudryavtsev[1], Yurii Makogon[2], Olena P. Pavlova[2], Sergey I. Sidorenko[2], Tatiana I. Verbitskaya[2]

1. *G.V. Kurdyumov Institute for Metal Physics National Academy of Sciences (IMP), Vernadsky Blvd. 36, Kyiv UA03680, Ukraine* **2.** *National Technical University of Ukraine KPI, pr.Peremogy 37, Kyiv 03056, Ukraine*

e-mail: kudr@imp.kiev.ua

The work aimed to demonstrate the potential of the spectroscopic ellipsometry approach for studying of the spontaneous and induced by thermal annealing solid state reactions in $(3.0\text{ nm Ti }/6.7\text{ nm Si})_{20}$ multilayered film (MLF) with overall stoichiometry of $TiSi_2$ deposited by DC-sputtering onto (001) single-crystalline Si kept at room temperature. The structural characterization of the Ti/Si MLF in the as-deposited state and after each step of heat-treatment has been performed also by the methods of x-ray diffraction (XRD) and resistometry. According to the results of the XRD-study the as-deposited Ti/Si MLF looks amorphous-like. Annealings at 470 -1020 K did not cause any visible changes in the XRD patterns. The optical tool reveals that definite changes in the MLF's structure appeared after annealing at 470 K. Comparing the experimental and modelled optical properties of the Ti/Si MLF based on different models of the MLF's structure, the conclusions on various types of short range orders in these amorphous-like Ti/Si MLF have been done. It was established that the regions with a stoichiometry close to TiSi are spontaneously formed in Ti/Si MLF during the deposition. The thickness of such a regions for the $(3.0\text{ nm Ti }/6.7\text{ nm Si})_{20}$ MLF was estimated to be 1 nm. Sequential annealings of the as-deposited Ti/Si MLF completely destroy the layered structure of the films and lead according to the optical data to the formation of C54-$TiSi_2$ crystalline film after annealing at 1170 K. These results nicely agree with the XRD data.

16:00 Poster F43

Cu-Si nanocomposites based on porous silicon matrix

Hanna Bandarenka[1], Aliaksandr Shapel[1], Marko Balucani[2]

1. *Belarusian State University of Informatics and Radioelectronics (BSUIR), P.Brovka str. 6, Minsk 220000, Belarus* **2.** *Universita 'La Sapienza' di Roma, Via Eudossiana 18, Roma 00184, Italy*

e-mail: vitaly51@mail.ru

Porous silicon (PS) is an artificially structured form of silicon to be used as a matrix for formation of nanocomposite materials by introducing different metals into PS. The fundamental understanding of the relationship between fabrication, structure and physical-chemical properties of porous silicon and porous silicon-based composites is essential for its further applications.

In the present work we demonstrate Cu-Si nanocomposites formed by chemical displacement deposition of Cu into porous silicon matrix. The basic reaction of this process is the substitution of silicon atoms by copper atoms. The fundamental advantage of displacement deposition with respect to other deposition methods is that it can provide deep penetration of metals inside pore channels in PS. Porous silicon layers with porosity from 30 % up to 80 % and with thicknesses from 1 to 10 micrometers were formed by anodizing of Czochralski (100) silicon wafers in HF electrolyte. PS porosity was controlled by varying the anodic current density in the range of 10 -150 mA/cm². After anodization, the HF electrolyte was replaced by a $CuSO_4$ + HF solution and Cu was deposited into porous silicon. SEM and X-ray microanalysis techniques were used to investigate the structure and elemental composition of Cu-Si samples. The distribution of the deposited metal, the structural features of Cu film and factors that influence Cu film structure are described. It is shown that variation of PS porosity and chemical displacement deposition regimes provide the formation of different nanocomposite PS-Cu structures. The potential fields of application of Cu-Si nanostructures are discussed: (a) electrical and mechanical Cu contacts with extremely high adhesion to PS; (b) nano- and micro-electromechanical systems; (c) assemblies of Si-nanowires carefully covered by Cu; (d) porous Cu membranes.

16:00 Poster F44

Effect of heat treatment on Ti(C,N)-SiC-Si_3N_4 -C ceramic nanocomposites

Anna Biedunkiewicz, Urszula R. Gabriel, Paweł Figiel

Szczecin University of Technology, Institute of Materials Engineering, Szczecin 70-310, Poland

e-mail: pfigiel@ps.pl

The studied nanocomposite was Ti(C,N)-SiC-Si_3N_4-C powder, produced by a sol-gel method. The main aim of the investigation was the selection of optimal parameters for annealing of the multiphase composites, in order to eliminate carbon vacancies and oxygen atoms. This approach was applied to obtain maximal stoichiometric composition of investigated phases, retaining minimal nanocrystallite size. Optimal conditions of the annealing of Ti(C,N)-SiC-Si_3N_4-C nanocomposite were determined on the base of a kinetic analysis of this process. The analysis was performed with application of the Coats-Redfern equation. Artificial Neural Networks were used to the direct assessment of experimental data and identification of kinetic models and parameters. Nanoparticle size, dispersion and phase composition before and after heat treatment were determined with HRTEM, SEM, XPS, XRD methods and total carbon analysis. TG measurements were carried out on samples heated in argon atmosphere up to 1773 K. Gaseous products were identified using MS while solid products by XRD and HRTEM techniques.

16:00 Poster F45

Hybrid nanocomposite coatings for application in construction materials: tribological study

Celia Silvestre[1], Mariajose López-Tendero[1], Manuel Cruz-Yusta[1], Noelia Baeza[1], Celia Guillem[1], Stephanie San Juan[1], Jose-Manuel Lloris[1], Tamayo Eduardo[2]

1. *Asociación Investigación Industrias de Construcción (AIDICO), Parque Tecnológico Valencia, Valencia 46980, Spain* **2.** *Universidad de Valencia-ICMUV (ICMUV), Polígono La Coma s/n, Valencia 46980, Spain*

e-mail: mlopezt@aidico.es

The Nanocomposite group of AIDICO and the Nanomaterials Group of University of Valencia collaborate in the development of new nanocomposite materials of epoxy matrix with application in construction materials. Tribological properties and good thermal stability are some of the achieved specifications for these applications. Some hybrid coatings based on the "in situ" formation of nanosilica are presenting in this work. Elastic modulus and hardness obtained from TDMA analyses and nanoindentation techniques, together with thermal stability by TGA, are the main properties analysed in this work in order to fit the requirements of stone coating applications. New routes for obtaining these coatings based on sol-gel have been explored. Structural characterization by SEM is also correlated with the final properties.

16:00 Poster F46

Production of fine-grained α-SiAlON ceramics from nanopowders

Ilmars Zalite, Natalja Zilinska, Janis Krastins

Institute of Inorganic Chemistry, Riga Technical University, Miera iela 34, Salaspils LV2169, Latvia

e-mail: ilmars@nki.lv

Ceramic materials on the basis of Si_3N_4 including sialons are characteristic with outstanding mechanical properties (hardness, bending strength etc.) at temperatures up to 1400 °C and good wear and corrosion resistance.

Because of low diffusion speed sintering processes of Si_3N_4-containg materials as well as microstructure and mechanical properties depend not only on the chemical composition of sialon, but also on the size of particles of the starting material. Therefore application of nanoparticles would be interesting for development of new materials.

The aim of this work was to find the dependence of sinterability, microstructure and properties of the mentioned α-sialons on the chemical composition of sialons by using nanopowder composites.

Investigation were made of 15 different Y-containing α- sialon composites corresponding to the formula $Y_{m/3}Si_{12-(m+n)}Al_{m+n}O_nN_{16-n}$ or near it. Si_3N_4 – 27 wt. % AlN nanocomposite was used as a raw material with the addition of Al_2O_3, Y_2O_3 and Si_3N_4 nanopowders. Sialon composites were made by mechanical mixing of raw powders. Final specific surface area of composite was of 70-100 m^2/g corresponding to the average particle size of 20-30 nm. Ceramic materials were obtained by sintering in nitrogen medium at 1400-1700 °C.

It was found that it is possible to obtain dense ceramic materials with relatively fine-grained structure (200-300 nm) from nanopowders beginning with 1500 °C and they differ from sialons obtained from traditional more coarse powders, because the density of them at such sintering temperatures does not exceed 60-70 %. Hardness of some sialon composites prepared at such sintering temperatures reaches even 23 GPa. Fracture toughness K_{1c} of samples obtained after sintering at 1600 °C is of 4-6 $MPa{\cdot}m^{1/2}$ and grows with the increase of sintering temperature. If the sintering temperature is increased over 1700 °C, the concentration of needle-shaped crystals in material grows increasing the mechanical strength of material.

16:00 Poster F47

Magnetic properties and caloric effect in the $Gd(Ni_{1-x}Fe_x)_3$ /Cu nanocomposites

Anna Bajorek[1], Artur Chrobak[1], Grażyna Chełkowska[1], Marzena Kwiecień[1], Małgorzata Karolus[2], Grzegorz Haneczok[2]

1. *University of Silesia, August Chełkowski Institute of Physics, Department of Solid State Physics, Uniwersytecka 4, Katowice 40-007, Poland* **2.** *University of Silesia, Institute of Material Science, Bankowa 12, Katowice 40-007, Poland*

e-mail: anna.bajorek@us.edu.pl

During the last decades the Greenhouse effect, caused also by emission of chlorofluorocarbons, is considered to be an increasing problem for our environment. One solution for this problem is to eliminate traditional refrigeration by a modern technique based on the magnetocaloric effect (MCE). Materials used for this application should exhibit different opposing properties such as a relatively high magnetocaloric effect, a high thermal conductivity and a Curie point near room temperature.

It appears that magnetic nancomposites consisting of rare earth and transition metal particles nanodispersed in a conductive matrix will have great potential for the use in refrigeration. Therefore, the aim of the presented work is to study magnetic properties of the Gd(Ni_{1-x} Fe_x)$_3$ nanopowder embedded into a copper matrix with a caloric effect of high efficiency near room temperature. Apart from that it is important to compare the magnetic properties of the examined nanocomposites and crystalline phase of the magnetic component.

The Gd(Ni_{1-x} Fe_x)$_3$ compounds were obtained by arc melting technique, the compounds were ground by making use of mechanical ball milling and finally the mixture of milled nanopowder and copper was compacted. As it is shown the best material for the room temperature refrigeration exhibit samples with 0.1<= x <=0.2 for which the T_c is 266 K and 376 K respectively. However the highest magnetocaloric effect was observed for Ni- rich samples.

16:00 Poster F48

Characterization of Nano-sized Ba-Mg Ferrite Powders Prepared through Self-propagating High Temperature Synthesis Reaction and Mechanical Milling

Yong Choi

Sunmoon University, 100 Kalsan-Ri Tangjeoung-Myun, Asan 336-840, Korea, South

e-mail: yochoi@sunmoon.ac.kr

Nano-sized $Ba_xMg_{1-x}Fe_2O_4$ ferrite powders were prepared with the initial reactant powders of Fe, BaO, MgO and Fe_2O_3 by self-propagating high temperature synthesis (SHS) reaction followed by mechanical milling. Magnetic properties and non-stoichiometric number of the SHS products were determined by vibrating sample magnetometry and neutron diffractometry, respectively. As the initial composition of barium oxide and magnesium oxide changed from 0.5 to 4.0, the coercive force and residual magnetization and maximum magnetization increased about 34%, 70% and 60% respectively. Neutron diffraction revealed that the change of the magnetic properties was related to the non-stoichiometries of the ferrite powders. Numerical modeling of the SHS reaction will be presented.

16:00 Poster F49

Enhanced gas sensing behaviour at room temperature of doped Ga_2O_3 nanowire grown by thermal evaporation method

Weekyung Kang[1], Kyungrae Kim[1], Dong-Kuk Kim[2]

1. *Dept. of Chemistry, Soongsil University, 511, Sangdo-dong, Dongjak-ku, Seoul 156-743, Korea, South* **2.** *Kyungpook National University (KNU), Daegu 702-701, Korea, South*

e-mail: wkang@ssu.ac.kr

Monoclinic gallium oxide (Ga_2O_3) is a versatile wide band gap semiconductor material. Ga2O3 thin film-based gas sensors are very promising to detect O_2, H_2, CH_4 and CO at high temperature. At elevated temperature, the conductivity of Ga_2O_3 can be influenced by an ambient atmosphere. But at low temperature, the oxygen-vacancies diffusion is frozen and the bulk electrical conductivity no longer responds to the change in the gas composition. The high working temperature limits the application of Ga_2O_3-based gas sensors. One-dimensional (1D) nanomaterials are considered as ideal candidates for applications due to their large surface area-to-volume ration and the size effect. The 1D nanostructures of well-established gas sensing materials have shown higher sensitivity, fast response, and enhanced capability to detect low concentration gases compared with the corresponding thin film materials. Gas sensors made from 1D nanomaterials showed lower optimal operating temperature, which is favourable for power saving and device integration. Gallium oxide nanowires are synthesised on Au-patterned Si substrate by simple thermal evaporation method from milled gallium oxide powder and graphite powder under Ar atmosphere at 1100□. The morphology and size of the nanowires are characterized by X-ray diffraction, scanning electron microscopy high resolution transmission electron microscopy and energy dispersive X-ray spectroscopy. Electrical properties of Ga_2O_3:X nanowires (X=Sn, Mn, Fe.......) constructed on Au electrode are measured at room temperature for application to gas sensor materials. The conductivity change of n-type semiconducting Ga_2O_3 nanowires is sensitive to NO_2 or H_2S gas at room temperature.

This work was supported by the Seoul R&D program.

16:00 Poster F50

Colouring anodization of AZ31 Mg alloy

Kyungmun Lee[2], Soo-young Doh[1], Eun-Jung Lee[1], Ji Eun Lee[3], Jeung-Soo Huh[2], Dong-Kuk Kim[3]

1. *NUC Electronics Co., Ltd. (NUC), 679 Chimsan3Dong, Bukgu, Daegu 702-053, Korea, South* **2.** *Kyungpook National University (KNU), Daegu 702-701, Korea, South* **3.** *Kyungpook National University, Department of Chemistry, Daegu 702-701, Korea, South*

e-mail: happyching@hanmail.net

The colouring of magnesium alloy articles that have been anodized (or otherwise chemically oxidised) has defeated most attempts by experimenters attempting to provide a range such as is available for anodized aluminium. A new anodizing process based on an environmentally friendly electrolyte solution that contains none of chromate, phosphate of fluoride can do colouring and give a luster on AZ31 Mg alloy surface. Anodizing behaviours of magnesium and its alloys are influenced by many factors, including the constituents and concentrations of electrolyte solution, the nature of basis metal as well as applied current density of voltage, treatment time and solution temperature, etc. Therein, the electrolyte solution plays a determinant role. Applied constant current can ensure that anodic films grow at an almost uniform rate. Corrosion resistances of the films were analyzed from results of the anodic polarization measurement in 0.1 mass% NaCl solution. Microstructure and phase composition were analyzed by SEM and XRD. The basic mechanism of anodic coating formation is explained.

16:00 Poster F51

Synthesis of Cobalt ferrite nanowires using FeOOH as a template

Jose G. Camacho[1], Carlos A. Martínez[1], Humberto A. Monreal-Romero[2], Perla E. Garcia-Casillas[1]

1. *Universidad Autonoma de Ciudad Juarez, Ave. del Charro 450 Norte, Juarez 32360, Mexico* **2.** *Universidad Autónoma de Cd. Chihuahua, Ave. Escorza y Venustiano Carranza s/n, Chiuahua 3100, Mexico*

e-mail: perlaelviagarcia@yahoo.com

In this work cobalt ferrite nanowires were synthesized by chemical synthesis by the use of FeOOH as template. The FeOOH nanorods were obtained by the hydrolysis of ferric chloride, afterwards the cobalt ion (Co+2) was added and precipitated in order to interact with the FeOOH. The FeOOH nanorods has a diameter size of 19 and 65 nm length, these nanorods were grouped in packages with different orientation due to the cobalt interaction. These agglomerates were calcinated at different temperatures since 700 to 1000 °C, the obtained product was a cobalt nanowires with a diameter of 70 nm and some microns of length.

The average size of the nanorods and nanowires were determined by field emission scanning electron microscopy (FESEM). In order to understand the interaction mechanism between nanorods and the cobalt ions Fourier transform infrared spectroscopy (FTIR) was used. The transformation of these particles was studied by thermogravimetric and differential thermal analysis (TGA-DTA). The magnetic properties, intrinsic coercivity (H_c) and the saturation magnetization were determined by vibrating sample magnetometry (VSM). The identification of phases was made by X-ray Diffraction.

16:00 Poster F52

Fabrication of $Sm_{0.5}Sr_{0.5}CoO_3$ cathode thin films for IT-SOFC by Electrostatic Spray Depositon

Inyu Park, Jongmo Im, Sungeun Jang, Dongwook Shin

Hanyang University, 14-509, Heangdang-Dong, Seong-dong-Gu, Seoul 133-791, Korea, South

e-mail: 2000iu@hanmail.net

Strontium-doped samarium cobaltite ($Sm_{0.5}Sr_{0.5}CoO_3$, SSC) has good electrochemical properties for intermediate-temperature solid oxide fuel Cells (IT-SOFCs) because it has a mixed-conduction characteristic of electronic and ionic conductivities. It has higher ionic conductivities than other cathode materials for SOFCs such as LSM and LSGM. The Electrostatic Spray Deposition (ESD) method has some advantages such as being a simple apparatus, the convenience of controlling the microstructure of thin films and a variety of choices for precursor solution. In this study, the ESD method was applied to fabricate porous SSC thin films for a SOFC cathode. Samarium chloride hexahydrate ($SmCl_3 \cdot 6H_2O$), strontium chloride hexahydrate ($SrCl_2 \cdot 6H_2O$), cobalt nitrate hexahydrate ($Co(NO_3)_2 \cdot 6H_2O$) as starting materials and methyl alcohol as solvent were used to make precursor solution. The porous SSC films were deposited on Si substrate and the microstructure was dependent on processing parameters such as substrate temperature, distance from nozzle to substrate, applied voltage and flow rate of a syringe. Scanning Electron Microscope (SEM) and X-ray Diffractometer (XRD) measurement were used to investigate the microstructure and crystallinity of the SSC films. The ESD technique is shown to be an efficient method by which SOFCs' cathode films can be fabricated tailored for the desired phases and microstructures.

16:00 Poster F53

Lanthanum strontium manganite films prepared by air-blast spray deposition technique

Jongmo Im, Inyu Park, Seungun Jang, Dongwook Shin

Hanyang University, 14-509, Heangdang-Dong, Seong-dong-Gu, Seoul 133-791, Korea, South

e-mail: ijm73@hotmail.com

Air-blast spray deposition (ASD), using liquid droplets atomized by gas pressure, are based on the aerosol technique. This technique has shown many advantages over several conventional deposition techniques, such as a simple set-up, inexpensive and nontoxic precursors, high deposition rate and, in particular, easy control of the surface morphology of the deposited layers. This method also enables the thin film deposition in ambient atmosphere even if an additional heat treatment is required to obtain film with high degree of crystallinity.

In this work, ASD was applied to prepare porous lanthanum strontium manganite (LSM) films on silicon substrate for the electrolyte application in Solid Oxide Fuel Cell. The morphology of LSM film was dependant on the process parameters such as substrate temperature, liquid flow rate, deposition time, and nozzle-substrate distance. The effects of heating temperature on the crystal structure of films were investigated with X-ray diffraction (XRD) in the heating temperature range of 400 ^{o}C to 1000 ^{o}C. The porous LSM film was successfully prepared in the solution flow rate range of 1 l/min to 3.5 l/min, the substrate temperature of 149 ^{o}C to 243 ^{o}C, the nozzle-substrate distance range of 1 cm to 10 cm, and the deposition time of 0.5 min to 30 min.

16:00 Poster F54

A solid-state route for the synthesis of metal nanocluster composite glasses

Elti Cattaruzza[1], Francesco Gonella[1], Patrizia Canton[2], Tiziana Cesca[3], Ali Shahid[3]

1. *Physical Chemistry Dept, Università Ca' Foscari Venezia, Dorsoduro 2137, Venezia I-30123, Italy* **2.** *Physical Chemistry Dept, Università Ca' Foscari Venezia, via Torino 155/b, Venezia-Mestre I-30170, Italy* **3.** *CNISM, Physics Dept, Università di Padova, via Marzolo 8, Padova I-35131, Italy*

e-mail: cattaruz@unive.it

To dope silicate glasses with mono- and/or multivalent ions, an approach based on field-assisted solid state ion exchange (FASSIE) is used. The diffusion of dopant ions originating from a film deposited onto the glass surface takes place owing to an external electric field across the glass slide. After doping, metal precipitation to form nanoparticles is induced by irradiation with either energetic ion or high power laser beams. The characterisation of soda-lime silicate glass samples doped with different metals was performed by Rutherford backscattering spectrometry, optical absorption and transmission electron microscopy, in order to correlate the irradiation parameters to the cluster formation process.

16:00 Poster F55

Photoluminescent properties of doped ZnO nanopowders

Bohdan K. Kotlyarchuk[1], Bohdan K. Ostafiychuk[3], Dmytro I. Popovych[1,2], Andrew S. Serednytski[1]

1. *Institute of Applied Problems of Mechanics and Mathematics (IAPMM), 3B Naukova Str., Lviv 79060, Ukraine* **2.** *National University "Lvivska Polytechnika", Bendera St. 12, Lviv UA-79013, Ukraine* **3.** *Precarpathian National University named after Vasyl Stefanyk, 57 Shevchenko, Ivano-Frankivsk 76025, Ukraine*

e-mail: popovych@iapmm.lviv.ua

Zinc oxide is one of the most important II-IV compound semiconductors with a wide bandgap of about 3.37 eV at room temperature which can be used in a number of optoelectronic devices (UV photodetectors, light emitting diodes, laser diodes, gas-sensors) [1].

This work is devoted to experimental research of the photoluminescence features of ZnO nanopowder (d~30÷40 nm) doped by impurities of Mn, Ti, Cr, V (~2÷3 at. %). Doping was accomplished by the method of thin film (h~5÷8 nm) laser deposition of the doping material onto nanopowder followed by laser implantation and activation of the doping impurity [2].

For initial ZnO at a room temperature intensive ultraviolet (λ_{max}=387 nm) and yellow-orange luminescence (λ_{max}=600 nm) was observed and also a weak radiation in the green range of the spectrum (λ_{max}=510 nm). A decrease of the intensity of the yellow luminescence in comparison with undoped material and the occurrence of a new luminescence maximum (λ_{max}=535 nm) in zinc oxide doped by Cr and Ti has been observed . In ZnO:Ti appears also a green luminescence with λ_{max}=525 nm, which could be the result of a formation of TiO_2 particles in the nanopowder . Doping of zinc oxide by Mn and V leads to a significant increase of the intensity of the yellow luminescence which can be used effectively for the increase of the sensitivity in gas detection.

[1] Zinc Oxide Bulk, Thin Films and Nanostructures. Processing, Properties and Applications. *Edited by: Chennupati Jagadish and Stephen Pearton* (2006).

[2] B.K.Kotlyarchuk, D.I.Popovych, A.S.Serednytski, I.F.Myronyuk. *Features of Photoluminescent Properties of Doped ZnO Nanopowders* // COLA 2007, 9th International Conference on Laser Ablation, September 24-28, 2007, Tenerife, Spain, PTU-73.

16:00 Poster F56

Obtaining of luminescent core-shell hetero-nanoparticles SiO_2(core)/ZnO(shell) for photonic application

Iuliia V. Iermolaieva, Yuriy N. Savin, Alexander V. Tolmachev

Institute for Single Crystals NAS of Ukraine (ISC), 60 Lenin Ave., Kharkov 61001, Ukraine

e-mail: yermolayeva@isc.kharkov.ua

In last decade, development of essentially new class of the functional optical materials on the basis of the active photonic crystals has the considerable interest. Zinc oxide is well known wide band-gap semiconductor with large exiton binding energy (60 meV) and intensive UV-luminescence (l_{max}~380 nm) at room temperature. This semiconductor in the low-dimensional state is considered as one of the most promising materials for making active luminescent photonic crystals, light-emitting devices for UV lasers.

Obtaining of ZnO nanocrystals (ZnO NC) in opal-like structures mostly formed by spherical silica particles (SiO_2) with nano- and ultramicron sizes by the infiltration methods is described in many papers. However, negative consequence of the precursor's infiltration into voids of the matrix with further thermal treatment is the process of concomitant zinc silicate formation and worsening of the luminescence characteristics. As an alternative, it is possible to prevent such undesirable effects for that layers of ZnO NC can be formed upon silica spheres (i.e. to obtain hetero-nanoparticles) before theirs compacting.

In the present work SiO_2(core)/ZnO NC(shell) core-shell hetero-nanoparticles with a silica core (200-300 nm) and a shell of NC ZnO (20-30 nm) have been obtained. NC ZnO the given sizes at a narrow size distribution (< 15 %) have been grown up from non-water solutions by a sol-gel technique in the presence of silica spheres. The size, morphology and phase composition of synthesized SiO_2/ZnO hetero-nanoparticles have been examined by means of electron microscopy and X-ray photoelectric spectroscopy methods. Optical and luminescent properties of received SiO_2/ZnO hetero-nanoparticles have been investigated. UV-luminescence (λ_{max} ~ 390 nm) in the all experimental samples is prevailing. It is shown that structure of the luminescence band (presence and intensity of the defect band at 500-600 nm) depends on the ZnO NC synthesis method.

16:00 Poster F57

Characterization of n-$Mg_xZn_{1-x}O$/ZnO/p-GaN double heterostructure grown by pulsed laser deposition

Ju-Young Lee[1], Bo La Jang[1], Hong Seung Kim[1], Hyung Koun Cho[2], Won-Jae Lee[3]

1. *Korea maritime university (KMU), Yongdo-gu, dongsam-dong, Busan 606-791, Korea, South* **2.** *Sungkyunkwan University (SKKU), 300, Chunchun-Dong, Jangan-Gu, Suwon 440-746, Korea, South* **3.** *Dong-Eui University, 995 Eomgwangno, Busan-Jin-Gu, Busan 614-714, Korea, South*

e-mail: somi4001@hhu.ac.kr

For optoelectronic applications in the ultraviolet spectral range, besides GaN-based materials, ZnO and its alloys have attracted much attention in the last few years due to the possibility of using excitonic effects at room temperature in ZnO based materials. Recently, high quality ZnO has been grown with excellent properties. Bandgap engineering in ZnO can be accomplished using alloys with MgO because the ionic radius of Mg^{2+} (0.57Å) is close to that of Zn^{2+} (0.6Å). $Mg_xZn_{1-x}O$/ZnO alloy is considered to be a suitable potential barrier material. Although most of the previous works were focused on the fabrication of $Mg_xZn_{1-x}O$ alloy thin films and of $Mg_xZn_{1-x}O$/ZnO QW, we found only few reports about PLD grown MgZnO/ZnO double heterostructure (DHS). Recently we reported on the demonstration of p-n junction LEDs fabricated from n-ZnO/p-GaN single heterostracture (SHS). In this study, we are going to investigate the structural, optical and electrical properties of n-$Mg_xZn_{1-x}O$/ZnO/p-GaN double heterostructure (DHS) grown by pulsed laser deposition. DHS design is expected to improve optical and thermal characteristics of LEDs with ZnO-based active regions.

The $Mg_xZn_{1-x}O$/ZnO films were deposited by PLD using a KrF excimer laser operating at 248 nm, on p-GaN/sapphire substrate. The growth temperature is 600 ^{o}C. The structures of ZnO films were studied by an X-ray diffractometer and the surface morphologies of the thin films were investigated by a scanning prove microscope in the AFM mode. Also, the photoluminescence (PL) was measured under excitation with He-Cd laser operation at 325 nm. The enhancement of the Mg incorporation at high temperature is due to the stronger bonding strength of Mg-O than that of Zn-O, which induced a blueshift of the PL emission. In addition, the deposition at high temperature enhanced the UV peak intensity and the intensity ratio of UV/deep-level emission.

16:00 Poster F58

Charge Carrier Transport Investigation in Oxide Matrix Containing Silicon Nanocrystals of Different Size

Yury V. Ryabchikov[1], Alexey S. Gavrilyuk[1], Pavel A. Forsh[1,2]

1. *M.V. Lomonosov Moscow State University, Vorobyevy gory, Moscow 119992, Russian Federation* **2.** *Russian Research Center "Kurchatov Institute", Moscow 123182, Russian Federation*

e-mail: yury_r@vega.phys.msu.ru

Properties of silicon nanocrystals in silicon dioxide matrix (nc-Si/SiO_2) were investigated in detail because of its effective photoluminescence. Methods of preparation allow changing the sizes of nanocrystals in wide range. Formation mechanisms and photoluminescence properties of silicon nanocrystals were described in literature but the mechanisms of charge carrier transfer in nc-Si/SiO_2 structures were insufficiently investigated. It is necessary to know electrophysical properties of these structures at the room temperature to produce light-emitting devices. The purpose of our work was the investigation of influence of nc-Si size and concentration on charge carrier transport in nc-Si/SiO_2 structures.

The nc-Si/SiO_2 structures were prepared by a method of high temperature annealing of SiO/SiO_2 layers which had been deposited by reactive evaporation on n-type monocrystalline silicon. The thermal annealing was made in the N_2 atmosphere at a temperature of 1100 ^{0}C. The size of silicon nanocrystals varied from 3 to 6 nm. The conductivity of nc-Si/SiO_2 structures was measured by picoammeter/voltage source Keithley 6487.

The current-voltage characteristics of nc-Si/SiO_2 structures with silicon nanocrystals of different size nanocrystals were investigated at room temperature. A strong decrease of the conductivity of nc-Si/SiO_2 structures was found with increasing silicon nanocrystals number. It was shown that in case of one nc-Si/SiO_2 layer the resistance of investigated samples was generally determined by potential barrier resistance on Si/SiO_2 interface. The conductivity of these structures increased significantly with the growth of nc-Si/SiO_2 layers and the process of charge carrier transfer was determined by this region.

The model of charge carrier transfer in nc-Si/SiO_2 structures was suggested. The temperature dependence of nc-Si/SiO_2 structures conductivity was investigated. The possibility of temperature influence on charge carrier transport was analyzed.

16:00 Poster F59

Optical and magneto-optical studies of composite materials containing semimagnetic semiconductor nanoparticles

Andriy I. Savchuk, Volodymyr I. Fediv, Tetyana A. Savchuk, Ihor D. Stolyarchuk, Yevheniy O. Kandyba, Dmytro I. Ostafiychuk, Svitlana A. Ivanchak, Vitaliy V. Makoviy

Chernivtsi National University (ChNU), 2 Kotsubinsky Str., Chernivtsi 58012, Ukraine

e-mail: savchuk@chnu.cv.ua

Composite films containing semimagnetic semiconductor nanoparticles have been prepared by different physical and chemical techniques. $Cd_{1-x}Mn_xTe$ based films were fabricated by RF magnetron sputtering from a composite target. The incorporation of semiconductor nanoparticles into the SiO_2 matrix was achieved with a pulsed laser deposition technique. A new chemical approach for the synthesis of $Cd_{1-x}Mn_xS$ nanoparticles in a polymer matrix of polyvinylalcohol has been proposed. A similar polymer matrix was used also for embedding of $Pb_{1-x}Mn_xI_2$ and $Zn_{1-x}Mn_xO$ nanoparticles. The optical absorption edge for $Cd_{1-x}Mn_xTe$ nanoparticles and the exciton structure in the spectra of $Cd_{1-x}Mn_xS$, $Pb_{1-x}Mn_xI_2$, $Zn_{1-x}Mn_xO$ nanoparticles shifted to the higher-energy side compared to those for bulk crystals due to the quantum confinement effect. The magneto-optical Faraday effect for non-magnetic semiconductor/glass nanocomposites demonstrate only small changes as compared with that of bulk semiconductors. The revealed peculiarities in spectral and magnetic field dependence of the Faraday rotation for the semimagnetic semiconductor based composite films can be attributed to the influence of the dimensionality on spin exchange parameters for such kind of nanostructures. According to the magnetic field dependence of the Faraday rotation all the studied composite samples exhibit paramagnetic behaviour. The magneto-optical properties of the nanocomposites suggest possible applications for optical isolators and magnetic sensors. The work was supported by a grant from the Ministry of Education and Science of Ukraine.

16:00 Poster F60

Synthesis of metal-containing nanoparticles fixed on the SiO_2 matrix

Andrey Volkov[1], Ksenia Katok[2], Yuliya Bolbukh[2], Oleg V. Popkov[1], Gleb Yurkov[1]

1. *Kurnakov Institute of General and Inorganic Chemistry RAS (IGIC), Leninsky prospect, 31, Moscow 119991, Russian Federation*
2. *Institute of Surface Chemistry, Generala Naumova 17, Kiev 03164, Ukraine*

e-mail: iourkov@rambler.ru

In this study, we suggest an original method for synthesizing Fe_3O_4 and Fe_2O_3 nanoparticles localized on the surface silica nanoparticles. Iron oxide nanoparticles were prepared via precipitation from inverse suspensions containing silica modified with amino groups in the argon atmosphere under vigorous stirring at 40°C with further heating to 60°C. The modification of the silica was realized via interaction of surface silanol groups with γ-aminopropyltriethoxy silane at a mild condition in the toluene media. The size distribution and composition of the Fe-containing nanoparticles in the samples produced were investigated by means of TEM and XRD. Synthesis of silver nanoparticles was carried out in result of interaction between silver nitrate solution and silica modified with functional groups that possess reducing properties. After reduction procedure silica with attached to surface silver particles or in mixture were dried at 20 or 120 °C. Obtained composites were studied by UV-Vis spectra. On Figure the UV-spectra of ferric oxide (1-3) and silver (4) particles synthesized in the presence of modified silica are represent. Curve 5 corresponds to modified silica without metal. Presence of surface plasmon band in visible region at 400 nm provided evidence for silver nanoparticles formation.

This work was partial finance supported by the Russian Foundation for Basic Research (grant nos. 06-03-72031-MSTI, 07-03-00885, 07-08-00523, 08-03-00681, 08-08-90250), INTAS-05-1000008-7834, the grant of the President of the Russian Federation MK- 253.2007.3, Russian Science Support Foundation, ISTC nos. 3457, the Russian Academy of Sciences of the research programs «Development of methods for synthesis of chemical substances and creation of new materials» and «Creation of effective methods of the chemical analysis and investigations of structure of substances and materials».

16:00 Poster F61

Thermal conductivity of the nanocomposites with chaotic structure

Vitaly V. Novikov, Nadiya Dmitrieva

Odessa National Polytechnical University (NVV), Shevchenko Prospekt, 1, Odessa 65044, Ukraine

e-mail: novikov@te.net.ua

Today big attention is expressed for nanocomposites. One of the basic characteristics of nanocomposites is the ultra small dimensions of filler particles (d<100nm) and a structure which is irregular fractal. Creating a theoretical basis to prognosticate the effective properties of nanocomposites is a topical important task nowadays.

In this work, the fractal structural model and the iteration averaging method based on the idea of a renormal group transformation is proposed to predict the thermal conduction of a filled polymer nanocomposite. The averaging on mesolevels is done with the help of a Voronoi polyhedron.

In general, the definition of effective properties can be carried out according to the following scheme: firstly, properties of different configurations are found at the initial stage, then they are averaged, and after that they are handed over to the next step.

We single out two kinds of sets of bond configurations: connecting sets of “conducting” bonds (CS), and non-connecting sets (NCS).

The formulae obtained on the basis of variation evaluations are used to calculate the conductivity of the connecting and non-connecting sets.

The conductivity of the connecting set at the *k-th* iteration step is defined as:

$$\lambda^{(k)}{}_{con}=x_{k-1}\lambda^{(k-1)}{}_{con}+(1-x_{k-1})\lambda^{(k-1)}{}_{non}-$$

$$-[(x_{k-1}\cdot(1-x_{k-1})(\lambda^{(k-1)}{}_{con}-\lambda^{(k-1)}{}_{non})^2)/(x_{k-1}\cdot\lambda^{(k-1)}{}_{non}+(1-x_{k-1})\lambda^{(k-1)}{}_{con}+2\lambda^{(k-1)}{}_{con})],$$

where $\lambda^{(0)}{}_{con}=\lambda_1$, $\lambda^{(0)}{}_{non}=\lambda_2$; $x_k=Y(x_{k-1})$, at this $x_0=x$ - is the concentration of the component with a conductivity of λ_1.

The iteration procedure continues until the effective conductivity of the composite, λ, is equal to:

$$\lim_{k\to\infty}\lambda^{(k)}{}_{con}=\lim_{k\to\infty}\lambda^{(k)}{}_{non}=\lambda$$

The obtained results can be further used to analyze the dependence of the conductivity of the composite on such characteristics as the fractal dimension, the percolation threshold, the radius of particle, the ratio of the interface layer thickness to the particle’s radius and the thermal conduction of the interface layer.

Morphology and dynamics of nanostructures and disordered materials via atomic-scale modelling

Symposium G

Welcome

This symposium will be a forum of interaction and exchanges among scientists involved in the atomic-scale, computer based modeling of nanostructures (encompassing clusters, isolated or supported on substrates, complex molecules and supramolecular structures adsorbed at surfaces, and bulk systems for which nanostructural units can be clearly identified) and disordered systems, in particular those based on collections of constitutive units (such as network-forming glasses and liquids). It appears that modern approaches of modeling are applied to these two classes of systems on the basis of identical methodological requirements. These are targeted to provide the most accurate characterization of structure and migration mechanism. Therefore, a scientific meeting rooted on the consideration of nanostructures and disordered systems on the same theoretical footing becomes fully legitimate. To ensure adequate exposure and interaction with the experimental counterpart, two leading scientists reporting on experimental open issues and recent achievements in the area of nanostructures and disordered materials will be involved (one for each class of systems).

SCIENTIFIC COMMITTEE MEMBERS

Luciano Colombo (Cagliari, Italy)

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Alfredo Pasquarello (Lausanne, Switzerland)

Alain Pasturel (Grenoble, France)

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Organisers

Dr. Carlo Massobrio, Institut de Physique et de Chimie des Matériaux de Strasbourg, 23 rue du Loess, BP 43, F-67034 Strasbourg Cedex 2, France.

Prof. Fabrizio Cleri, Institut d'Electronique, Microélectronique et Nanotechnologie, Université de Sciences et Technologies de Lille, F-59652 Villeneuve d'Ascq, France.

Prof. Rafal Kozubski, Institute of Physics, Jagellonian University, Reymonta 4, 30-059, Krakow, Poland.

Proceedings

Solid State Sciences has agreed to publish
research articles related to the participation to this
Symposium. Papers submitted to Solid State Sciences will be reviewed according to rigorous international standards.

Acknowledgements

This symposium has obtained the label of the European Science Foundation (ESF) within the framework of the ESF activity entitled 'Molecular Simulations in Biosystems and Material Science'. We acknowledge the support of the European Science Foundation. We are also grateful to the "Institut of Physique et Chimie des Matériaux de Strasbourg (France)" and to "Institut d'Electronique, Microelectronique et Nanotechnologie de Lille" affiliated to the "Université de Science et Technologie de Lille (France)". Support has also been kindly provided by the Scientific Office of the French Embassy in Poland.

Programme

Monday, 15 September

Opening & Plenary Session

Czochralski Award Ceremony
Monday morning, 15 September, 10:00
Small Hall (237)

Lunch break

Monday afternoon, 15 September, 12:30
Inner Courtyards

Parallel Session

Molecular dynamics and phase transformations
Monday afternoon, 15 September, 14:00
Room 144
Chair: Carlo Massobrio

14:00 Invited oral

Pressure induced phase transformations of nanocrystals studied with transition path sampling simulations

Christoph Dellago, Michael Grünwald

University of Vienna, Faculty of Physics, Boltzmanngasse 5, Wien 1090, Austria

e-mail: Christoph.Dellago@univie.ac.at

In a series of recent experiments, Alivisatos and coworkers demonstrated that the pressure-induced transition from the four-coordinate wurtzite structure to the six-coordinate rocksalt structure in CdSe nanocrystals is strongly influenced by crystal size. On a molecular time scale, the transition is a rare event and the resulting long time scales present a challenge for computer simulations [1]. Using this example, I will discuss how the transition path sampling methodology provides a framework to treat systems with widely disparate time scales and, in particular, to study the mechanism and the kinetics of first order phase transformations close to experimental conditions [2]. From our transition path sampling simulation we obtain the preferred transformation pathway and determine activation enthalpies and volumes, which permit to make contact to experimental results.

[1] M. Grünwald, E. Rabani, and C. Dellago, "Mechanisms of the wurtzite to rocksalt transformation in CdSe nanocrystals", Physical Review Letters 96, 255701 (2006).
[2] M. Grünwald, P. L. Geissler, and C. Dellago, "An efficient transition path sampling algorithm for nanoparticles under pressure", Journal of Chemical Physics 127, 154718 (2007).

14:45 Invited oral

Changing shape under pressure: a study of semiconductor nano-crystals by metadynamics

Carla Molteni

King's College London (KCL), Strand, London WC2R2LS, United Kingdom

e-mail: carla.molteni@kcl.ac.uk

Pressure can be used as a tool for inducing structural transformations between distinct crystalline and/or amorphous phases. Polymorphic and polyamorphic phenomena can be studied by means of constant-pressure molecular dynamics simulations in both bulk- and nano-materials. In particular semiconductor nano-crystals exhibit, under pressure, a range of interesting size-dependent properties, which needs to be dealt with specific techniques for non-periodic systems. Still constant-pressure molecular dynamics simulations suffer from shortcomings due to the limited accessible time-scale, that result in the need of overpressurizing the system under investigation in order to see the transformation within a reasonable time. To address such problem we use the metadynamics method, that has proven to be very successful in accelerating rare events and in efficiently exploring free energy surfaces of complex polyatomic systems. Results for cadmium selenide and silicon bulk- and nano-crystals will be presented, highlighting in particular the role of shape in structural phase transformations.

Coffee break

Monday afternoon, 15 September, 15:30
Main Hall

Joint Poster Session 1

Monday & Wednesday
Monday afternoon, 15 September, 16:00
Main Hall

Tuesday, 16 September

Parallel Session

Nanosystems and diffusion 1
Tuesday morning, 16 September, 9:00
Room 144
Chair: Rafal Kozubski

9:00 Oral

Transition states in pressure-induced structural transformations of nanocrystals

Michael Grünwald, Christoph Dellago

University of Vienna, Faculty of Physics, Boltzmanngasse 5, Wien 1090, Austria

e-mail: michael.gruenwald@univie.ac.at

We identify transition states in structural transformations of CdSe nanocrystals under pressure using transition path sampling techniques. In agreement with nucleation theory, the critical nucleus of the high pressure phase grows in size with decreasing pressure. Activation volumes and enthalpies, calculated for typical trajectories of the transition path ensemble, show the same trend with crystal size as found in experiments. This result gives strong evidence for the correctness of the observed transformation mechanism, which consists of single nucleation events and growth along parallel crystal planes.

9:30 Oral

Graph-based sampling of fully-coordinated silica $(SiO_2)_N$ clusters

Edwin Flikkema[1], Stefan T. Bromley[2]

1. *University of Aberystwyth (UWA), Aberystwyth SY233BZ, United Kingdom* **2.** *Universitat de Barcelona, Marti i Franques 1, Barcelona 08930, Spain*

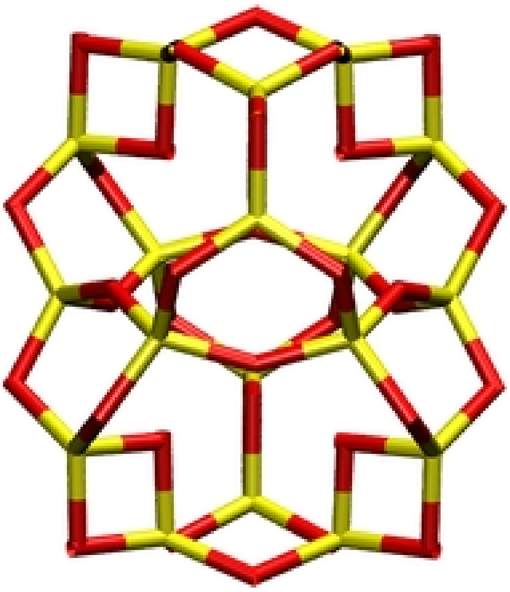
e-mail: edf@aber.ac.uk

Silica (SiO_2) is a versatile material with many different bulk polymorphs. Whereas bulk silica has been studied extensively, much less is known about silica clusters. The authors have studied silica clusters before, using global optimisation and a simple potential that had been reparameterised to get closer agreement with Density Functional Theory calculations [1,2]. This presentation focuses on a study of a special class of cluster geometries: fully-coordinated silica clusters, i.e. geometries where each silicon atom is chemically bonded to four oxygen atoms and each oxygen atom is bonded to two silicon atoms. While this is a common feature in the bulk, defects such as dangling oxygens are often found in clusters. In this presentation we will be discussing an algorithm for specifically generating fully-coordinated cluster geometries.

In our earlier study of silica clusters we used the standard Basin Hopping algorithm, which is based on performing Monte Carlo moves in coordinate-space followed by local optimisations. In our present study we propose to perform Monte Carlo sampling on the set of graphs (i.e. the networks of silicon-oxygen bonds) rather than in coordinate-space, since it is much easier to design Monte Carlo moves in graph-space that retain fully-coordinatedness than in coordinate-space. At each step a three dimensional realisation of the graph is sought, using a cascade of optimisations involving two cost-functions and our silica potential. With this method we have generated databases of low-energy fully-coordinated cluster geometries in a size range of up to 30 SiO_2 units. The proposed method can be generalised to other network-forming systems.

[1] Edwin Flikkema and Stefan T. Bromley, "A new interatomic potential for nanoscale silica", Chem. Phys. Lett. 378: 622, 2003
[2] Stefan T. Bromley and Edwin Flikkema, "Columnar-to-disk structural transition in nanoscale $(SiO_2)_N$ clusters", Phys. Rev. Lett., 95:

185505,



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10:00 Oral

Phenomenological Analysis and Monte Carlo Simulation of Diffusion in Hollow Binary Alloy Nanospheres

Alexander V. Evteev, Elena V. Levchenko, Irina V. Belova, Graeme E. Murch

The University of Newcastle, University Drive, Newcastle 2308, Australia

e-mail: Alexander.Evteev@newcastle.edu.au

In this paper a theoretical and computational study of the thermal instability of hollow binary alloy nanoparticles due to vacancy diffusion is described along with comparison with previous reported results [1-3].

The main results of the present work are:

1. A general treatment of the Gibbs-Thomson effect for a hollow nanosphere was made. Unlike the earlier treatment [1] the present analysis allows a vacancy composition profile across the nanoshell to be represented by a continuous decreasing function as well as by a continuous function with a minimum;

2. The range for the controlling parameter of the vacancy motion within a binary alloy nanoshell has been determined in terms of the phenomenological coefficients as well as the (measurable) tracer diffusion coefficients of the atomic components and the geometric correlation factor for the lattice by means of the Moleko, Allnatt and Allnatt [4] and Manning [5] diffusion kinetics theories;

3. From the theoretical description and kinetic Monte Carlo simulations, it is demonstrated that for a hollow random binary alloy nanosphere with an *equi-atomic* (initially homogeneous) composition and at an approximation that neglects the radial dependence of the vacancy formation free energy, the controlling parameter of the shrinking rate in the case when one element diffuses much faster than the other can be estimated with reasonable accuracy as the geometric mean of the tracer diffusion coefficients of both components.

[1] K.N. Tu and U. Gösele, Appl. Phys. Lett. **86** 093111 (2005).

[2] A.M. Gusak, T.V. Zaporozhets, K.N. Tu, U. Gösele, Phil. Mag. **85** 4445 (2005).

[3] A.V. Evteev, E.V. Levchenko, I.V. Belova.E. Murch, Phil. Mag. **87** 3787 (2007).

[4] L.K. Moleko, A.R. Allnatt and E.L. Allnatt, Phil. Mag. A **59** 141 (1989).

[5] J.R. Manning, Phys. Rev. B **4** 1111 (1971).

Coffee break

Tuesday morning, 16 September, 10:30
Main Hall

Parallel Session

Nanosystems and diffusion 2
Tuesday morning, 16 September, 11:00
Room 144
Chair: Rafal Kozubski

11:00 Oral

Molecular Dynamics Study of Formation by Interdiffusion of Pd-Ni and Ag-Ni Nanoparticles

Alexander V. Evteev, Elena V. Levchenko, Irina V. Belova, Graeme E. Murch

The University of Newcastle, University Drive, Newcastle 2308, Australia

e-mail: elena.levchenko@newcastle.edu.au

Nanoparticles are very promising materials for advanced magnetic, catalytic, optical, electronic, photonic, pharmaceutical and biomedical applications, due to their specific structure and unique physical and chemical properties at the nanoscale, which cannot be observed in bulk material. In principle, the properties of alloy nanoparticles can be tuned by varying the composition, size, shape and atomic ordering, but exactly how this can be achieved remains largely unknown.

In the case of alloy nanoparticles, surface segregation plays the major role for the understanding of their structure and functional properties. In this work, we have carried out a series of long-time scale molecular dynamics simulations of Pd-Ni and Ag-Ni nanoparticles with different compositions and sizes using many-body potentials. We have demonstrated that a novel kind of structure of Pd-Ni alloy nanoparticles can be self-assembled by interdiffusion from an initial Ni (core)-Pd (shell) f.c.c structure. In this self-assembled structure, the Ni atoms mostly accumulate in a layer just below the surface. Meanwhile, the Pd atoms cover this Ni layer from inside and outside by two Pd layers. In sharp contrast to the Pd-Ni system, in the system Ag-Ni, Ag and Ni have almost complete insolubility. The initial state was the f.c.c. structure wherein a core of Ag atoms was surrounded by shell of Ni atoms. Then during isothermal annealing at various temperatures we observed a tree-shell Ag-Ni-Ag structure of the nanoparticles formed by segregation of Ag atoms to the surface. We established that Pd-Ni and Ag-Ni alloy nanoparticle structure is likely to depend strongly on alloy composition and nanoparticle size. Our results indicate a new possibility for controlling the chemical ordering in Pd-Ni and Ag-Ni system at the nanoscale level. Such segregated nanoparticles should have unique physical and chemical properties (applications).

11:30 Oral

Atomic Ordering in Metal-Doped Graphene: Statistical Thermodynamics and Kinetics

Taras M. Radchenko, Valentyn A. Tatarenko

Institute for Metal Physics, N.A.S.U., 36 Vernadsky Boulevard, Kyiv 03142, Ukraine

e-mail: Taras.Radchenko@gmail.com

We consider a model of two-dimensional binary substitutional solid solution based on a graphene-type crystal lattice. The question is as follows: how do doped metal atoms and carbon atoms distribute at the sites of graphene-type lattice (for a given temperature and concentration)—by means of ordered or disordered manner? Statistical-thermodynamics and kinetics models are proposed for atomic ordering in two-dimensional plane graphene-type lattice with stoichiometric concentrations, 1/8, 1/4, 1/2. (The unified 'physical nature', which causes mechanisms of atomic ordering in nanoscale and macroscopic mixed systems, is assumed.) Impossibility of atomically ordered distribution with stoichiometries of 1/6, 1/3 in such lattice is ascertained (at least, in case of a short-range interactions between substitutional atoms). If stoichiometry is 1/4, the structure with one long-range order (LRO) parameter is more advantageous thermodynamically than with two or three parameters. As revealed, kinetics curves of LRO parameters can be non-monotonic for structures described by two or three LRO parameters (because graphene-type crystal lattice consists of two sublattices and 'mixing' energies are different for them). Kinetics results confirm statistical-thermodynamic ones: firstly, equilibrium values of LRO parameter coincide within the both models; secondly, equilibrium (and instantaneous) values of LRO parameter in non-stoichiometric binary two-dimensional graphene-based phase can be higher than they are in stoichiometric one.

12:00 Oral

Shape and faceting of Si nanocrystals embedded in an amorphous glass matrix

Romain Soulairol, Fabrizio Cleri

e-mail: fabrizio.cleri@univ-lille1.fr

The growth of Si nanocrystals from a Si-rich, oxyde matrices, e.g. those obtained from thermal treatment of an amorphous or organic (sol-gel) silica-based glass, is a subject with both fundamental and applied science implications. In particular, nanocrystals can be precipitated from the Si-rich matrix with the simultaneous addition of foreign species, such as Er atoms, so as to exploit at the same time the effects of quantum confinement and active doping. Experiments have shown that the optical gain of such systems can be improved by orders of magnitude, therefore opening the way to all-silicon optoelectronics. However, the detailed thermodynamics and kinetics of the precipitation and aggregation is not understood up to date.

With the aim of elucidating the role of interfacial interactions on the Si nanocrystal final shape and size, we used molecular dynamics simulations based on empirical potentials to study the equilibrium structures of Si nanocrystals embedded in an amorphous glass. Atoms at the nanocrystal-glass interface were allowed to interact via mixture of Stillinger-Weber and BKS potentials, while assigning an effective charge to surface Si atoms, adjusted so as to reproduce qualitative results from ab initio calculations.

We calculated the relaxed, minimum energy structures of free-standing Si clusters of different diameters, going from about 3 to 5 nm, and found them to be spherical up to the maximum sizes studied. Both the static structure factor and phonon spectra indicate that the surface layer of the spherical Si cluster is more mobile than the bulk, and tends to be rather disordered. Subsequently, clusters of similar volume, but with either spherical or faceted shapes, were inserted into the a-SiO2 matrix, and their free energies were calculated in the quasi-harmonic approximation. Such a calculation allows to assess the size limit above which the clusters prefer a faceted shape, under the constraint and stress of the surrounding matrix.

Lunch break

Tuesday afternoon, 16 September, 12:30
Inner Courtyards

Parallel Session

Dynamics at surfaces
Tuesday afternoon, 16 September, 14:00
Room 144
Chair: Fabrizio Cleri

14:00 Invited oral

An STM investigation of the influence of topography and electronic structure on diffusion

Karina Morgenstern

Universität Hannover, Institut für Festkörperphysik (FKP), Appelstrasse 2, Hannover D-30167, Germany

e-mail: morgenstern@fkp.uni-hannover.de

STM allows to follow dynamical changes on surfaces directly in real space. In particular, diffusion and decay of nanoislands and diffusion of single atoms can be followed on the time scale of the changes. Though original work [1] could be well described within a framework of mean-field theory, more recently the influence of the surface state has been found in several instances. On fcc(111) surfaces the fast decay of stacks of islands originally attributed to the surface state [2] was shown to be of different origin [3]. However, the motion of single atoms and dimers [4] as well as the slow decay of an island [5] were shown to be indeed related to the surface state. Furthermore, the increased diffusivity and reduced decay of small copper islands on Ag(100) will be discussed [6].

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14:45 Invited oral

Fast surface exchange processes determining local concentration profiles in heteroepitaxial nanometric islands

Francesco Montalenti

University of Milano-Bicocca, Department of Materials Science, via Cozzi 53, Milano 20125, Italy

e-mail: francesco.montalenti@unimib.it

Thin-film growth as determined by various experimental deposition techniques commonly takes place under non-equilibrium conditions. In order to build a comprehensive understanding of the phenomenon it is therefore fundamental to understand the actual *kinetic scenario*. This requires evaluating the activation energies for the most relevant diffusion events, after having determined possible diffusion paths. In the first half of this talk, I shall review some key methodology which was introduced within the last decade, allowing one to tackle the well-known problem of estimating the rates of (initially unknown) rare events. Accelerated molecular dynamics [1], the Nudged Elastic Band Method [2], the Dimer Method [3], and Metadynamics [4] will be briefly reviewed. Afterwards, I shall present recent results exemplifying how exploiting state of the art methods it is possible to accurately characterize complex exchange-mediated diffusion events involving several atoms at the same time. Applications to popular Ge/Si systems (for both flat films and 3D islands) will be discussed [5,6], with the aim of understanding recent experimental results concerning the Si/Ge concentration profiles in nanoislands [7] .

I acknowledge financial support from the EU (STREP Project d-DOT-FET, contract 012150) and from the Cariplo Foundation (SIMBAD project).

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Coffee break

Tuesday afternoon, 16 September, 15:30
Main Hall

Parallel Session

Dynamics in nanostructures and alloys
Tuesday afternoon, 16 September, 16:00
Room 144
Chair: Fabrizio Cleri

16:00 Oral

Surface effect on atomic ordering in nano-layered $L1_0$ AB binaries: multiscale Monte Carlo Simulation

Rafal Kozubski[1], Mirosław Kozłowski[1], Jan Wróbel[2], Tomasz Wejrzanowski[3,4], Krzysztof J. Kurzydlowski[3], Christine Goyhenex[5], Véronique Pierron-Bohnes[5], Marcus Rennhofer[6], Savko Malinov[7]

1. *Jagiellonian University, Institute of Physics (IF UJ), Reymonta 4, Kraków 30-059, Poland* **2.** *Warsaw University of Technology, Faculty of Physics, Koszykowa 75, Warszawa 00-662, Poland* **3.** *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland* **4.** *Interdisciplinary Centre for Materials Modelling (ICMM), Woloska 141, Warszawa 02-507, Poland* **5.** *Institut de Physique et Chimie des Materiaux de Strasbourg, UMR7504, CNRS - ULP, 23, rue du Loess, BP 43, Strasbourg CEDEX 2 67034, France* **6.** *University of Vienna, Institute of Materials Physics, Wien, Austria* **7.** *Queen's University Belfast (QUB), Stranmillis Road, Belfast BT9 5AH, United Kingdom*

e-mail: rafal.kozubski@uj.edu.pl

Combined nano- and mesoscale simulation of chemical ordering kinetics in nano-layered $L1_0$ AB binary intermetallics was performed. In the nano- (atomistic) scale Monte Carlo (MC) technique implemented with vacancy mechanism of atomic migration and diverse models for the system energetics were used. The meso-scale microstructure evolution was, in turn, modelled by means of a Monte Carlo procedure simulating antiphase-domain-boundary motion as controlled by antiphase-boundary energies evaluated within the nano-scale simulations. The study addressed FePt thin layers considered as a material for ultra-high-density magnetic storage media and revealed metastability of the $L1_0$ c-variant superstructure with monoatomic planes parallel to the layer surface and off-plane easy magnetization. The layers, originally perfectly ordered in a c-variant of the $L1_0$ superstructure, showed homogeneous disordering running in parallel with a spontaneous re-orientation of the monoatomic planes leading to a mosaic microstructure composed of a- and b-$L1_0$-variant domains. The domains nucleated heterogeneously on the free surface of the layer and grew discontinuously inwards its volume. Finally, the domains relaxed towards an equilibrium microstructure of the system. Two “atomistic-scale” processes: (i) homogeneous disordering and (ii) nucleation of the a- and b-$L1_0$-variant domains showed characteristic time scales. The same was observed for the meso-scale processes: (i) heterogeneous $L1_0$-variant domain growth and (ii) domain microstructure relaxation. The above complex structural evolution modelled by means of the multiscale Monte Carlo simulations has recently been observed experimentally in epitaxially deposited thin films of FePt [1].

[1] M. Rennhofer, B. Sepiol, G. Vogl, M. Kozlowski, R. Kozubski, B. Laenens, A. Vantomme, J. Meersschaut, Diffusion Fundamentals **6** (2007) 45.1 - 45.2

16:30 Oral

Simulation of atomic migration in CoPt ordered alloys

Tounsia Bouzar[2], Christine Goyhenex[1], Romaric V. Montsouka[1], Hamid Bouzar[2], Véronique Pierron-Bohnes[1]

1. *Institut de Physique et Chimie des Materiaux de Strasbourg, UMR7504, CNRS - ULP, 23, rue du Loess, BP 43, Strasbourg CEDEX 2 67034, France* **2.** *Laboratoire de Physique et Chimie Quantique, Université Mouloud Mammeri (LPCQ), Faculté des Sciences, Département de Physique, Tizi-Ouzou 15000, Algeria*

e-mail: goyhenex@ipcms.u-strasbg.fr

The $L1_0$ systems are extensively studied as good candidates for high density magnetic storage media due to their high magnetic anisotropy, which is related to their chemical order anisotropy. In recent experiments, epitaxied thin bilayers NiPt/FePt/MgO(001) grown at 700K were annealed at 800K and 900K. At 800K, the $L1_0$ long range order increases without measurable interdiffusion. Surprisingly further annealing at 900K leads to interdiffusion that takes place without destroying the $L1_0$ long range order [1]. The same phenomenon has been observed by Rennhofer et al. [2] in the case of $L1_0$ FePt multilayers suggesting that interdiffusion can occur through a series of atomic mechanisms while keeping the $L1_0$ structure. As this point is important for the growth of high quality layers of alloys, we have investigated the possible atomic processes through numerical simulations for such diffusion without order change. We have used Molecular Dynamics in the second moment approximation of the tight binding method taking as reference CoPt that orders in the $L1_0$ tetragonal structure like FePt and NiPt. In a first stage, molecular statics calculations were performed in order to study the vacancy migration and to determine in particular if some jump cycles are feasible with an energy barrier low enough to make possible a diffusion without order change. For instance we find that a 6 jump cycle mechanism is favourable from an energy point of view relatively to a second nearest neighbour jump that has a much higher energy barrier. We have also checked mechanisms involving two or three vacancies. The static results are supported by a statistical study for which large series of constant energy simulations are performed at the temperatures of interest (900-1000 K) in order to check the actual occurrence of each elementary step of the previously identified jump cycles.

[1] R. V. Montsouka et al., Phys. Rev. B 74, 144409 (2006)
[2] M. Rennhofer et al., Phys. Rev. B 74, 104301 (2006)

17:00 Oral

Quenched molecular dynamics simulations of the vacancy behaviour near the (001) surface of an ordered CoPt alloy

Christine Goyhenex[1], Ovidiu Ersen[1], Leila Messad[1,2], Hiroshi Numakura[3], Katsushi Tanaka[4], Véronique Pierron-Bohnes[1]

1. *Institut de Physique et Chimie des Materiaux de Strasbourg, UMR7504, CNRS - ULP, 23, rue du Loess, BP 43, Strasbourg CEDEX 2 67034, France* **2.** *Laboratoire de Physique et Chimie Quantique, Université Mouloud Mammeri (LPCQ), Faculté des Sciences, Département de Physique, Tizi-Ouzou 15000, Algeria* **3.** *Department of Materials Science, Osaka Prefecture University, Sakai 599-8531, Japan* **4.** *Kyoto University, Department of Materials Science and Engineering, Kyoto, Japan*

e-mail: vero@ipcms.u-strasbg.fr

We present quenched molecular dynamics simulations of the vacancy behaviour near the surface of an $L1_0$ ordered CoPt alloy.

We calculate the following parameters:
- amount of relaxation for the two possible terminations and surface formation energies,
- formation and migration energies of a vacancy within the different planes,
- formation energies of the antisites,
- migration energies of a vacancy between the different planes,
- formation and migration energies of adatoms on the different surfaces.

We find that as expected the alloy surface is preferentially a Pt plane. There are typically 2 planes where the migration and formation energies are different from the bulk. Whereas the activation energy of the vacancies is higher than 2.5 eV in the bulk, near to the surface some mechanisms have an activation energy smaller than 1 eV. The anisotropy of the structure involves an anisotropy of the diffusion.

The values of the energies obtained for the different processes are used to understand the chemical ordering in CoPt(001) thin films grown at different temperatures. These films present indeed a concentration modulation along the growth direction with 2 temperature ranges. We analyse this behaviour in terms of chemical ordering using a classical phenomenological diffusion law with the values of the energies deduced by quenched molecular dynamics.

The energy profiles in bulk are also used to extend the model developed by Schober [1] to the $L1_0$ structure and to deduce from the phonon spectra measured using neutron inelastic scattering on a single variant single crystal CoPt [2] a migration energy that is compared to the calculated values.

[1] H.R. Schober et al, J. Phys.: Cond. Matter, 4 (1992) 9321 ; E. Kentzinger and H.R. Schober, J. Phys.: Cond. Matter, 12 (2000) 8145.

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17:30 Oral

Atomic Mechanisms of Structural Reconstruction of Nanocrystal FCC at an Impulsive Deformation

Mikhail D. Starostenkov, Aleksandr V. Yashin, Nikita V. Sinitsa

Altai State Technical University (ASTU), Lenin st.46, Barnaul 656038, Russian Federation

e-mail: genphys@mail.ru

Atomic mechanisms of structural reconstruction having place in the block of nanocrystal at an impulsive tension deformation were studied by the method of molecular dynamics. The block of nanocrystal was presented by a rectangular parallelepiped with the sides corresponding to the planes [100] of FCC lattice. The number of atoms of the calculated block ranged from 2*10^4 to 10^5.Free boundary conditions were applied along tension direction. The velocity of the change of deforming loading amounted to 20 m/s. The model blocks of crystals of pure metals Ni, Al and Ni3Al intermetallide with the atomic pacing corresponding to the structure L12. It was supposed that there were no defects in the calculated block. Four main stages are distinct seen on the graphs of the change of the stored energy of deformation on the value of the applied deforming stress. They are the following: 1) quasielastic deformation, 2) plastic deformation, 3) flow, 4) fracture. The first stage is characterized by the growth of energy according the parabolic low. The formation and storing of dynamic pairs of point defects vacancies and interstitial atoms is observed at this stage. The formation of dislocation loops and the displacements of crystal parts along the planes [111] took place at definite concentrations of such defects. Sharp jump-like decrease of energy is seen on the graph of the dependence of the stored energy on time (value of deforming loading). The stage of plastic deformation is characterized by a new growth of stored energy but the growth process takes place more slowly. In this connection, the storing of dislocations and the appearance of the neck is observed. At the flow stage, the stored energy is not practically changed up to the fracture. The comparison of the curves of deformation development was made for the alloys under study and Ni3Al.

18:00 Oral

Calculation of direct and indirect excitons in $\mathrm{GaAs/Ga_{1-x}Al_xAs}$ coupled double quantum wells: electric and magnetic fields and hydrostatic pressure effects

Carlos A. Duque, Sonia Y. López

Universidad de Antioquia (UA), Calle-67-N-53-108, Medellín 05001000, Colombia

e-mail: cduque_echeverri@yahoo.es

The variational procedure, in the effective-mass and parabolic-band approximations, is used in order to investigate the effects of hydrostatic pressure and applied electric and magnetic fields on the exciton states in $\mathrm{GaAs/Ga_{1-x}Al_xAs}$ coupled double quantum wells. The exciton envelope wave function is obtained through a variational procedure using a hydrogenic 1s-like wave function and an expansion in a complete set of trigonometric functions for the electron and hole wave functions.
We take into account intersubband mixing brought about by the Coulomb interaction of electron-hole pairs in double quantum wells and present a detailed analysis of the properties of direct and indirect exciton states in these systems.
Calculated results are found in good agreement with available experimental measurements on the photoluminescence peak position associated with direct and indirect excitons in $\mathrm{GaAs\text{-}Ga_{1\text{-}x}Al_xAs}$ double quantum wells under growth direction applied electric field both for growth direction and in-plane applied magnetic fields.

Wednesday, 17 September

Parallel Session

Growth and diffusion in non-homogeneous systems
Wednesday morning, 17 September, 9:00
Room 144
Chair: Massimo Celino

9:00 Invited oral

Growth phenomena and optoelectronic properties of mixed-phase amorphous-crystalline nanosystems

Alessandro Mattoni, Luciano Colombo

CNR-INFM SLACS and Dipartimento di Fisica, Università di Cagliari, Cittadella Universitaria, Monserrato (Cagliari) I-09042, Italy

e-mail: alessandro.mattoni@dsf.unica.it

Mixed-phase amorphous-crystalline (a-c) systems are both of technological and theoretical relevance.[1] In particular, this is the case of nanocrystalline (nc) materials, where a distribution of nanosized crystal grains is embedded into an amorphous matrix. nc-systems are useful for advanced optoelectronics, structural engineering, and many other technological applications.

nc-systems are in most cases thermodynamically metastable. Since the free energy is larger in the amorphous phase than in the corresponding crystalline one, a-c systems tend to recrystallize.[2] It is possible to take advantage of this property in order to synthesize new materials by solid phase crystallization.[3] A comprehensive physical understanding and theoretical modeling of the recrystallization phenomena is mostly needed and useful for technological impact.

We investigate at the atomic scale the microstructure evolution of a two-phase amorphous-crystalline system. We focus on the case of textured nanocrystalline silicon here described as a distribution of cylindrical grains embedded into an amorphous matrix.

We prove that the growth of an isolated grain is nonuniform and it can be described by a power law model.[2] Furthermore, we study the case of a distribution of grains in absence of nucleation. The atomistic results are used to work out a comparison with Kolmogorov-Johnson-Mehl-Avrami (KJMA) mesoscopic model describing the kinetics of a first-order phase transformation. Deviations from the KJMA are observed that are mainly due to atomic-scale features. We include such effects by using an improved version of the KJMA theory. Finally, the optoelectronic properties of the nc-systems are studied during the recrystallization process by means of large scale empirical tight binding calculations.

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[2] A. Mattoni and L. Colombo, Phys. Rev. Lett. **99** 205501 (2007)

[3] A. Mattoni and L. Colombo, Phys. Rev. B **69** 045204 (2004)

9:45 Invited oral

Surface diffusion on inhomogeneous surfaces

Hervé Bulou

Institut de Physique et Chimie des Materiaux de Strasbourg, UMR7504, CNRS - ULP, 23, rue du Loess, BP 43, Strasbourg CEDEX 2 67034, France

e-mail: herve.bulou@ipcms.u-strasbg.fr

The present talk aims to review the current theoretical understanding of mass transport on inhomogeneous surfaces. Such surfaces, inhomogeneous on a structural and/or chemical point of view, are more and more used as functionalized substrates for organizing the matter at nanoscale by over deposition of atoms. We will first focus on a description of the different types of inhomogeneous surfaces such as the reconstructed surfaces and the vicinale ones. Both natural and ``heteroepitaxial-induced'' reconstructed surfaces will be describe. The second part will be dedicated to the theoretical approaches used to investigate the mass transport phenomena on such surfaces. Both energy functionals, used to imitate the interatomic bonds, and methods, employed to determine the dynamic behavior of the atoms, will be considered. Especially, we will show that the concerted use of classical molecular dynamics, to determine the actual involved microscopic processes, and energy minization procedures to calculate potential energies along diffusion pathways, allows a comprehensive description of the intricated atomic processes in such complex systems. In the last part, we will list some issues characteristic of diffusion on inhomogeneous surfaces as obtained following the previously described working procedure. Specific processes occurring at the inhomogeneous surface, such as preferential nucleation, diffusion anisotropy[1], strain-induced exchange[2] and solitonic diffusion[3], will be describe.

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Coffee break

Wednesday morning, 17 September, 10:30
Main Hall

Parallel Session

Interfaces of nanosystems
Wednesday morning, 17 September, 11:00
Room 144
Chair: Massimo Celino

11:00 Oral

Interlayer effects in Multi walled Carbon Nanotubes and Carbon Nanopeapods

Roberto Scipioni, Atsushi Oshiyama, Takahisa Ohno

e-mail: scipioni.roberto@nims.go.jp

Interlayer effects in Multi walled Carbon Nanotubes and Carbon Nanopeapods

Roberto Scipioni[1] , Atsushi Oshiyama[2], and Takahisa Ohno[3]

1International Center for Young Scientists (ICYS), National institute for Materials Science, 1-1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan.

[2]Department of Applied Physics, University of Tokyo,Hongo, Tokyo 113, Japan and JST-CREST, Kawaguchi, Saitama, Japan.

[3]Computational Materials Science Center (CMSC) and International Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan

We discuss the role of the interlayer region in double walled carbon nanotubes encapsulating fullerenes. We find that electrostatic effects as well as the long range interactions give rise to an increased stability in multiwalled carbon Nanopeapods as compared to the SWNT case. The interlayer state acts as a repository of charge to minimize the electrostatic repulsion. Thus, the number of layers is an important parameter to assess the properties of these systems. The characteristics of similar systems composed of intercalated fullerenes in graphite is also currently investigated.

11:30 Oral

Ab initio study of a metal contacted organic-inorganic heterostructure

Matthieu Soulis, Fabrizio Cleri

Institute for Electronics and Nanotechnology, Lille 60069, France

e-mail: matthieu.soulis@isen.iemn.univ-lille1.fr

This work consists in first-principles calculations applied to the study of bulk heterojunctions composed of organic molecules deposited onto Si surface. These molecules are composed of an insulating alkyl chain completed by ap-bonded headgroup. A metal layer finally caps everything, and formsa Schottky contact.

Thus, calculations were carried out for a Si-molecule-metal multilayer of the type experimentally realized at the IEMN laboratories. We calculated the energy band and vacuum-level alignment between Si, molecular semiconductor, and metal layers, according to the bulk semiconductor theory, in order to describe the electronic structure and electrostatic properties of such complex.
The electron density and the electrostatic potential were evaluatedacross the various interfaces of the multilayer. We compared the open circuit arrangement (a void slab of about 10 Å separates the top and bottom free surfaces) tothe closed circuit one(an additional Al-Si interface is present). Our aim is to underline the role of the interface structure and defects in establishing such quantities as the relative potential and wavefunction drop, the attending (mis)alignment of vacuum levels, and the band offset at the organic-inorganic semiconductor interface.

Our model mimics the simplest of the experimental arrangements. Stacked along the supercell (001) direction, we find: four 2x2 planar units of Si (100), with the bottom free surface terminated by H; one layer of silane-terminated, 8-mer alkyl chain, with a phenyl head linked by a double-oxygen bridge, or $H_3Si(CH_2)_8COO–CH_2$(1,phenyl); and four 2x2 planar units of Al (100). The resulting inverse density of the molecular monolayer is equal to 29.2 $Å^2$/mol, a value well in the range of the experimental data.

12:00 Oral

Computer simulation of high reversible hydrogen sorption on surfaces of a carbon nanotube

Serge A. Beznosyuk, Mark S. Zhukovskiy, Tatyana M. Zhukovsky, Olga A. Maslova

Altai State University (ASU), Lenin St., 61, Barnaul 656049, Russian Federation

e-mail: zhukovsky@list.ru

In quantum-field chemistry approach computing simulation of high reversible hydrogen sorption in carbon nanotube is presented. It is shown that hydrogen molecules accumulation is coursed by strong spin-dependent exchange interactions between activated hydrogen biradical H_2^* and carbone nanotube's surfaces. Investigation of the interaction between the hydrogen atoms and molecules and atoms of carbon are carried out by density functional method in non-local density approximation. Our results are in accordance with experimental data, which are corresponding with "super"- Van der Waals forces or "weak" covalent bonds in other works. Thus, it has been marked, that interaction energy between hydrogen and carbon nanostructure (20 - 40 кJ/mol) exceed interaction (distraction) energy of Van-der-Waals bonds in ten times, which is characteristic for physical hydrogen adsorption by carbon materials, Potentials of strong spin-dependent exchange interactions is ten times lower than distracting energies of covalent C-H bonds, which are characteristic for chemisorptions. We examine the self-assembling hydrogen adsorption both on internal, and on external surfaces of carbone nanotube. It is shown that thermodynamically stability of hydrogen bi-radical H_2^* adsorbate set in at mass-concentrations of hydrogen amount above 3%. Inside carbon nanotube the stabilization occurs easier. Computer experiment reveals thermodynamic stability of some self-assembly spiral nanostructure forms in the hydrogen bi-radical H_2^* adsorbate aggregation distribution. In case of exothermic processes of self-assembling adsorption on internal surface of nanotube, when concentrations of hydrogen amounts spontaneously increasing from initial 3% up to 7,7 mass. %, a thermal effect increases, as follows: 7 кJ/mol (3.7%), 27 кJ/mol (5.6%), 36 кJ/mol (7.7%). That provides both a thermodynamic stability of adsorbate with high hydrogen concentration and an easy reversibility of hydrogen sorption and desorption.

Lunch break

Wednesday afternoon, 17 September, 12:30
Inner Courtyards

Parallel session

Dynamics of complex and biological systems 1
Wednesday afternoon, 17 September, 14:00
Room 144
Chair: Phil Salmon

14:00 Oral

The fragile to strong dynamic crossover transition in confined water: molecular dynamics results

Paola Gallo[1], Mauro Rovere[1], Sow-Hsin Chen[2]

1. *Physics Department, University Roma Tre, Via della vasca navale 84, Roma 00146, Italy* **2.** *Massachusetts Institute of Technology (MIT), Cambridge, MA 02139, United States*

e-mail: gallop@fis.uniroma3.it

Molecular dynamics simulations of supercooled water confined in a silica nanopore of MCM-41 type have been performed down to T=200 K. We find evidence of a fragile-to-strong dynamic crossover transition at a temperature T=220 K, close to the experimental finding. This crossover has been localized by looking at the diffusion coefficient behavior that shows a crossover point from a non-Arrhenius to an Arrhenius behavior. We also analyze the glassy behavior of the mean square displacement and of the self intermediate scattering function upon crossing the dynamic crossover. We discuss the results on the framework of a physical picture of a fragile high density liquid that evolves to a strong low density liquid upon approaching the glass transition temperature.

14:30 Oral

Large-scale density-functional theory study of gramicidin A ion channel geometry and electronic properties

Milica Todorovic[1], Tsuyoshi Miyazaki[1], Takahisa Ohno[1], David R. Bowler[2], Michael J. Gillan[2]

1. *National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba 305-0047, Japan* **2.** *London Centre for Nanotechnology (LCN), Gower St, London WC1E6BT, United Kingdom*

e-mail: todorovic.milica@nims.go.jp

Gramicidin A is a small but highly selective ion channel, an antibiotic protein embedded in the cell membrane, whose inner pore conducts cations in a single-file geometry. Given the difficulties in describing the energetics of its ion transport using classical potentials, a full density-functional theory study was conducted using the linear-scaling code CONQUEST. This code computes electronic structure through the conventional exact diagonalisation method, but also an approximate method of variable accuracy, which scales linearly with system size and makes it possible to apply quantum mechanics to large numbers of atoms. Since the function of this channel is closely related to structure, two experimental structures featuring slightly different helix properties and peptide residue orientation were selected for comparison in an initial, isolated channel investigation performed using the diagonalisation method. Comprehensive structural optimisations led to geometries that are close to respective initial structures, and situated in different local minima of the Born-Oppenheimer surface. The lower energy experimental structure was also closer to an energy minimum and notably more stable during optimisation, while the other geometry underwent an expansion in helix pitch that is difficult to reconcile with other experiments. Despite the lack of channel environment in this preliminary study, the relative stability trend is in agreement with that predicted by long-time classical potential molecular dynamics of fully solvated channels.

Electronic properties of the isolated channel were explored with respect to changes in its helix characteristics and peptide residues and found to be more sensitive to helix features. Order-N calculations of the isolated channel agree very well with the diagonalisation result. Future order-N studies of this system will probe gramicidin A in a phospholipid membrane and explore the interactions between the channel and its environment.

15:00 Oral

Molecular dynamics simulations of lysozyme in water/sugar biopreservative solutions

Affouard Frederic[1], Adrien Lerbret[2], Alain Hedoux[1], Yannick Guinet[1], Marc Descamps[1]

1. *Universite des Sciences et Techniques de Lille CNRS (USTL), cite scientifique Villeneuve d'Ascq, Lille 59655, France* **2.** *Cornell University, 425 Philips Hall, Ithaca, NY 14853, United States*

e-mail: frederic.affouard@univ-lille1.fr

Sugars have received a huge interest over the past few decades for their preservation capabilities of biosystems such as cells, vaccines, or therapeutic proteins employed in the pharmaceutical industries. Indeed, disaccharides can be added to biologically active solutions to overcome the limited stability range of proteins (pH, temperature,...). These additives prevent the partial or even total degradation of biomolecules due to the lethal thermal or dehydration stresses encountered during industrial conservation methods (lyophilization). However, the molecular mechanisms at the origin of the biopreservation phenomenon itself still remain unclear. Several hypotheses (glass transition temperature, water molecules replacement, hydrogen bonding destructuring effect, preferential excluded volume,…) have been proposed, but none of them can be considered as fully accepted.

In order to better understand the physical properties of sugars and their influence on the protein stability we have performed Molecular Dynamics investigations of hen egg-white lysozyme in presence of three homologous disaccharides: trehalose, sucrose and maltose. This study shows that the hydrogen bonds network of water is highly dependent on the presence of sugars and contributes to the stabilization of lysozyme. The privileged interaction of trehalose with water is confirmed below a threshold weight sugar concentration. Above this concentration, trehalose becomes less efficient to distort the tetra-bonded HB network of water than maltose. This result is interpreted as a competition between sugars and lysozyme to bind to water molecules. At high sugar concentration, trehalose molecules are found less capable to perturb water molecules which bind preferentially to lysozyme consistently with the preferential hydration hypothesis. The analysis of the relative concentration of water oxygen atoms around lysozyme suggests that lysozyme is preferentially hydrated.

Coffee break

Wednesday afternoon, 17 September, 15:30
Main Hall

Joint Poster Session 2

Wednesday afternoon, 17 September, 16:00
Main Hall

Thursday, 18 September

Parallel symposia

Dynamics of complex and biological systems 2
Thursday morning, 18 September, 9:00
Room 144
Chair: Mark Wilson

9:00 Invited oral

Computational analysis of protein-protein interfaces and implications for ligand design

Annick P. Dejaegere

University Louis Pasteur, Strasbourg, France

e-mail: annick@igbmc.fr

A free energy decomposition scheme based on the MM-PBSA approach is presented and used to identify interaction hot-spots in biomolecular complexes. The calculations identify protein amino acids that make important contributions to the interaction energy of the complexes. Small structural variations on the energetics of binding are accounted for through the use of multiple conformations. We also define the concept of "efficient amino acids" which can provide an assessment of the binding potential of a particular hot spot interaction. This information, in turn, can be useful in the rational design of small molecules that interfere with protein-protein binding. Applications to different protein-protein and protein-ligand complexes are presented. The work shows that a free energy decomposition scheme can be employed to identify regions of a biomolecular complex that could be subsequently targeted by small molecules inhibitors. Applications of the method to ligand recognition by nuclear receptors also underlines general principles of molecular recognition that are useful for ligand design.

9:45 Invited oral

Substrate conformational changes in carbohydrate binding enzymes. Insights from ab initio simulations.

Carme Rovira[1,2], Xevi Biarnés[1], Albert Ardèvol[1], Antoni Planas

1. *Parc Científic de Barcelona (PCB), Baldiri Reixac 10-12, Barcelona 08028, Spain* **2.** *Institució Catalana de Recerca i Estudis Avançats (ICREA), Passeig Lluís Companys 23, Barcelona 08018, Spain*

e-mail: crovira@pcb.ub.es

The important roles that carbohydrates play in biology and medicine have stimulated a rapid expansion of the field of glycobiology.[1] The structures of glycoside hydrolases, the enzymes involved in the degradation of glycosidic bonds, are now being elucidated in molecular detail.[2] It is becoming increasingly accepted that only a complex interplay of electronic/structural properties can explain the perfect docking between the substrate and the enzyme. In this presentation, we will show how the conformational changes of one sugar unit of the carbohydrate affect the efficiency of these enzymes.[3] The structure and dynamics of the enzyme-substrate complex will be investigated by means of ab initio QM/MM simulations.[4]

[1] Hurtley, S., Service, R., and Szuromi, P. (eds) *Science* 291, 2263–2502 (2000).

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[4] Biarnés, X. Nieto, J., Planas, A., and Rovira, C. *J. Biol.Chem.* 281, 1432-1441 (2006).

Coffee break

Thursday morning, 18 September, 10:30
Main Hall

Parallel Session

Disordered systems: structure and dynamics 1
Thursday morning, 18 September, 11:00
Room 144
Chair: Mark Wilson

11:00 Invited oral

Ordering in Network Liquids and Glasses

Philip S. Salmon

University of Bath, Department of Physics, Claverton Down, Bath BA27AY, United Kingdom

e-mail: P.S.Salmon@bath.ac.uk

The structure of liquid and glassy materials is a formidable problem to solve because the atomic sites are topologically disordered and the presence of two or more chemical species adds further complexity. In this talk, some new in-roads are reported that have emanated from the application of neutron and x-ray diffraction methods. Specifically, it is found that the topological and chemical ordering are both described by at least two different length scales at distances greater than the nearest-neighbour. The interplay between the ordering on these length scales and the physical properties of liquid and glassy networks is discussed.

11:45 Invited oral

Distortions and low symmetry environments in liquids : alkalis at high pressure.

Jean-Yves Raty, Eric Schwegler, Isaac Tamblyn, Stanimir Bonev

University of Liege (ULg), B5, Liège 4000, Belgium

e-mail: jyraty@ulg.ac.be

The melting curve of sodium measured in exhibits totally unexpected features under pressure : the melting temperature, Tm, reaches a maximum around 30 GPa followed by a sharp decline from 1000 K to 300 K in the pressure range from 30 to 120 GPa.

In the present study, the structural and electronic properties of molten sodium and lithium are studied using first principles theory. With increasing pressure, both liquids evolve by assuming a more compact

local structure, which accounts for the maximum of Tm at 30 GPas in Na and the flattening of the melting curve in Li. However, at pressure around 65 GPa in Na and 20 GPa in Li a transition to a lower coordinated structure takes place, driven by the opening of a pseudogap at the Fermi level. Remarkably, the 'broken symmetry' liquid phase emerges at rather elevated temperatures and above the stability region of a closed packed free electron-like metal. The theory explains the measured drop of the sodium melting temperature, down to 300 kelvin at 105 GPas. The behavior of Li at higher pressure is even more surprising as we evidence the emergence of tetrahedrally (slightly) bonded clusters as due to increased core-core overlap.
The properties of the proposed new liquid phases and the implications of our findings for the stability of low-symmetry
solids will be discussed.

This work was supported by NSERC and CFI. Computational resources were provided by ACEnet, IRM Dalhousie, Westgrid, and Sharcnet. . J.Y.R. acknowledges support by the FNRS, and the FAME NoE. E.S. worked under the auspices of the U.S. Dept. of Energy at the University of California/LLNL.

Lunch break

Thursday afternoon, 18 September, 12:30
Inner Courtyards

Parallel Session

Disordered systems: structure and dynamics 2
Thursday afternoon, 18 September, 14:00
Room 144
Chair: Carlo Massobrio

14:00 Oral

Atomic and electronic structure of GST phase change materials

Christophe Bichara[1], Jean-Yves Raty[2], Céline Otjacques, Jean Pierre Gaspard

1. *Centre de Recherche en Matière Condensée et Nanosciences (CRMCN-CNRS), Campus de Luminy, case 913, Marseille 13288, France* **2.** *University of Liege (ULg), B5, Liège 4000, Belgium*

e-mail: xtof@cinam.univ-mrs.fr

Understanding the structure of phase change (PC) materials in their amorphous and metastable crystalline phase and their working mechanisms is of major importance.

While many groups have focused their attention on the structure of the crystalline or amorphous states, we start from studies of the liquid state of germanium tellurides. Combining experiments on liquids (thermodynamics, neutron scattering, EXAFS) and computer simulations (RMC, first principles Molecular Dynamics) we end up with a model emphasizing the role of electronically driven distortions of the local octahedral order in the peculiar behavior of these liquids (see references).

We will present DFT based molecular dynamics simulations of $Ge_2Sb_2Te_5$ alloys in crystalline, liquid and amorphous states. The interpretation of these results in the same framework leads to a simple and original picture that helps understanding the structure and properties difference between the crystalline and amorphous phases, thus paving the way for the development of new phase change alloys.

Raty J.-Y., Godlevsky V., Ghosez P., Bichara C., Gaspard J.-P., Chelikowsky J. R., *Evidence of a reentrant Peierls distortion in liquid GeTe.* Phys. Rev. Lett., 85, -9-, 1950-3, 2000.

Bergman C., Bichara C., Gaspard J.-P., Tsuchiya Y. *Experimental investigation of the water-like density anomaly in liquid $Ge_{15}Te_{85}$ eutectic alloys.* Phys. Rev. B67, 104202, 2003.

Coulet M.-V., Testemale D., Hazemann J.-L., Gaspard J.-P., Bichara C.,*A Reverse Monte Carlo analysis of the local order in liquid $Ge_{.15}$ $Te_{.85}$ alloys combining neutron scattering and X-Ray Absorption Spectroscopy.* Phys. Rev. B, 72, 174209, 2005.

Bichara C., Johnson M., Raty J.-Y.,*Temperature-induced density anomaly in Te-rich liquid germaniumtellurides: p versus sp^3 bonding?* Phys. Rev. Lett., 95, 267801, 2005.

C. Bichara, M. Johnson, J.-P. Gaspard*Octahedral structure of liquid $GeSb_2Te_4$ alloy : first principles molecular dynamics study* Phys. Rev. B 75, 060201R, 2007.

14:30 Oral

Partial Structure Factors of Molten and Glassy Zinc Chloride

Anita Zeidler[1], Philip S. Salmon[1], Richard A. Martin[1], Philip E. Mason[2], Gabriel J. Cuello[3]

1. *University of Bath, Department of Physics, Claverton Down, Bath BA27AY, United Kingdom* **2.** *University of Bristol, Tyndall Avenue, Bristol BS8 1TL, United Kingdom* **3.** *Institut Laue Langevin (ILL), 6 Rue Jules Horowitz, Grenoble, France*

e-mail: az207@bath.ac.uk

Liquid zinc chloride is a binary molten salt having the AX_2 composition. Anhydrous zinc chloride melts from a δ-ZnCl2 crystal structure where the chloride ions are packed densely in a hexagonal lattice and the zinc ions occupy 1/4 of the tetrahedral holes [1, 2]. However, zinc chloride, like beryllium fluoride, is different from other molten salts in the sense that it can be supercooled into a glass. The molten state is very highly viscous close to its freezing point and its electrical conductivity is small [3]. The partial structure factors for liquid zinc chloride were measured by Biggin and Enderby [3] at a temperature of 327 ºC but the instrumentation has greatly improved since 1981 and information is now obtainable on the possible occurrence of edge sharing tetrahedra in liquid zinc chloride as suggested by Raman scattering [4]. Also, the structure of liquid zinc chloride reported by Biggin and Enderby has recently been called into doubt by combining x-ray and neutron diffraction data [5]. A new set of partial structure factors was obtained which suggests that the first sharp diffraction peak (FSDP) is not due the zinc-zinc correlations but to the zinc-chlorine correlations.

We applied the method of isotopic substitution in neutron diffraction to measure the partial structure factors for liquid and glassy zinc chloride.

[1] J. Brynestad and H. L. Yakel, Inorg. Chem. 17, 1376 (1978).

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[4] S. N. Yannopoulos, A. G. Kalampounias, A. Chrissanthopoulos, and G. N. Papatheodorou, J. Chem. Phys. 118, 3197 (2007).

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15:00 Oral

Silica glass models from first-principles molecular dynamics approach

Masahiko Matsubara, Simona Ispas, Walter Kob

Université Montpellier II, Laboratoire des Colloïdes, Verres et Nanomatériaux (LCVN), place Eugène Bataillon, Montpellier 34095, France

e-mail: Masahiko.Matsubara@LCVN.univ-montp2.fr

Silica glass is a typical example of disordered material. Theoretically, molecular dynamics computer simulation is a common and effective way to investigate microscopic structural and dynamic properties of silica glass, such as pair correlation functions, bond angle distribution, vibrational density of states and so on.

In this work, we have prepared several different silica models solely within the framework of first-principles approach of the order of hundred atoms (38 Si and 76 O atoms) and analyze their structural, electronic and vibrational properties.

The SiO_2 models have been generated by quenching liquid silica (equilibrated at 3600 K and with a density equal to 2.20 g/cm^3) to room temperature (300 K) using different

cooling rates. We have compared the microscopic properties with experimental and previous simulation results. We have found that the cooling rate affects the properties of generated silica models and that the slowly quenched model gives better agreement with the experimental results.

These models have been gradually compressed up to 2.67 g/cm^3 density, which corresponds to about 7 GPa: just below the elastic to plastic transition regime (estimated around 8 to 10 GPa) of silica glass. To characterize microscopic properties of compressed silica models below the transition pressure is an important step to investigate the mechanism of the transition with further compressed silica models (above the transition pressure). We show the properties of these compressed silica models and compare them with those of the uncompressed ones.

Another type of models are also generated by compressing and equilibrating the liquid silica at 3600 K to 2.67 g/cm^3 and then quenched to 300 K. The microscopic properties of these models will be also presented and discussed.

Coffee break

Thursday afternoon, 18 September, 15:30
Main Hall

Parallel Session

Disordered systems: structure and dynamics 3
Thursday afternoon, 18 September, 16:00
Room 144
Chair: Carlo Massobrio

16:00 Invited oral

First-principles modelling of some simple silicate glasses: local structural distortions vs specific macroscopic properties

Simona Ispas

Laboratoire des Colloides, Verres et Nanomateriaux, Univ Montpellier II (LCVN), Place Eugene Bataillon, Montpellier 34095, France

e-mail: simona.ispas@lcvn.univ-montp2.fr

Tackling precisely the microscopic properties of minerals and glasses is a very complex multidisciplinary issue: It has been, and continues to be, a subject of investigation in many fields of fundamental science, from solid state physics to geochemistry, and of major interest for various applications. Despite this very strong interest from the scientific community, an important number of molecular mechanisms remain unfortunately unclear even for silicates with a simple composition. In this talk, we will present first-principles density functional theory calculations which may be used to better understand two peculiar mechanisms present in silicate glasses.

Firstly, we will discuss the structural properties of two (Li/Na) single-alkali silicate glasses with the same cation content. The influence of the network modifier nature on the relevant structural parameters will be further examined in terms on their correlations to the first-principles calculated NMR parameters of our glassy models. This comparative study may be helpful to obtain a precise microscopic insight into one of the unsual properties of oxide glasses, namely the so-called mixed alkali effect.

Secondly, we will provide a description of some initial mechanisms of hydration and hydrolysis of a calcium aluminosilicate glass. It is found that hydrolysis, among all the regular bridging bonds, is only allowed at specific sites. The existence of such reactive sites is likely a general feature of amorphous systems, and it may be used to describe qualitatively some experimental trends common to silicates and aluminosilicates.

16:45 Invited oral

Multiple Length-Scale Ordering in Network-forming Ionic Liquids

Mark Wilson

Oxford University, Physical and Theoretical Chemistry Laboratory, South Parks Road, Oxford OX1 3QZ, United Kingdom

e-mail: mark.wilson@chem.ox.ac.uk

Recent developments in the molecular dynamics computer simulation of network-forming liquids are discussed. Relatively simple potential energy models, in which many-body (dipolar) polarization is accounted for, are able to reproduce a range of static and dynamic properties. Ion polarization is shown to account for the network topology via controlling the number of edge- and corner- sharing polyhedral units. The nature of this intermediate-range order (as probed by the Bhatia-Thornton structure factors) is shown to depend subtly on the fractions of such linkages. Furthermore, the presence of the intermediate-range order is shown to have important implications for both the low temperature liquid relaxation dynamics and the presence of extended-range order.

17:30 Oral

Defective icosahedral order in undercooled copper

Massimo Celino

ENEA, via Anguillarese 301, Roma 00123, Italy

e-mail: celino@casaccia.enea.it

No consensus there is on the role played by the icosahedral short range order on the stability of undercooled simple metals. Furthermore, experiments are not in agreement on the nature of the local icosahedral structures. The stability of undercooled copper is analyzed by performing classical molecular dynamics simulations based on an empirical interatomic potential. Icosahedral order is quantified in terms of a common neighbor analysis in several conditions of temperature and pressure. It is possible to show that not only perfect but also defective icosahedra, embedded in a disordered matrix, partecipate to stabilize the atomic structure preventing crystallization.

Friday, 19 September

E-MRS & EPDIC Joint Plenary Session

Friday morning, 19 September, 9:00
Small Hall (237)

Coffee break

Friday morning, 19 September, 10:30
Main Hall

Posters

Monday, 15 September

Joint Poster Session 1

Monday & Wednesday
Monday afternoon, 15 September, 16:00
Main Hall

16:00 Poster G01

Kinetic Monte Carlo simulation of homoepitaxial growth of magnesium oxide thin films by molecular deposition

Ekaterina Antoshchenkova[1], Marc Hayoun[1], Fabio Finocchi[2], Gregory Geneste[3]

1. *Laboratoire des Solides Irradies, CEA, CNRS, Ecole Polytechnique (LSI), Ecole Polytechnique, Palaiseau 91128, France* **2.** *Institut des nanosciences de Paris (INSP), 140 rue de Lourmel, Paris 75015, France* **3.** *Ecole Centrale Paris, SPMS, UMR CNRS-ECP (ECP), Grande voie des vignes, Chatenay-Malabry 92295, France*

e-mail: ekaterina.antoshchenkova@polytechnique.edu

We have developed a Kinetic Monte Carlo (KMC) code adapted to the homoepitaxial growth of MgO. The KMC approach is an efficient tool for modeling a complex sequence of simple events. The events, which form the growth of the oxide, are the followings: deposition, various diffusion mechanisms, evaporation and chemical reactions. These events and their probabilities obtained from their frequencies are the input data of the KMC simulations. We have used *ab initio* calculations (Density Fonctional Theory) at T=0 K [1] and Molecular Dynamics (MD) computations based upon phenomenological potentials at T=1000 K [2] to guess and discover the possible events occurring and their corresponding frequencies.
KMC allows us to bridge the time scale gap between diffusion events (nanoseconds) and deposition events (seconds). Our KMC code simulate the homoepitaxial growth by Molecular Beam Epitaxy. The simulations where carried out on a MgO(001) monocrystalline substrate using a cell with periodic boundary conditions. The dimensions of the system can reach a few hundred thousand of molecules.
We simulated the MgO homoepitaxial growth at different temperatures and pressures of the molecular beam and at a chosen roughness of the MgO substrate. We investigated and compared the effects of each event in order to estimate the role of diffusion in crystal growth and the contributionof every diffusion mechanism. To obtain a realistic model, we varied the event probabilities as a function of the neighboring of the migrating molecule: near defects (steps, vacancies) and centers of nucleation (clusters). We have also used MD as a tool to check the validity of some hypothesis made within KMC.

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16:00 Poster G02

Morphology and topological Shannon's information interdependence for self-assembling nanoparticle agglomeration

Serge A. Beznosyuk, Mark S. Zhukovskiy, Yakov V. Lerh

Altai State University (ASU), Lenin St., 61, Barnaul 656049, Russian Federation

e-mail: zhukovsky@list.ru

The computer simulation on self-assembling growth of aggregates of nanoclusters dispersed in randomly medium of colloidal solution is suggested. The Cluster-Cluster Aggregation model for original research self-organizing aggregations of nanoparticles is used. For description of random dynamics of nanoparticles dispersed in bounded volume, their aggregation is located inside a cubic cage of physical space with base length n = 30 composed from 27000 (30×30×30) equal-sized cubic cells. Aggregates of cubic-form nanoparticles are synthesized at different concentrations (10% - 100%). Time of evolution is dimensioned with discrete steps. On the first time step cubic particles occupy the cage of physical space randomly. On every time step particles migrate in one of the twenty six sectors. Every particle has nearest-neighbor vicinity, consisted from twenty six cells. As long as other particles come in this vicinity, the aggregate will be generated from these particles. Aggregates migrate in one of twenty six sectors just as well particles. If another particles or formed aggregates come in vicinity of this aggregate, it will cause new aggregate generation from these particles and/or aggregates. Process is to be continued, unless one cluster will include all particles generations. Analyzing topological graph of aggregates, in which vertexes denote particles, whereas ribs of graph denote chemical-physical bonds of neighboring particles, it is shown that increasing of number of aggregate graph ribs decreases enthalpy. That is a main gathered factor. The novelty of the exploration is a model validation that a maximum of the Shannon's information of the aggregate topological graph reflects some self-assembling trends. When numbers of ribs countering each vertex increase from zero to a possible value it is revealed that the extreme property of Shannon's information functional dependence on the concentration of nanoparticles reflects main morphologic features of the agglomeration.

16:00 Poster G03

Theory and computer simulation of interconnection between femtosecond dynamics and corporative phenomena in nanosystems

Serge A. Beznosyuk, Mark S. Zhukovskiy, Stanislav V. Vazhenin

Altai State University (ASU), Lenin St., 61, Barnaul 656049, Russian Federation

e-mail: zhukovsky@list.ru

The precise description of evolution processes is one of the most important problems in the field of nanoscience. Especially there are specific nonequilibrium corporative phenomena of self-assembling and self-organization. In present work the problem of nonequilibrium corporative algorithmic motion of nanosystems is investigated. As regards the corporative motion, it is observed both in equilibrium and in nonequilibrium electron-nuclear systems. In the former this results in the existence of adiabatic lattice of nuclei and phonon acoustic modes, whereas in the latter corporative effects involve non-adiabatic algorithmic processes including self-assembly and self-organization, generating nanostructures. Initialization such kind operations require at least three conditions: (a) nonequilibrium, (b) corporative and (c) algorithmic dynamics of nanosystem. The fundamental scheme of evolution is considered as applied to nonequilibrium nanosystems, whose discontinuous and non-adiabatic motion in configuration space is controlled by quantum correlations with topologic structures of Bose-condensate vacuum states of physical fields. By the example of nickel and graphene nanoparticles it is investigated time-dependent algorithmic behavior of consolidated quantum-sized field systems. It is shown that time quanta of discrete nanoparticle transformations amounts to a femtosecond. Today femtosecond and sub-femtosecond range turns out to be beyond resolution power of the up-to-date devices of nanotechnology. In the circumstances it is really significant to know the availability of theoretical approaches, used for description of the nanoscale dynamics. The model considered allows one to forecast the discrete forms of nanoparticle structural organization under variable experimental conditions. This, in turn, clears the way to directional effect on widely applicable structures in technologies and industry practice for the purpose of control the nanoparticle femtosecond dynamics.

16:00 Poster G04

Hydrostatic pressure and $\Gamma - \mathrm{X}$ mixing effects on the exciton and impurity related optical properties in GaAs-Ga$_{1-x}$Al$_x$As quantum wells

Carlos A. Duque[1], Sonia Y. López[1], Miguel E. Mora-Ramos[2]

1. *Universidad de Antioquia (UA), Calle-67-N-53-108, Medellín 05001000, Colombia* **2.** *Universidad (UAEM), Av.-Universidad-1001, Cuernavaca 62209, Mexico*

e-mail: cduque_echeverri@yahoo.es

The mixing between the Γ and X conduction-band valleys in GaAs-Ga$_{1-x}$Al$_x$As quantum wells is investigated by using both a phenomenological and a variational models which take into account the effects of applied hydrostatic pressure. The dependencies of the calculated photoluminescence peak-energy transitions on the applied hydrostatic pressure and quantum-well width are presented. A systematic study of the $\Gamma - \mathrm{X}$ mixing parameter is also reported. In particular, it is shown that the inclusion of the $\Gamma - \mathrm{X}$ mixing explains the non-linear behavior in the photoluminescence peak of confined exciton states that has been experimentally observed for pressures above 15 kbar in GaAs-Ga$_{1-x}$Al$_x$As quantum wells.

16:00 Poster G05

Thermodynamics of supercooled water in solutions and in confinement

Paola Gallo, Dario Corradini, Mauro Rovere

Physics Department, University Roma Tre, Via della vasca navale 84, Roma 00146, Italy

e-mail: gallop@fis.uniroma3.it

Results of molecular dynamics simulations of TIP4P water in a hydrophilic and hydrophobic environments are presented. The study is done upon supercooling to investigate the modifications induced by these environments in the temperature of maximum density line and in the liquid-gas spinodal.

The first system is done with water confined in a hydrophobic disordered matrix of soft spheres. The second is an aqueous ionic solution of NaCl at low molality. Studies are done for several isochores from 350 K down to 210 K.

Qualitatively these systems behave like the bulk. The spinodal curve is monotonically decreasing and the line of maximum density bends avoiding a crossing of the spinodal. There are however changes in shape and/or position of these curves in the two systems that will be discussed in comparison with other studies in confinement and in connection with the possible position of a second critical point.

16:00 Poster G06

Dynamical properties of homocysteine near carbon nanotube – MD simulation

Krzysztof M. Górny, Przemysław Raczyński, Zygmunt Gburski

University of Silesia, Institute of Physics, Uniwersytecka 4, Katowice 40-007, Poland

e-mail: kgorny@us.edu.pl

Molecular dynamics (MD) studies are presented for the ensembles of homocysteine molecules surrounded single walled carbon nanotube. We have investigated several dynamical observables of homocysteine at the physiological temperature T = 309 K: radial distribution function, mean square displacement, diffusion coefficient, translational velocity correlation function, … *etc*. We also calculate the total dipole moment autocorrelation function of homocysteine molecules and dielectric loss of both samples.

16:00 Poster G07

Molecular dynamics of 5CB mesogene molecules covering graphene layer – computer simulation

Krzysztof M. Górny, Wojciech Gwizdała, Zygmunt Gburski

University of Silesia, Institute of Physics, Uniwersytecka 4, Katowice 40-007, Poland

e-mail: kgorny@us.edu.pl

The ultrathin film of mesogenous molecules 5CB covering a graphene wall has been investigated by molecular dynamics (MD) technique. The dynamical observables of 4-cyano-4-n-pentylbiphenyl (5CB) were calculated for several temperatures: the mean square displacement, diffusion coefficient, translational and angular velocity autocorrelation function, … *etc*. The comparison with the properties of pure 5CB cluster (without graphene) is presented and discussed.

16:00 Poster G08

Dielectric relaxation of homocysteine layer between graphite walls – computer simulation

Przemysław Raczyński, Krzysztof M. Górny, Zygmunt Gburski

University of Silesia, Institute of Physics, Uniwersytecka 4, Katowice 40-007, Poland

e-mail: kgorny@us.edu.pl

Molecular dynamics (MD) studies are presented for the homocysteine $C_4H_9NO_2S$ layer located between parallel graphite walls. We have calculated several dynamical observables of homocysteine at the physiological temperature $T \approx 309$ K. Several physical characteristics: the radial distribution function, the mean square displacement, the translational velocity autocorrelation function and its Fourier transform, the second rank order parameter have been calculated. The attention was focused on the total dipole moment autocorrelation function, the dielectric loss spectrum $\varepsilon''(\nu)$ and absorption coefficient $\alpha(\nu)$. The comparison with the dielectric relaxation of pure homocysteine sample (without graphite wall) is also presented and discussed.

16:00 Poster G09

Effect of silicate nanosheets on nanochannel morphology of polymeric ionomers

Mohammad M. Hasani-Sadrabadi[1,2,3], Reza Ghaffarian[1]

1. *Amirkabir University of Technology (AUT), Hafez, Tehran 15914, Iran* **2.** *Young Researcher Club, Tehran 15655-461, Iran* **3.** *National Foundation for Elites, Tehran 19615-334, Iran*

e-mail: mahdi.hasani@gmail.com

Nafion, the fluorinated membrane from DuPont has been intensively used for fuel cells as proton exchange membranes(PEMs). This polymer combines the mechanical strength and chemical/thermal stability with high proton conductivity and methanol permeability. In order to overcome methanol cross-over, the tortuous pathways can be introduced by dispersion of inorganic fillers. A Nafion membrane consists of an interconnecting network of nanoscopic aqueous domains surrounded by a fluorocarbon backbone. The size and extent of the aqueous domains or nanochannels control proton and methanol diffusion, and it is one of the factors controlling the maximum current densities generated by a cell. Understanding the effects of nanoclay addition on morphology of Nafion channels was the main aim of current study. In current research, organically modified montmorillonite(MMT) are introduced in Nafion, for reduction in methanol permeability. Nafion composite membranes were fabricated by ultra-sonic mixing and solution-casting method. Exfoliated structure of clay in polymeric matrix is approved by X-Ray Diffraction patterns. For membranes to be used in liquid DMFC, it is highly desirable to obtain the structural data of the electrolyte membranes at conditions close to that in practical fuel cells. Accordingly, we equilibrate the Nafion membranes with different MMT loading in methanol solution. The relationships between the Bragg spacing and the transport of methanol and protons in the nanocomposie membranes are discussed and the data are compared with those of Nafion117 as a commercial PEM. The proton conduction properties of the membranes have been investigated by impedance spectroscopy. The network cluster model is employed to retrieve the structural information from the scattering and proton conductivity data. While the nanocomposie membranes have narrower pathways for methanol/water permeation, the pure Nafion membranes have wider channels, resulting in higher methanol permeability.

16:00 Poster G10

Modelling of nanooscillators

Roman I. Hrytskiv, Ivan M. Bolesta

Ivan Franko National university of Lviv (LNU), Lviv 79017, Ukraine

e-mail: roman.hrytskiv@gmail.com

For last decades carbon nanotubes (CNT's) are intensively studied due to their unique structure and wide range of potential applications. Recent experiments have shown that CNT's can serve as elements of electromechanical systems such as nanoengines, nanooscillators, nanoresistors, nanotermometers and nanoactuators. Some of these devices have already laboratory prototypes. Furthermore, such systems will form a basis for future development of nanomechanics.

Nanooscillators are systems constituted by a pair of CNT's put into each other, able to move periodically when not in equilibrium state. Such systems are studied mainly by means of computer simulations.

In presented work nanooscillators were investigated using molecular dynamics. Covalent interactions between carbon atoms inside a CNT were described by Tersoff potential while interactions of particles in the different tubes were modeled using Lennard-Jones potential.

Various systems formed by tubes with different geometry and with different initial conditions (such as temperature) were studied. Corresponding time dependences of frequency, amplitude and other characteristics obtained. In particular, the oscillator consisting of (9, 0) and (18, 0) tubes both of length 21 Å was considered. For this oscillator sustained oscillations were observed. The frequency has increased from 118 GHz at the beginning of the simulation up to 120 GHz in the end (the simulation was run for 1 ns time). The oscillations were found to be damped: amplitude has decreased for about 2.5% from the initial value after 1 ns. Periodical changes in the amplitude were discovered, which we assume to result from superposition of oscillator vibrations and longitudinal vibrations of inner and outer tubes. These vibrations of tubes are induced by Van der Waals forces acting during oscillations. The frequency of tubes oscillations was found to be two times higher than main oscillator frequency. This proves abovementioned assumption.

16:00 Poster G11

Formation of stacking defects at surfaces: From atomistic modelling to DFT calculations.

Ali Jaafar, Christine Goyhenex

Institut de Physique et Chimie des Materiaux de Strasbourg, UMR7504, CNRS - ULP, 23, rue du Loess, BP 43, Strasbourg CEDEX 2 67034, France

e-mail: ali.jaafar@ipcms.u-strasbg.fr

Stacking fault formation is at the origin of nanostructuration phenomena at close-packed like in the case of the famous Au(111) herrigbone reconstruction. The balance energy between FCC stacking and HCP stacking is conditionning also the structural homogeneity of an epitaxial growing deposit on such surfaces. In this context we apply a sp-d tight binding model to study the evolution of the stacking fault energy at (111) surfaces of metals. We show in this way the relative importance of sp-d hybridation both in the formation of defects at the surface of metals and in reconstruction phenomena as a function of band filling especially for the end of transition series. In our work, we also use a method of DFT, precisely the SIESTA method, which is based on orbital atomic localized, which allows us to compare sp-d tight binding model with a more accurate values. Finally, we compare our results with atomistic simulations. It is concluded that although atomistic calculations are powerful tools to investigate relaxation mechanisms at surfaces, a higher degree of accuracy on electronic structure could be necessary to quantify the energy of some defects at surfaces like FCC stacking and HCP stacking. In particular long range interactions associated to less localized sp electrons are clearly playing a non negligible role in reconstruction phenomena for metals like platinum and gold.

16:00 Poster G12

Ab initio Molecular Dynamics study of the dynamic behaviour of a «floppy» guest complexed in Mo_{12} cage

Ali Kachmar[1,2], Marie-Madeleine Rohmer[2], Carlo Massobrio[1], Marc Benard[2]

1. *Institut de Physique et Chimie des Materiaux de Strasbourg, UMR7504, CNRS - ULP, 23, rue du Loess, BP 43, Strasbourg CEDEX 2 67034, France* **2.** *Institut de Chimie (CNRS/ULP), 4, rue Blaise Pascal, Strasbourg 67000, France*

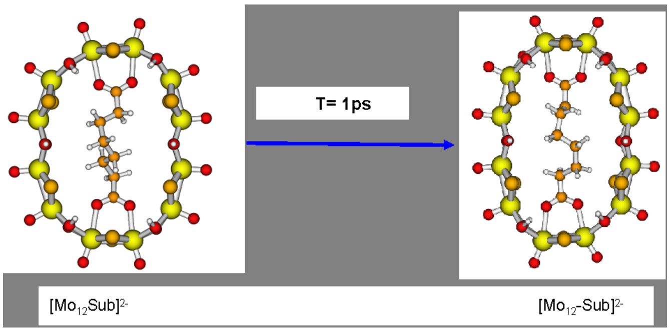
e-mail: kachmar@quantix.u-strasbg.fr

Polyoxometalates (POMs) are inorganic metal-oxygen anionic clusters of nanometric size. They represent a wide family of molecules with versatile properties, which have been shown to be potentially attractive for catalysis, medicine, magnetism, or supramolecular chemistry.

We present DFT calculations and geometry optimizations carried out on three host-guest complexes labelled $[Mo_{12}Adip]^{2-}$, $[Mo_{12}Pim]^{2-}$ and $[Mo_{12}Sub]^{2-}$. The host is a neutral, ring-like oxothiomolybdate with formula $Mo_{12}O_{12}S_{12}(OH)_{12}$.[1] This structure was shown to encapsulate dicarboxylate anions with linear, flexible chains with formula $[O_2C\text{-}(CH_2)_n\text{-}CO_2]^{2-}$, such as adipate (n=4), pimelate (n=5), and suberate (n=6). The stability of the host-guest systems decreases as the alkyl chain becomes longer, due to the increasing constraints affecting the guest.[2]

Car-Parrinello molecular dynamics (CPMD) simulations have also been carried out on these three host-guest complexes, in order to visualize the mutual adjustment of the host and guest fragments. Simulations have been carried out on both the free dicarboxylates and the whole host-guest complexes in order to point out and visualize the rotations occurring around the C-C bonds of the alkyl chains, resulting in conformational changes in the carboxylate.

Such changes could be characterized at relatively high temperatures (500 K), without leading however to the decomposition of the complex. They seem to occur more easily for suberate, the dicarboxylate with the longest carbon chain, illustrating the higher flexibility of this “floppy” molecule.



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16:00 Poster G13

The spatial-temporal structures as a model system for used microheterogeneous structure of aqueous-alcohol solutions

Svetlana Karitskaya

Urals State Technical University (USTU-UPI), Mira,19, Ekaterinburg 620002, Russian Federation

e-mail: sv.karitskaya@rambler.ru

The investigation of the properties of micellar systems is of great practical importance, since the microheterogeneous structure, in particular, of aqueous-organic solutions can be used to create reaction centers with designed properties, which will make it possible to increase the efficiency of processes associated with the intra-molecular conversion of the electronic excitation energy of a molecule. In the present paper, such model systems are the spatial-temporal structures (STS) formed as a result of photophysical and photochemical reactions, whose time characteristics are highly sensitive to a change in the solvent compositions.

Previously, the phenomenon of formation of the STS in alcohol solutions of anthraquinone at various ketone concentrations was investigated. It was shown that the luminescent photoproduct (ketyl radical) of anthraquinone is responsible for the formation of structures in this system. The STS evolution processes are slow and the structures formed have macroscopic sizes, which makes the system under consideration a convenient object for experimental studies.

We have investigated water-alcohol solutions with a different mass content of analytically pure isopropyl alcohol, which was varied from 10 to 95% with a step of 5%. Analysis of the obtained spectral characteristics of the solutions under investigation has shown that in the water-alcohol solutions of anthraquinone, independent of the mass concentration of alcohol, the ketyl radical is responsible for the luminescence.

The microheterogeneous structure of water–alcohol solutions produces a strong effect on the intermolecular energy transfer rate, which in turn affects the behavior of luminescent STSs. A considerable decrease in the induction period of the appearance of an STS (t_{ind}<1 sec) was registered under irradiation by UV light of solutions with a 70% mass content of alcohol in the matrix, which corresponds to a simplified structure of the alcohol–water mixture.

16:00 Poster G14

amorphous materials - x-ray studies

Małgorzata Karolus

University of Silesia, Institute of Material Science, Bankowa 12, Katowice 40-007, Poland

e-mail: karolus@us.edu.pl

In this paper there is presented the general view on the experimental aspects of amorphous material structure analysis for different kind of materials (e.g. thin amorphous films). From the classical point of view the structure of the amorphous materials might be done by the Radial Distribution Function and Pair Distribution Function analyses. The radii and numbers of coordination spheres are the results of such analyses. Basing on that information it is possible to create the spherical structure model of the amorphous material. Moreover, comparing the received values to the values characteristic for the typical crystalline structure models it is possible e.g. to guess the way of crystallization process. Basing on the "microcrystalline structure model" the Rietveld method might be used for refinement of the "unit cell" of searching material and further for the crystallite size, and lattice strain calculations or the calculation of the change of unit cell parameters etc. The results are comparable with the results of other experimental method as HR-EM.

16:00 Poster G15

Computer simulation of structure and hydrogen capacity of nanoporous carbon

Valeriy V. Kartuzov[1], Yury Gogotsi[2], Oleksandr O. Kryklia[1]

1. *Institute for Problems in Materias Science (IPMS), 3, Krzhizhanivsky Str., Kiev 03680, Ukraine* **2.** *Drexel University, 3141 Chestnut St, Philadelphia 19104, United States*

e-mail: vvk@ipms.kiev.ua

In our previous work [1] was described a model of nanoporous carbon produced from SiC. However, that computational model did not produce a clear description of the structure of porous space that can be used later for sorption and other applications (for example, hydrogen storage or sorption and transport of certain molecules in the porous structure).

This work deals with computer modeling of porous space with a well-defined porous structure and with the density of the sample conforming to the experimental value (0.96 g/cm^3) [3,4]. The objects of modeling are clusters of nanoporous carbon with characteristic dimensions less than 10 nm and the number of carbon atoms less 20 000, with different pore sizes, b: 0.2 - 2 nm and distances between pore channels d: 0.2-1.5 nm. The porous space contains parallelepipedic corridors. Cross-sections of pores include square, circle, hexagon, and octagon. Resulted cluster structures were generated and computed by molecular dynamics methods [2] at different temperatures. Specific surface area (SSA) and various geometrical distributions of cluster structure were calculated. For all clusters, hydrogen capacity was computed using the developed geometrical model. Porous space with the optimal porosity fro hydrogen storage was built.

For experimental b and SSA [3,4], the obtained structures were stable at different temperatures. For example, for $b = 0.8$ nm and SSA = 2000 m^2/g, the cluster density without pores was 2.44 g/cm^3, with pores - 0.98 g/cm^3, open pores share - 0.59. Inner structure of the cluster may be graphite-like with some additional carbon atoms or sp^3-bonded clusters with closed pores.

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16:00 Poster G16

Contact Resistance Limited Thermal Transport of Carbon Nanotube Mats

Pawel J. Keblinski[1], Fabrizio Cleri[2], Ravi Prasher[3], Jack Hu[3]

1. *Rensselaer Polytechnic Institute (RPI), 110 - 8th St., MRC-218, Troy, NY 12180, United States* **2.** *Institute for Electronics and Nanotechnology, Lille 60069, France* **3.** *Intel Corporation, Chandler, AZ 85226, United States*

e-mail: keblip@rpi.edu

Experimental measurement on pressure compressed single-walled and multi-walled carbon nanotube mats demonstrated low thermal conductivity of the mats which is bellow that exhibited by isotropic amorphous polymers. Using molecular dynamics simulations and theoretical analysis we propose that the very low thermal conductivity of carbon nanotube mats originates with low thermal conductance of contacts between carbon nanotubes which is due to very large mismatch between strong covalent bonds within the tubes and week Van der Waals bonding between the tubes. We discuss the possibility of good thermoelectric properties of carbon nanotube mats due to their low thermal conductivity

16:00 Poster G17

Characterization of Ni-P surface layers produced by the chemical method in a multicomponent solvent with additions of ionic liquids

Maria Trzaska, Piotr Moszczyński

Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland

e-mail: moszczu@gmail.com

Nickel-phosphorous alloys are of great commercial interest as of their mechanical and corrosion resistance properties. A proprietary, high efficiency process of chemical reduction has been developed to produce the Ni-P surface layers exhibiting useful tribological properties resulted from a modification of the solvent by ionic liquids.

The goal of the present paper is to report the results of performed investigations on the influence of additions of different quantities of ionic liquids into a multi-component solvent on properties of Ni-P layers prepared by the method of chemical reduction. The results of analyses of topography, morphology and lubricating properties of the Ni-P layers prepared with and without liquid ions additives are also presented.The structural analyses are performed by using X-Ray diffractometer PW-1830. Morphology and topography of examined layers are performed by scanning electron microscopy S-3600N.

Results of investigations presented in this paper have showed that the introduction of ionic liquids into the bath leads to important increase in mechanical properties of the Ni-P surface layers.

16:00 Poster G18

Modeling of order-disorder phase transition in intermetallic compounds

Marek Muzyk, Krzysztof J. Kurzydlowski

Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland

e-mail: muzyk@inmat.pw.edu.pl

Phase ordering has a strong influence on many properties of intermetallic alloys. In particular mechanical properties, such as creep resistance, which decreases drastically when phase transition occurs. Since the transition takes place at elevated temperatures and is influenced by materials purity, it is experimental investigations are time consuming. On the other hand, new modeling techniques, such as ab initio pseudo potential calculations including phonon contributions make it possible to study ordering-disordering process in ideally pure systems. In particular, the temperature of such phase transition can be predicted. The results of the investigations are discussed with respect to the date obtained experimentally.

16:00 Poster G19

Dynamical simulation of SiO_2/4H-SiC C-face interface oxidation process at 1500K

Toshiharu Ohnuma[1], Atsumi Miyashita[2], Misako Iwasawa[1], Masahito Yoshikawa[2], Hidekazu Tsuchida[1]

1. *Central Research Institute of Electric Power Industry (CRIEPI), Tokyo 201-8511, Japan* **2.** *Japan Atomic Energy Agency (JAEA), 1233 Watanuki, Takasaki, Gunma 370-1292, Japan*

e-mail: ohnuma@criepi.denken.or.jp

We performed first-principles molecular dynamics calculation of the oxidation process in the SiO_2/4H-SiC C-face interface. The calculations have been performed by the Vienna ab initio simulation package (VASP) with plane waves, supercells, and the projector augment wave method. The slab model is used for the simulation. The molecular dynamics simulation is carried out at 1500K using the time step of 1 fs. The calculation was held on the Earth Simulator. The oxygen molecules are added one by one every 15 ps to the empty sphere in the SiO_2 layer near the interface in the simulation of the oxidation process. The oxygen molecules are dissociated in the SiO_2 layer or at C atoms of the interface. Dissociated O atoms oxidize not only at the C atoms of the interface but also at the Si atoms in the second atomic layer of the SiC region. It was found that bilayer oxidation occurres at the SiO_2/4H-SiC C-face interface.

16:00 Poster G20

Desorption of H_2 molecules from hydrogen doped TiC_2H_2 exohedral fullerene nanosystem

Adam Piątek, Aleksander Dawid, Zygmunt Gburski

University of Silesia, Institute of Physics, Uniwersytecka 4, Katowice 40-007, Poland

e-mail: afriday@interia.eu

The titanium-decorated $C_{60}(TiC_2H_2)_6$ fullerene matrix doped with molecular hydrogen (H_2) was studied by MD simulation. The process of hydrogens' desorption from the solid matrix was investigated by analyzing several physical quantities: the radial distribution function, the mean square displacement, the translational and angular velocity autocorrelation functions, translational diffusion coefficient, etc. over a wide range of temperature.

16:00 Poster G21

Dynamical and structural properties of OH - decorated fullerene cluster: computer simulation study

Adam Piątek, Aleksander Dawid, Zygmunt Gburski

University of Silesia, Institute of Physics, Uniwersytecka 4, Katowice 40-007, Poland

e-mail: afriday@interia.eu

Using classical molecular dynamic (MD) simulation we have studied an ensemble made of $C_{60}(OH)_{24}$ molecules. The system has been studied in a wide range of temperatures, from solid to the gaseous state. Several physical characteristics of exohedral fullerene: the mean square displacement, the translational and angular velocity autocorrelation function, translational diffusion coefficient, etc. have been calculated for several temperatures. We have observed the reduction of rotational freedom of fullerene decorated by OH functionality groups, comparing to the pure fullerene sample.

16:00 Poster G22

The properties of fullerenol nanosystem $(C_{60}OH_{24})_7$ - MD simulation

Adam Piątek, Aleksander Dawid, Zygmunt Gburski

University of Silesia, Institute of Physics, Uniwersytecka 4, Katowice 40-007, Poland

e-mail: afriday@interia.eu

The nanosystem composed of only as few as seven fullerenols $C_{60}(OH)_{24}$ molecules was studied using the molecular dynamics (MD) technique. The interaction was taken to be the full site-site pairwise additive Lennard-Jones (LJ) potential, which generates both translational and anisotropic rotational motions of each fullerenol. The radial distribution function, the mean square displacement, the Lindemann index, the translational and angular velocity correlation functions of fullerenol have been calculated for several energies of the nanosystem. We provide also the in-depth evidence of the solid-liquid phase transition in the investigated cluster. The comparision with the properties of pure fullerene cluster $(C_{60})_7$ is provided. The study are motivated by the expected diverse biological applications of water-soluble fullerenols.

16:00 Poster G23

SEM investigations of the surface and cross-section features of ZnO nanowires under focused ion beam treatment

Gagik Shmavonyan

State Engineering University of Armenia, Yerevan 0002, Armenia

e-mail: gshmavon@yahoo.com

We investigated VPE-grown ZnO NWs on a Si substrate by SEM. SEM investigations show that there are single NWs and ensembles of NWs, among which we found straight and bend, perfect (with regular facets and smooth surfaces) and non-perfect (with irregular facets, not smooth surfaces, variable width, damages and particles) NWs, as well as NWs with clean surfaces and surfaces with the dark spots and features. After FIB polishing we found that every NW has a clean homogeneous surface, which allow us to conclude that all those dark spots and surface features of the NWs really are just surface features. The FIB milling gives information of the deeper interior of the NWs, i.e. buried structures within the NWs and whether those structures are propagating within the NWs. But also here we found that there are no buried structures inside the NWs and the dark spots and features are not propagating within the NWs, which leads to the result that the NWs are totally homogeneous. The hexagonal facets of the NWs were observed on SEM images, which emphasizes the good crystalline quality of the NWs. The sizes of the NWs were determined: the length is about 2-24 μm, and the width and height are about 200-500 nm.

16:00 Poster G24

The Formation of Aggregates from Ni Atoms at the Impulsive High-Intensive Influences on Ni3Al Intermetallide

Mikhail D. Starostenkov, Aleksandr V. Yashin, Olga A. Tereschenko, Olga V. Pozhidaeva, Nikolay N. Medvedev

Altai State Technical University (ASTU), Lenin st.46, Barnaul 656038, Russian Federation

e-mail: genphys@mail.ru

The process of nanoclusters aggregatization containing of Ni atoms in the structure of Ni3Al intermetallide is studied in the present paper. The process takes place at the internal high-intensive influences-radiation and deformation ones. The researches were made by the method of molecular dynamics. The calculated block of crystal contained 2*10^5 atoms and it repeated outside the crystal block by the introduction of periodical boundary conditions. The temporary step of re-calculation of the system of the movement equation was equal to 5*10^(-15) s. The temperature was given by the initial velocities in correspondence with Maxwell distribution. The directions of initial velocities were given randomly, but the total impulse of the atoms of the calculated block was given to zero. Simulation the radiation influence in the calculated crystal block, the definite number of Frenckel pairs – vacancies and interstitial atoms was introduced. But condition had to be fulfilled: stoichiometry of intermetallide composition. The formation and accumulation of Frenckel pairs took place at the definite levels and the velocities of an impulsive deformation of tension in the material. Such pairs recombined partially, the left pairs could unite into the aggregates in the migration process. The vacancies and interstitial atoms begin to form the aggregates such as flat accumulations in a form of dislocation loops volume crowdion complexes and tetrahedrons of fault defects at high concentrations of point defects. It was found that Ni atoms having less effective sizes in comparison with Al atoms tended to the formation of the above presented complexes Al atoms recombined on the structural vacancies as less mobile one. The intensivity of similar processes increases with the increase of temperature value and velocity of an impulsive deforming loading and duration of a computer experiment.

16:00 Poster G25

The Problems of the Construction of Many-Body Potentials

Mikhail D. Starostenkov, Gennadiy M. Poletaev

Altai State Technical University (ASTU), Lenin st.46, Barnaul 656038, Russian Federation

e-mail: genphys@mail.ru

One of the most important conditions of a realistic simulation of the processes taking place in metals and alloys at an atomic level is a proof description of interatomic interactions. The most wide-spread potentials at present time are many-body Finnis-Sinclair potentials and potentials, obtained by the embedded atom method. The advantage of many-body potentials in comparison with pair ones is their validity from the point of view of solid state theory. The potential energy of the system of atoms is presented as the sum of contribution of atoms pair interactions and many-body contribution identified with the energy of conductivity electrons. The use of Finnis-Sinclair potentials in the work showed that there was one essential drawback in the methods of the construction of many-body potentials. The problem is in the absence of reliable criterion to evaluate the contribution of many-body part of atoms interaction energy during the calculation of potential parameters. The only criterion that can define the contribution is the Cauchy pressure (the other characteristics can be described by a pair potential). But, the calculation values of elastic modules, as a rule, are not exactly corresponded to experimental data and the Cauchy pressure is calculated with an error. Besides, this criterion is corresponded to an ideal crystal lattice. That is why the contribution of many-body component of a structure near a defect can not be evaluated beyond all doubt. In this connection, many-body component of potential can have underestimated or overestimated contribution. In the first case, many-body potentials behave like pair potentials, and the results obtained with their use slightly differ from the results obtained by pair potentials. In the second case, metal structures tend to the increasing of coordination number (local density), sometimes even in damage to a long order of crystal because of the excessive contribution of many-body component.

16:00 Poster G26

Morphology of three-dimensional Ge nanoclusters growing on SiO_x (x<2) film

Yuriy N. Kozyrev[1], Vasilij K. Sklyar[1], Marija Y. Rubezhanska[1], Andrii V. Sushyi[1], Christian Teichert[2], Christian Hofer[2]

1. *Institute of Surface Chemistry NAS of Ukraine, 17 General Naumov, Kyiv 03164, Ukraine* **2.** *Montanuniversitaet Leoben, Franz Josef Str 18, Leoben 8700, Austria*

e-mail: kozyrev@iop.kiev.ua

Since newly elaborated optoelectronic and nanoelectronic devices require more and more small sizes of their structural components, the thickness of investigated silicon oxide layers was reduced to several nanometers. Three-dimensional Ge nanoclusters about 20 nm in height and 30 nm in the basis were prepared by molecular-beam epitaxy on initially amorphous SiO_x (x<2) film of the thickness varying from 2 to 8 nm. Their distribution density over the substrate surface exceeded 10^{11} cm^{-2}. In contrast to traditional heteroepitaxial formation of Ge quantum dots on Si(100) or growth of Si nanoclusters on SiO_x, when the correlation between the nanocluster height and lateral size is usually about b~8-10 and pronounced facets {113} are formed, in our case the nanoclusters were almost hemispherical with b~1-2.

Formation mode of three-dimensional Ge nanoclusters on initially amorphous SiO_x film is a question under discussion. Taking into consideration the fact that adhesion of Ge adatoms may be rather essential, the mechanism of 2D®3D transformation corresponds to the conditions of Stranski-Krastanov epitaxial growth realized in the presence of a lattice mismatch between the growing surface and Ge. We suppose that a large number of randomly aligned compound nanocrystallites, for example $Si_{1-x}Ge_xO_y$, can be formed on the surface in our case. The presence of oxygen in these nanocrystallites even at a low concentration may essentially enlarge the strain relaxation. That is why the forming Ge nanoclusters take a shape of hemispheres with a low b coefficient and high distribution density over the surface that is more typical to Volmer-Weber epitaxial growth.

The work has been performed in the framework of Austra-Ukrainian joint scientific and technical collaboration supported by the Austrian Academic Exchange service under project #UA05/2007. Also this work is supported by the program of fundamental investigations “Nanosystems, nanomaterials and nanotechnologies”.

Crossing frontiers in designing of bio-inspired materials - a novel breakthrough in material science

Symposium H (as a part of Symposium L)

Welcome

Although, since many decades scientists have been attracted by solutions found in nature, yet only recent developments of experimental techniques allow for designing and full characterizations of materials inspired by nature. The growing amount of results concerning studies on bio-inspired materials necessitates the exchange of ideas concerning this subject.

More and more materials scientists search their inspiration for creating new materials in nature to achieve well defined, controllable properties by design. Therefore multi-disciplinary research is focused on using and expanding fundamental understanding of the formation and hierarchical construction of biological materials such as viruses, cells, and bio-minerals (bones, teeth, seashells etc.) and the subsequent transfer of the know-how gathered in this fundamental work for materials design. Also solutions observed for animals can be used as templates for the construction of novel materials. The Symposium will attract scientists and engineers working on the design of materials inspired by nature: so-called bio-mimetic materials, which can be used for technical and engineering applications. A good example of biomimetic system is the development of motion sensors based on superficial sensor cupulae of fish for which the morphology and mechanical responses comprising the elastic modulus and retardation time were investigated. Having collected all the above mentioned information the structure and composition of living organisms can be imitated.

The potential of microscopic and spectroscopic experimental methods, which were extensively presented in the Symposium J at the E-MRS Fall Meeting 2007, should be now extended to bio-inspired materials, with the aim of promoting this novel approach in materials science.

Contributions dealing with designing and fabrication of novel bio-inspired materials for engineering applications will be presented. In this context, micro and nanoscale experimental methods such as: electron microscopy, surface probe microscopy and spectroscopy, mechanical testing as well as nanotribology allowing the full understanding of bio-inspired materials properties will be favored.

The participants are encouraged to present their most recent studies concerning transfer of solutions used and developed by nature biomimetic materials, by focusing rather on the material properties than on the biological aspects.

Organisers

Dr. Ireneusz Piwoński
University of Lodz
Department of Chemical Technology and Environmental Protection
Pomorska 163; 90-236 Lodz, Poland
Dr. Magdalena Parlińska-Wojtan
Empa Materials Science and Technology
Laboratory for Nanscale Materials Science
Ueberlandstrasse 129; CH-8600 Dübendorf, Switzerland
Prof. Vladimir Tsukruk
Georgia Institute of Technology,
School of Materials Science and Engineering &
School of Polymer, Textile, and Fiber Engineering
771 Ferst Dr., NW, Atlanta, GA 30332-0245; USA
Karolina A. Rzepiejewska-Małyska
Empa Materials Science and Technology
Materials Measurement Research Group
Feuerwerkerstr. 39
3602 Thun, Switzerland

Proceedings

The proceedings of Sympoium H will be published in JMS-Materials in Medicine or Polymers International (IF=1.5). The best papers will be published in Tissue Engineering (IF=3.7).

Programme

Monday, 15 September

Joint Poster Session I
Monday & Wednesday
Monday afternoon, 15 September, 16:00
Main Hall

Tuesday, 16 September

Session 1
as a part of Symposium L
Tuesday morning, 16 September, 9:00
Room 213

9:00 Invited oral

Functional Self-organizing Surface Structures in Biology and Engineering

Christoph Neinhuis[1], Kerstin Koch[2], Wilhelm Barthlott[2]

1. *Technische Universität Dresden, Institut für Botanik, Zellescher Weg 20b, Dresden 01069, Germany* **2.** *University of Bonn, Nees-Institute for Biodiversity of Plants, Meckenheimer Allee 170, Bonn 53115, Germany*

e-mail: christoph.neinhuis@tu-dresden.de

A thin extra cellular membrane, called the cuticle, covers all primary surfaces of plants except roots. In many species, the cuticle itself is covered by small structures composed of various lipids, usually called waxes. Their size the ranges from 200 nanometres to several micrometers. For many wax structures a crystalline nature has been proven. These wax crystals in most cases are formed by self-assembly upon the surface after individual molecules moved through the cell wall and the cuticle. AFM investigations allow demonstrating the formation processes of wax crystals on the molecular level and that the crystallisation process is highly dynamic. The epicuticular wax layer represents a multifunctional interface between the plant and its environment. Wax crystals directly influence many interactions such as the reduction of wettability or the adhesion of particles or insects. Therefore it is of interest to manufacture biomimetic technical surfaces with similar properties. By choosing suitable conditions, self-assembly of waxes can be mimicked in vitro and may be controlled by choosing substrates of variable surface properties such as polarity or crystal order. In addition, other techniques such as electrochemical approaches allow structuring large metal surfaces according to natural models again by using self-assembly. Examples for both systems will be presented and possible applications discussed.

9:30 Invited oral

Spider silk – production and processing of a fascinating biomaterial

Thomas Scheibel

Universität Bayreuth, Universitätsstr. 30, Bayreuth 95440, Germany

e-mail: thomas.scheibel@uni-bayreuth.de

Biological materials often exceed the characteristics and properties of man-made ones. One well-known example is spider silk with superior mechanical properties such as strength and toughness. During 400 million years of evolution spiders became outstanding silk producers. In contrast to insects, such as caterpillars of the mulberry moth *Bombyx mori* (commonly known as silkworms), spiders can produce different silks – orb web spiders even up to seven different ones. Orb web spiders can precisely control their production and application. Most spider silks are used for building the web, which reflects an optimized trap for flying prey.

Already thousands of years ago the excellent mechanical properties and low immunogenicity of spider webs have been acknowledged by men, employing them as fishing nets or as wound closure devices. During industrialization, attempts to breed spiders and to collect their silks have been intensified. However, large-scale farming of spiders has been quickly abandoned due to the territorial and cannibalistic behavior of most spiders.

In order to avoid such complication, we developed a bio-inspired system using bacteria as production hosts which produce silk proteins mimicking the natural spider silks. Besides the protein fabrication, we have developed a spinning technique to produce spider silk threads closely resembling natural silk fibers. Importantly, we can employ the bio-inspired silk proteins also in other application forms such as hydrogels, spheres or films.

Our bio-inspired approach serves as a basis for new materials in a variety of medical, biological, or chemical applications.

10:00 Invited oral

Oligomers isohelical to DNA: DNA-binding properties and applications for construction of nano-scaled devices

Georgy V. Gursky, Alexei M. Nikitin, Anna N. Surovaya, Victor A. Nikolaev, Natalia P. Bajulina, Michail V. Golovkin, Sergei L. Grokhovsky

Engelhardt Institute of Molecular Biology RAS (EIMB), Vavilova 32, Moscow 119991, Russian Federation

e-mail: gursky@eimb.ru

There are two possible applications of DNA as a structural material for construction of nano-scaled devices. Metallization of DNA was invented as a perspective method for the construction of conductive wires for nano-scaled electrical circuits. The DNA can also be used as a scaffold for the clamping of the DNA-binding ligands that possess appropriate electrical, optical and magnetic properties. An obvious advantage of this approach is that DNA is accessible for modification with an aid of different enzymes. Using a systematic computational search, new single-stranded and two-stranded structural motifs isohelical to double-stranded DNA were found. These motifs can be used for design and synthesis of new generations of sequence-specific DNA-binding oligomers. Isohelical oligomers that possess conjugated p electron systems can serve as conductive wires in nano-scaled devices.Template-assistant organic synthesis and photopolymerization can be used to generate very long oligomers. New strategies are developed for synthesis of sequence specific DNA -binding oligomers which recognize long DNA sequences. Bis-netropsins were synthesized which contain two netropsin-like fragments attached to a pair of peptides Gly-Cys-Gly-Gly-Gly and Gly-Val-Gly-Cys-Gly-Gly-Gly bridged by S-S bonds. These conjugates possesses a composite binding specificity: the peptide dimers recognize sites with sequences GCCG and GCCCCG on DNA, whereas the netropsin fragments bind selectively to runs of four AT-base pairs. A series of new ligands were synthesized by a modular assembly of pyrrole carboxamides and isohelical pseudopeptides of the form (XY)n . Here Y is a glycine residue; n is the degree of polymerization. X is an unusual amino acid residue containing five - membered aromatic ring (furan, thiazole, oxazole, imidazole). Studies on binding of these compounds to DNA will be reported.

Wednesday, 17 September

Session 2

as a part of Symposium L
Wednesday afternoon, 17 September, 14:00
Room 213

14:00 Invited oral

Lotus-Effect®: Biomimetic super-hydrophobic surfaces and their application

Wilhelm Barthlott, Henning Immink

University of Bonn, Nees-Institute for Biodiversity of Plants, Meckenheimer Allee 170, Bonn 53115, Germany

e-mail: immink@uni-bonn.de

Biological surfaces exhibit a large diversity of structures. Especially the cuticles of many plant species are not smooth but microstructured, often additionally covered with wax crystals in the nanometer-dimension. This combination of micro- and nanostructures, together with the hydrophobic chemistry of the waxes, produces a fascinating phenomenon defined as super-hydrophobicity: Water droplets on these surfaces exhibit contact angles exceeding 140°. Due to the reduced contact area dirt particles cannot adhere and are removed by running water. This property is called “self-cleaning”. The principles of this self-cleaning effect were successfully applied to technical prototypes. The technical conversion was patented and the trade mark Lotus-Effect® was introduced. In the mid-1990s a large cooperation project started with industrial partners. Since then several Lotus-Effect® products have been marketed: a facade paint and a rendering by Sto, a coating for glass and metal surfaces by Ferro, a spray and a nano-particle powder (Aeroxide LE®) for multipurpose applications by Evonik. In 2005 a new project linked with Lotus-Effect® got under way. It focuses on floating plants and semiaquatic animals which have surface structures enabling them to retain an air film under water. A first textile prototype based on the principles of these structures has already been developed. A major target of this project is to develop surfaces that create stable underwater air films. Such films applied in ships and pipelines result in significant drag reduction and yield considerable savings of energy. Experiments with a biomimetic prototype on the hull of a model ship showed a drag reduction of up to 10 percent. Further information: www.lotus-effect.com

14:30 Oral

Self-organised nano-dot structures on titanium surfaces with tuneable dimensions for evaluation of cell response to nano-topography

Terje Sjöström, Jason P. Mansell, Bo Su

University of Bristol, Tyndall Avenue, Bristol BS8 1TL, United Kingdom

e-mail: omxts@bristol.ac.uk

The surface topography of an implant is one of the factors determining the success of its osseointegration. Since the surface of bone tissue exhibits nano-sized topography it is of interest to fabricate similar bio-inspired topographies on implant surfaces and to understand the interaction between these surfaces and their biological surroundings. For systematic in vitro/in vivo investigation it is desirable to work with surface topography features with tuneable dimensions.

We have used a mask anodization method to create tuneable nano-sized dot features on polished titanium sheets to be used for evaluation of nano-topography effects on osteoblast-like cells in vitro. By depositing a layer of aluminium onto polished titanium samples and subsequently anodizing the aluminium, a self-organised porous alumina mask was created on top of the titanium substrate. Further anodization transferred the mask pattern to the titanium substrate resulting in dot-like nano-sized titanium oxide features beneath the alumina pores. The porous alumina mask was finally removed in a selective chemical etch to reveal the titania features. The diameters, centre-centre distances and heights of the titania dots could be varied between ~20 nm - 100 nm by changing the anodization parameters. An oxalic acid electrolyte was used for all anodizations to ensure equivalent surface chemistry. The dot size range could be further increased by using other electrolytes. The anodized surfaces have been characterized using SEM, AFM and TEM.

The formation process of the titania dots changed depending on the mounting of the aluminium/titanium samples. When titanium was exposed to the electrolyte during anodization, the titania structures were formed on top of the alumina pore bottoms and were therefore etched off the surface during the selective chemical etch of the alumina mask. Possible formation mechanisms have been discussed.

14:45 Oral

Cerium-based coating for enhancing the corrosion resistance of bio-degradable Mg implants

Wai Fong Ng, Man Hon Wong, Fai Tsun Cheng

Department of Applied Physics, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong 00852, Hong Kong

e-mail: 07900582r@polyu.edu.hk

Recently there has been interest in employing degradable metallic implants for internal fixation in bone fracture healing. The major advantage of using degradable implants is to avoid a second surgery to remove the implants when bone healing has completed. The concept is similar to that of resorbable suture. Mg, by virtue of its desirable mechanical properties, degradability, and biocompatibility, is an ideal potential candidate except that its corrosion rate *in vivo* is too high. Thus increasing the corrosion resistance of Mg is the key problem to address in the development of degradable Mg implants. One possible route is by way of surface treatment, which would lower the corrosion rate at the initial phase of bone healing, the period during which the implant provides mechanical support for the broken bone. In the present study cerium oxide coating was prepared on pure Mg by immersion or by cathodic deposition in cerium nitrate solution. The coated samples were characterized by scanning-electron microscopy (SEM) and X-ray diffractometry (XRD). The corrosion resistance in Hanks’ solution (a simulated body fluid) was studied using polarization method and electrochemical impedance spectroscopy (EIS). With properly chosen processing parameters, an adherent cerium oxide coating was formed on Mg. The corrosion resistance of cerium oxide coated Mg in Hanks’ solution at 37 °C and pH 7.4 was significantly higher than that of bare Mg.

15:00 Oral

Highly oriented dense calcium fluorapatite biomimetically grown on metal substrates

Oleksandra S. Kryzhanovska, Andrey G. Doroshenko, Yuriy N. Savin, Alexander V. Tolmachev

Institute for Single Crystals NAS of Ukraine (ISC), 60 Lenin Ave., Kharkov 61001, Ukraine

e-mail: alexkryzh@isc.kharkov.ua

Bioinspired aqueous synthesis of calcium hydroxyapatite $Ca_{10}(PO_4)_6OH_2$ and calcium fluorapatite $Ca_{10}(PO_4)_6F_2$ (FAP) is widely used for designing of dental, bone or restorative materials. One of the most actual questions in the study of bioinspired formation of nanocrystalline apatite materials is the role of physical and chemical factors in crystallographic orientation and shape evolution of crystals in biocomposite structure. Taking proper account of natural capability for selfassembly and preferred growth direction along *c* axis of apatite crystals one can use a substrate to provide highly textured dense apatite in the form of bulk material or coating, varying crystallinity and porosity of material by solution composition and experimental conditions.

The purpose of the current work is studying the effect of supersaturation, temperature and growth inhibitors on microarchitecture of inorganic material by the example of bioinspired growth of FAP crystals on 2D template in $Ca^{2+} – PO_4^{3-} – F^- – H_2O$ system.

Highly (0001) oriented polycrystalline calcium fluorapatite (FAP) on fictionalized titanium substrates is obtained. The characterization of obtained apatite material (composition, structure, crystal domain size) is performed by means of electron and X-ray diffraction, X-ray photoelectron spectroscopy, scanning and transmission electron microscopy. Texture degree is determined by means of rocking curves. Intervals of parameters of monophase fluorapatite formation are determined. It is shown that the initial step of fluorapatite formation in aqueous solution is amorphous calcium phosphate. Physical and chemical conditions required for FAP texturing during column crystals formation are determined. It is shown that lower supersaturation leads to formation of highly textured dense FAP whereas coloumn FAP structures grow at high supersaturations. It is shown that the presence of aminoacids in solution reduces density and texture of polycrystalline FAP.

15:15 Oral

Bioinspired design of $SrAl_2O_4$:Eu^{2+} phosphor

Mariya H. Kostova[1], Cordt Zollfrank[1], Miroslaw Batentschuk[2], Albrecht Winnacker[2], Peter Greil[1]

1. *University of Erlangen-Nürnberg, Glass and Ceramics, Martenstr.5, Erlangen 91058, Germany* **2.** *University of Erlangen-Nürnberg, Elctrical Engineering Materials, Erlangen 91054, Germany*

e-mail: mariya.kostova@ww.uni-erlangen.de

A cellular phosphor material based on $Sr_{0.97}Al_2O_4$:$Eu_{0.03}$ was manufactured via vacuum assisted infiltration of wood tissue (*Pinus sylvestris*) with a precursor nitrate solution. The major crystalline phase was monoclinic $SrAl_2O_4$, detected by X-ray diffraction (XRD). Due to the uniform arrangement of rectangular shaped tracheidal cells of the pine wood specimens, the nitrate solution penetrated homogeneously into the porous structure. The microstructure of the biotemplated $Sr_{0.97}Al_2O_4$:$Eu_{0.03}$ phosphor was examined by scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Energy-dispersive X-ray analysis (EDX) proved the homogeneous conversion of the wood cell wall into $Sr_{0.97}Al_2O_4$:$Eu_{0.03}$ struts. The optical properties of the resulting phosphor material were determined by photoluminescence spectroscopy (PL) at room temperature and cathodoluminescence spectroscopy (CL) in the SEM. The biotemplated $Sr_{0.97}Al_2O_4$:$Eu_{0.03}$ showed a characteristic green emission at 530 nm (2.34 eV). Shaping biomorphous $SrAl_2O_4$:Eu^{2+} phosphor with a microstructure pseudomorphous to the bioorganic template anatomy offers novel approach for designing highly oriented phosphor materials to be used in two dimensional detector arrays.

Joint Poster Session II

Poster Award Ceremony
Wednesday afternoon, 17 September, 16:00
Main Hall

Thursday, 18 September

Session 3

as a part of Symposium L
Thursday morning, 18 September, 9:00
Room 213

9:00 Invited oral

Bacilli, green algae, diatoms and red blood cells – how biology inspires novel materials in nanoarchitectural applications

Ille C. Gebeshuber

Institut fuer Allgemeine Physik, Vienna University of Technology (IAP), Wiedner Hauptstrasse 8-10/134, Wien 1040, Austria Austrian Center of Competence for Tribology (ACCT), Viktor Kaplan-Strasse 2, Wiener Neustadt 2700, Austria

e-mail: gebeshuber@iap.tuwien.ac.at

Biogenic material with functional units in the micro- and nanometer regime has already inspired novel micro- and nanotechnological applications [1].

Examples presented comprise

- scanning force spectroscopy investigations on UV-resistant bacterial spores, showing distinct differences in indentation depth to UV-sensitive spores [2],
- highly efficient biogenic single photon detectors [3],
- natural micromechanical systems made of nanostructured silica [4],
- a novel method for rapid screening of diabetes in lab-on-a-chip applications, based on nanodiagnostics on red blood cells performed with atomic force spectroscopic methods [5], and
- the application of bioinspired nanotechnology in architecture and building industry.

The outlook and discussion will deal with the possible activation of architectural elements by integration of sensing and actuation devices and nanotechnology in building technology (filters etc) and bioinspired nanotechnology still in the research stage.

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[2] Hekele O., Goesselsberger C.G., Brandstetter M., Aumayr M., Sommer R. and Gebeshuber I.C. “Atomic force microscopy and spectroscopy study of the sporulation of *Bacillus subtilis*”, under review

[3] Gruenberger C., Ritter R., Aumayr F., Stachelberger H. and Gebeshuber I.C. (2007) “Algal biophysics: *Euglena gracilis* investigated by atomic force microscopy”, Mat. Sci. Forum **555**, 411-416

[4] Gebeshuber I.C. and Crawford R.M. (2006) “Micromechanics in biogenic hydrated silica: hinges and interlocking devices in diatoms”, Proc. IMechE Part J: J. Eng. Tribol. **220**(J8), 787-796

[5] Hekele O., Goesselsberger C.G. and Gebeshuber I.C. “Nanodiagnostics performed on human red blood cells with the atomic force microscope”, under review

9:30 Invited oral

Design rules for biomimetic materials: from adhesive structures to nanocomposites

Ralph Spolenak

ETH Zurich, Wolfgang-Pauli-Str. 10, Zurich 8093, Switzerland

e-mail: spolenak@mat.ethz.ch

Geckos, spiders, flies and beetles can climb vertical walls and even adhere to ceilings. Nacre exhibits superior toughness compared to its mineral constituents. This talk will try to explore the design principles that enable the properties found in nature, reduce them to the simplest formulation possible without loosing the essence, and transfer them to potential technological structures. Fibrillar adhesive structures are investigated for optimal material (Young's modulus), size, aspect ratio and spacing. For brick and mortar structure, on the other hand, as found in nacre, a variation in building block thickness and aspect ratio is explored. Surprisingly, the parameters found in nature are very close to the theoretical optimum.

10:00 Invited oral

Peptide Nanotubes: Physical Properties and Technological Applications

Gil Rosenman

e-mail: gilr@eng.tau.ac.il

Short aromatic dipeptides can self-assemble into ordered structures at the nano-scale. These assemblies include nanotubes, nanospheres, nano-plates and hydrogels with nano-scale order (Reches, Gazit, *Science*, 2003; *Nature Nanotechology*, 2006, 2007). Peptide nanotubes (PNT) represent a novel class of nanotubes of biological origin as an appealing alternative to carbon nanotubes.

It has been observed that these biological nanostructures possess paramount properties of different origin allowing to find at the intersection Biology-Physics-Engineering new advanced nanotechnological applications using the PNT building blocks.

The basis for the new nanotechnology presented in this report is recently developed new biomolecules deposition method. It may be applied to PNT coatings on unlimited area with high density and homogeneity, controllable thickness as well for fabricating patterned PNT structures. We show in the lecture that vertically oriented PNT affords to develop new envoromentally clean nanodevices.

We found that highly oriented peptide nanotubular bioinspired structures may demonstrate new surprising physical properties such as dielectric, electrochemical, and wettability. PNT "nanoforest" creates a biomimetic "lotus-type" structure and allow observation of pronounced superhydrophobic effect which might be used for self-cleaned smart windows and solar cells.

We report on new generic PNT-based technology toward "green" energy storage devices-Supercapacitors. Deposition of PNT arrays strongly increase efficiency of these electrochemical units due to high density PNT coating. In the developed electrostatic supercapacitors aromatic vertically oriented dipeptide nanotubes have been used for modification of supercapacitor carbon electrodes. We demonstrate that PNT-modified electrodes possess much higher double-layer capacitance than that the CNT-based electrodes.

Session 4

as a part of Symposium L
Thursday afternoon, 18 September, 15:50
Room 213

15:50 Oral

Bio-inspired actuated nanostructures

Boaz Pokroy, Joanna Aizenberg

Harvard University, 12 Oxford Street, Cambridge, MA 02138, United States

e-mail: bpokroy@seas.harvard.edu

There are a multitude of examples in nature of functional materials that exhibit superior properties as compared to man-made materials. Some examples of such advanced functionality are mechanical, optical, adhesive, self-cleaning, actuation and sensing properties.

It is fascinating to observe, that the common denominator of these vast designs is the use of fibers and high-aspect-ratio nano- and microstructures. For example the superhydrophobic surface of the lotus leaf, the Gecko's sticky feet, the fiber optical properties of the Venus's flower basket sponge and there are many other examples.

We aspired to design a finely tunable, multifunctional, responsive nanostructured material that will show combined properties such as actuation/sensing, self cleaning, and be superhydrophobic as well.

Recently we developed hydrogel-muscle reversibly actuated Si nanostructures, which dynamically changed their orientation in response to humidity, with a 60 ms response time[1]. Based on this we wanted to extend this bio-inspired design and use a materials approach to develop a low-cost procedure for producing an arbitrarily-designed actuated surface with high-aspect-ratio nanostructures that are themselves responsive to a variety of stimuli and have a finely-tuned geometry and stiffness. We have used soft lithographical techniques to replicate high aspect ratio structures from epoxy and have the ability to control the geometry of the high aspect ratio nano-posts (tilt, length and 2D array lattice and symmetry) as well as to tune the stiffness of the replicated material within 4 orders of magnitude (several MPa to a few GPa). We will present our fabrication method as well as show that these bio-inspired nanostructures can be actuated by different stimuli[2].

1. Science, 2007. **315**(5811), 487-490.
2. Submitted to Advanced Materials (2008).

16:05 Oral

Bioinspired templating of ZnO with blue luminescent characteristics

Cordt Zollfrank

e-mail: cordt.zollfrank@ww.uni-erlangen.de

A novel approach for the bioinspired synthesis of hierarchical zinc oxide (ZnO) microstructures using the polysaccharide chitosan (CTS) as templating agent is presnted. The hierarchically structured ZnO was prepared from Zn(II) nitrate solutions in the presence of dissolved CTS under acidic conditions by thermal decomplexation at 50 °C for 16 h. The resulting clear suspensions showed an intensive deep-level blue emission with a peak maximum at 447 nm (2.77 eV). The excitation spectrum of the acidic ZnO/chitosan suspensions exhibited a global maximum at 370 nm (3.35 eV). The UV-Vis spectra for acidic ZnO-

CTS suspensions showed a medium absorption at 302 nm (4.12 eV) and an absorption edge at 243 nm (5.10 eV), whereas the acidic CTS solution exhibited a broad absorption with a maximum at 283 nm (4.38 eV) and an absorption edge at 215 nm (5.77 eV). After drying the prepared ZnO microstructures revealed a rod like shape with lengths varying from 1-20 µm and diameters from 0.1-2 µm observed by scanning electron microscopy (SEM). The formation of ZnO (zincite) was confirmed by X-ray diffraction (XRD). Transmission electron microscopy (TEM) confirmed that the ZnO rods were composed of individual nanosized crystallites (~5 nm). Severe beam damage of the ZnO rods suggested the intimate presence of the organic templating agent CTS.

16:20 Oral

Nanoparticle Ligand-Solvent Interactions

Alison M. Funston, Paul Mulvaney

The Univeristy of Melbourne (UNIMELB), Grattan Street, Melbourne 3052, Australia

e-mail: afunston@unimelb.edu.au

Fluorescent semiconductor nanocrystals such as CdSe have a wide range of application within biology as well as energy conversion and transduction. The key criteria for CdSe nanoparticle use in biological systems are their fluorescence quantum yield, size and aqueous stability. The surface chemistry and properties of the ligands adsorbed onto the nanocrystal surface influence all these applications, as well as allowing transfer of the particles to different solvents via specific ligand-solvent interactions.

The ligand-solvent interactions of nanocrystals may be investigated using fluorescence correlation spectroscopy (FCS). FCS is a single molecule technique within which an excitation source is focussed to a diffraction-limited spot. A confocal pinhole eliminates out of plane light resulting in the detection of fluorescence from a volume of around one femtolitre. The fluorescence from a single molecule (or in this case, single nanocrystal) diffusing through the confocal volume is able to be detected via the use of efficient photon detectors.

We report here the investigation of ligand-solvent interactions in a variety of systems. The diffusion of spherical CdSe nanoparticles functionalised with a range of bio-compatible and organic ligands have been probed via FCS, allowing their hydrodynamic radius to be determined. The effect of buffer in aqueous solution on the hydrodynamic radius will be described along with the presence of different functional groups at the ligand tail. The relationship between the hydrodynamic radius and nanocrystal size has been found to be non-linear in organic solvents for particles with small diameters, these results will be presented discussed.

16:35 Oral

QTAIM Analysis of Weak Interactions in Bio-Inspired Substances: Derivatives of the L-α-Glutamic Acid and Cyclotriphosphazene

Mikhail F. Bobrov, Mikhail A. Vantsyan, Galina V. Popova, Vladimir G. Tsirelson

D.I.Mendeleyev University of Chemical Technology of Russia (MUCTR), Miusskaya Sq., Moscow 125047, Russian Federation

e-mail: mikel@muctr.edu.ru

Cyclotriphosphazene (CTP) is used in the production of new bio-inspired smart materials and medications because of its hypotoxic and high biodegradable properties. The directed synthesis of the CTP-polypeptide derivatives, which possess the valuable properties, demands to establish the most probable structural models of these compounds and to reveal the structural features responsible for their 3D-architecture.

The models of molecular architecture of the CTP, fenoxy-CTP, amino- and carboxyfenoxy-CTP and aminofenoxy-CTP including 1, 2 and 3 molecules of L-α-glutamic acid were established by using HF/6-31G(d,p) method. Quantum-topological analysis of electron density (ED) was further performed using the ED, Laplacian of electron density and density of kinetic and potential energies. The weak C–H•••C/C–H•••π interactions and C•••C stacking interactions between the atoms of nearby fenoxy-groups were found in terms of the Bader's Quantum Theory of Atoms in Molecules (QTAIM). The C–H•••O, C–H•••N, N–H•••N and N–H•••O interactions both between the glutamic acid units and fenoxy-groups were identified as well. This system of bonded non-covalent interactions provides the observed 3D-architecture of these substances.

The authors are grateful for financial support to Russian Ministry of Education and Science (Projects 5051 and 5118).

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Posters

Monday, 15 September

Joint Poster Session I

Monday & Wednesday
Monday afternoon, 15 September, 16:00
Main Hall

16:00 Poster H01

Stability of iron-based carbon nanotubes in biological media

Nataly V. Boshytska, Olena A. Ivashchenko, Emanuil V. Priloutsky, Iryna V. Uvarova

Institute for Problems of Materials Science, National Academy of Sciences of Ukraine, Krzizanovsky, Kyiv 38(044), Ukraine

e-mail: uvarova@ipms.kiev.ua

The interaction of nanotubes with antibodies, which are used in biomedicine for diagnostic of cancer decease, has been studied. Immune system generates antibodies, as response to the appearance of foreign antigens in organism. Taking into account advantages of carbon nanotubes as antibody carriers it is necessary to investigate their corrosion stability in biological media, such as human blood plasma and digestive juice.

For safe use of nanotubes in medicine, the knowledge of their behaviour in media of living organism is very important. These media are multicomponent complex systems. For example, digestive juice contains albumens, organic and inorganic acids, mucopolysaccharides, ferments, slime, which makes difficulties in preparation of samples for analysis.

Interaction of nanotubes prepared by reduction of carbon monoxide with human blood plasma and physiological solutions (0,9 % NaCl, Ringer, Ringer - Lokk) has been studied. It was shown that carbon nanotubes containing 33 and 50 mass % of iron are stable enough both in human blood plasma and in physiological solutions. The iron concentration in human blood plasma changed slightly after the interaction.

Magnetic characteristics of carbon nanotubes and sorbtion capability towards methylene-blue do not practically change after interaction with human blood plasma.
Thus, iron carbon nanotubes with 30-50 mass % iron slightly interact with human blood plasma and can be used as advanced carriers of specific antibodies for identification of cancer center in living organism.

16:00 Poster H02

Development of methods for rapid biochemical control

Olena A. Ivashchenko, Nataly V. Boshytska, Iryna V. Uvarova

Institute for Problems of Materials Science, National Academy of Sciences of Ukraine, Krzizanovsky, Kyiv 38(044), Ukraine

e-mail: uvarova@ipms.kiev.ua

The aim of the present work was to investigate interaction of iron-based powders with model biomedia in experiments in vitro. Objects to be investigated were nanosized powders obtained by reduction of iron oxalates under various process parameters. As a reference sample, extra-purity carbonyl iron was used. The reference carbonyl iron practically contains α-iron only. The powders produced from oxalates at 400-450 oC were composed of magnetite, which corresponded to the content of total iron ~65 mass%. The powders obtained by reduction of oxalates interact with all the model media 2-3 times weaker than carbonyl iron powder, except for the interaction of the powder obtained by reduction of oxalates in a of hydrogen medium with blood plasma. In the latter case, the quantity of the removed iron ions doubles that after interaction of carbonyl iron with the same medium. Therefore, the finer powder containing α-Fe, the more rapid its dissolution in blood plasma. All of the powders studied interact with the media containing human blood plasma more intensely than with the water media. The investigations carried out make it possible to draw a conclusion that processes in media containing blood plasma differ from those in water media: in the latter corrosion processes take place whereas in the former biotransformation occurs. This indicates that to understand processes in living organism, the use of media containing blood plasma is preferable in experiments in vitro. The rate of powder dissolution in blood plasma depends on the α-iron content and powder dispersity: the higher these parameters, the more intense process of powder transformation. Fe3O4 powders are resistant enough to the action of the model biomedia. The probability of organism intoxication upon using them is lower compared to carbonyl iron powders.

16:00 Poster H03

Biosensor for pesticides detection in food

Carmen Moldovan

National Institute for Research and development in Microtechnologies (IMT-Buchares), P.O.Box 38-160, Bucharest 023573, Romania

e-mail: carmen.moldovan@imt.ro

The chemistry of a deposited enzymatic layer (AChE enzyme) has been developed (concentration, enzymatic activity measuring, deposition protocol), the immobilization technique for AChE, the fabrication technique and the electrical characteristiques of the enzymatic sensor.
The acethylcholinesterase (AChE) immobilization was performed by ionic adsorption on chitosane or polyethilenglicol (PEG) bio-polymeric substrate, by including in the gel. The method for enzyme complexation to this support is simple, being based mainly on the potential interactions between the rests of amino acids from the enzyme molecule, the cationic character and the non-solubility of chitosane at high pH values. The membrane is obtained by drying the gel in air flow and loosing of water molecules facilitates the enzyme accessibility to the support linking sites, by the interactions between the rest of polar and non-polar amino acids, ionic forces, hydrogen bridges and van der Waals forces. The advantage of this method: the enzyme immobilization is performed at room temperature, in aqueous environment, assuring an adequate homogeneity of the sample and reducing the possibility for enzyme inactivation. The sensor substrate is silicon with gold interdigitated electrodes on top. The plasma treatment in O_2 + Surface functionalization with APTS (3 aminopropiltrietoxisilan**)**, 0.1µL have been performed.

The accurately deposition and immobilization only on the surface of the working electrodes has been achieved.

The microelectrodes fabrication, the functionalization of electrodes and deposition of biomaterials ideposition will be presented. The electrodes deposited with biomaterial have been inserted into the microfluidic channels and tested from electrical and microfluidic point of view, achieving the micro/nano bio integration. Insertion of electrolyte plus choline into the channels is leading to activate the enzyme and the measurements are realized under the strict control of temperature and pH.

16:00 Poster H04

Adhesion of composite carbon-hydroxyapatite coatings deposited on 316L stainless steel

Bożena Pietrzyk, Agata Niedzielska, Jakub Gawroński

Technical University of Lodz, Institute of Materials Science and Engineering, 1/15 Stefanowskiego, Łódź 90-924, Poland

e-mail: bozena.pietrzyk@p.lodz.pl

Hydroxyapatite (HAP) is the main inorganic component of natural bones and teeth. It has attracted widespread interest due to its biocompatibility and bioactivity properties. HAP coatings are used to promote osteoconductive bonding of metallic implants with bone. One of the main problems of these coatings is the low adherence. An interesting solution of the improving adhesion of HAP coating to metallic substrate can be using carbon interlayer.

In the present work carbon-HAP bilayer coating was prepared. The carbon film was deposited on the 316L stainless steel by RF PACVD method. Next, the HAP film was prepared by sol-gel or PLD methods. These films were characterized using FTIR, EDS and microscratch adhesion testing.
It was found that carbon interlayer significantly improved adhesion of HAP to steel substrate but character of adherence was quite different in depending on deposition method: adhesive for HAP deposited by PLD method and diffusive for HAP deposited by sol-gel technique.

16:00 Poster H05

The estimation of the ability of the titanium surface on growth of bone tissue by chosen methods.

Vadim Savich[1], Mikalai Shypitsa[1], Anatoly Andreev[1], Sergey Martsev[2], Alecs Vlasov[2], Oleg Smorygo[1]

1. *Research institute of powder metallurgy, Platonova 41, Minsk 220071, Belarus* **2.** *Reserche and Production Centre of Himatology and Transfusology, Dolginovski 160, Minsk 220053, Belarus*

e-mail: shipitsa@tut.by

The aim of research work is investigation of the influence of the processing type of the titanium surface on its ability to growth of bone tissue.

The original methods for evaluating this ability, based on the optical density change and the degree and kinetics of sedimentation of sample components (proteins) for human immunoglobulin G (9%) were developed. Wetting capability by immunoglobulin solution according to the laying drop method as well as electron function for processed sample surface by scanning Kelvin probe method were investigated additionally.

It has been established that hydrothermal processing for titanium sample surface, microarc oxidation, dispersion abrasive processing with attached ultrasound oscillations provide higher adsorption and wetting capability by solution in comparison to reference sample without processing. Though jet and abrasive processing is applied in implant production for improving osteointegration effect, it decreases protein adsorption degree.

The results obtained by three above-mentioned methods correlate with each other and allow for higher degree of probability to predict expected kinetics and growth of bone tissue on titanium surface samples.

16:00 Poster H06

The Cellulose Templates for Nanostructured Oxide Fibers Ulyanova T.M., Vityaz P.A., Krut'ko N.P., Titova L.V. Institute of General and Inorganic Chemistry of NAS of Belarus

Tatyana M. Ulyanova

Institute of General and Inorganic Chemistry of NAS of Belarus (IGIC), Surganov str., 9, Minsk 220072, Belarus

e-mail: ulya@igic.bas-net.by

The aim of the present work was to investigate the formation of nanostructured alumina, zirconia, magnesia, titanium oxide, etc. powders and fibers as well as to research their crystal and microstructure.

The initial preform for oxide nanostructured fibrous materials preparation were hydrated cellulose filaments, felt and fabrics. They were impregnated with aqueous metal salt solutions and then were dried. The hydrated cellulose was chosen because it was a polysaccharide of complex architecture: the latter consisted of crystallites – microfibrilles surrounded by amorphous and crystal fields with microcapillaries and micropores. In the act of being adsorbed, the solutions were elevated via the capillary channels into the interfibrillar space and penetrated first into an amorphous, then into a crystal component of polysaccharide macromolecules. In this case, the impregnating liquid was kept by cellulose at the capillary expense, absorbing forces and chemical bond energy.

The complex processes proceed at heating of cellulose fibers containing metal salts. The adsorbed water was first removed near 100^0C. Then there took place hydrolysis of crystal hydrated salts and thermolysis of hydrated cellulose fibers, followed by the loss of chemically bound water. As a result, cellulose fibers lost gaseous and liquid organic substances, and transformed into carbon filaments, containing high-dispersed metal hydroxide and oxide grains. At temperatures 300-500^0C carbon burnt out, metal hydroxide transformed into oxide grains that were annealed each other at their contact place to form a nanostructured fibers. It should be noticed, a macrostructure of oxide fiber was similar to the initial polymer architecture (bio-mimetic phenomenon). This investigation permit purposefully develop technologies of nanostructured inorganic fibers and powders.

Functional and Structural Ceramic and Ceramic Matrix Composites (CCMC)

Symposium I

Sponsors

Frantsevich Institute for Problems of Materials Science of National Academy of Science of Ukraine

National Academy of Science of

Programme

Monday, 15 September

Opening & Plenary Session

Czochralski Award Ceremony
Monday morning, 15 September, 10:00
Small Hall (237)

Lunch break
Monday afternoon, 15 September, 12:30
Inner Courtyards

Parallel Session
Monday afternoon, 15 September, 14:00
Room 208

14:00 Invited oral

Conductive and dielectric properties of functional ceramic composites

Valeriy V. Skorokhod

Frantsevich Institute for Problems of Materials Science (IPMS), 3, Krzhizhanivsky Str., Kiev 03680, Ukraine

e-mail: dir@ipms.kiev.ua

Usually ceramic functional materials are multi-phase systems where the physical properties of isolated phases are differed greatly. For example, relatively small amounts of conductive phase as spheroid, elongate or flattened inclusions are usually added to ceramic resistive composites with dielectric non-conductive matrix. In this case difference in absolute values of electrical resistivity for matrix and such inclusions achieve 10-15 orders depending on type of conductivity and operating temperature.

For the ferroelectrics differences in the values of dielectric permeability for ferroelectric ($\varepsilon = 10^3 - 10^4$) and paraelectric impurity (ε about some units) reach 3-4 orders. Furthermore sometimes small amount of conductive phase (theoretically $\varepsilon = \infty$) are added for the increasing of dielectric permeability.

Within the framework of self-consistent field the dependence of conductivity and dielectric permeability effective values from the volume phase concentration under the condition of major difference in properties is a result of solution of simplified quadratic equation where some terms of equation are ignored. The analysis of such solutions allows qualitative evaluating of the influence of phase geometry in ceramic composite both on the effective values of its conducting and dielectric properties and on its some critical parameters determining extreme conditions of its performance.

14:30 Invited oral

Colloidal processing of nanozirconia-MWCNT composites for biomedical applications

Nere Garmendia[1], Isabel Santacruz[2], Rodrigo Moreno[2], Isabel Obieta[1]

1. *INASMET-TECNALIA, San Sebastián 20009, Spain* **2.** *Consejo Superior de Investigaciones Cientificas ICV (ICV-CSIC), Kelsen nº5, Madrid 28049, Spain*

e-mail: rmoreno@icv.csic.es

Nanocrystalline zirconia has interesting properties for biomedical applications, such as its biocompatibility and good mechanical response, but it has a major problem concerning its low temperature ageing that reduces fracture toughness. The addition of a second phase reduces ageing and improves fracture toughness. The aim of this work was to produce nanostructured materials consisting of a nanocrystalline zirconia matrix reinforced with a second phase of multi-wall carbon nanotubes (MWCNT) for biomedical applications, viz. hip prosthesis, in order to improve the mechanical properties of the material and to enhance its mean life.

MWCNT were partially coated by nanosized zirconia under hydrothermal conditions. Suspensions of zirconia with and without zirconia-coated MWCNTs were processed by a colloidal route. Dispersing conditions were studied through particle size distribution, zeta potential and rheological behaviour of concentrated suspensions in terms of pH, deflocculant content, solids loading, suspension ageing, etc. The suspensions were slip cast in plaster moulds in order to obtain homogeneous green samples. The effect of different amounts of second phase of MWCNT in the zirconia matrix was studied through the rheological behaviour of the suspensions, and the characteristics of the cast specimens, such as the density and microstructural features.

15:00 Oral

The development of components for high-temperature ceramic matrix composites

Nikolay Lyakhov, Natalya Baklanova, Va Verveno

Institute for Solid State and Mechanical Chemistry of RAS, Novosibirsk 630090, Russian Federation

e-mail: lyakhov@solis.nsc.ru

Ceramic-matrix composites (CMC’s), mainly, SiC/SiC_f or SiC/C_f are advanced structural materials that have the high strength, toughness and low density. There are three critical components to CMC’s, namely, reinforcement (carbon, SiC fiber), the interface coating and SiC matrix. The overall mechanical behavior, the environmental stability and the failure mechanisms of fiber-reinforced CMC’s are strongly influenced by the interfacial phenomena at the fiber/matrix boundary. A weakening the fiber/matrix bond is a well-established requirement in CMC’s. This is achieved through a disposal of the special coating on each carbon or SiC filament. The design and development of appropriate candidates for interphase materials and the development of the appropriate techniques for the coating deposition will be discussed in details. It is shown that SiC/SiC composites with appropriate interphases display a nonbrittle damage behavior and the extensive pull-out phenomenon is observed.

Another important component of CMC’s is SiC matrix. The results of the infiltration of SiC matrix in the fiber architecture by polymer infiltration and pyrolysis (PIP) technique will be also presented.

For many reinforcement problems a carbon monofiber is required. We received some rather promising results which demonstrate the possibility to manufacture single carbon fibers from a coke peach as a precursor. This kind of fiber may be cheap enough to use it as a corn for SiC deposition. A successful technological progress in monofiber production is necessary to provide multiple industrial applications with reinforced plastics.

Coffee break

Monday afternoon, 15 September, 15:30
Main Hall

Joint Poster Session 1

Monday & Wednesday
Monday afternoon, 15 September, 16:00
Main Hall

Tuesday, 16 September

Parallel Session

Tuesday morning, 16 September, 9:00
Room 208

9:00 Invited oral

Size-Dependent and Interface Effects in Properties of Nanocomposites

Rostislav A. Andrievskiy

e-mail: ara@icp.ac.ru

Size-dependent effects (SDE, i.e. the characteristic size influence of grains, particles, phase inclusions, layers/laminates, pores, etc., on the properties of materials and substances have been studied in physics, chemistry and materials science for a long time. The development of advanced nanotechnology manifests some new problems such as the SDE identification in nanometer interval. The SDE role in nanostructured (nanocrystalline, nanophase or nanocomposite) materials is of great importance both for fundamental considerations and modern technology. The effect of the nanoparticle/nanocrystalline size on surface energy, melting point, phase transformations and phase equilibriums is considered as applied to nanostructured materials. The role of size-dependent effects in phonon, electronic, superconducting, and mechanical properties is also analysed. Special attention is paid to the contribution of other factors such as the interface structure, grain boundary segregations, residual stresses and pores, non-uniform distribution of grain zise, and so on. The most interesting examples of the interface effect on the melting point (superheating) and strength/ductility of nanomaterials are described in detail. In particular, the importance of computer experiments and the study *in situ* of nanosubjects in high-resolution transmission electron microscopy is pointed. The little explored and unressolved problems are pointed and discussed.

9:30 Invited oral

About encyclopedic edition ”Inorganic Materials Science”

George Gnesin

Institute for Problems of Materials Science, National Academy of Sciences of Ukraine, Krzizanovsky, Kyiv 38(044), Ukraine

e-mail: geognesin@yandex.ru

This edition is generalization and systematization of modern views on scientific principles and fundamentals of inorganic material science, as well as concentrated exposition of facts about inorganic materials, their properties, production, technologies and fields of application. Author’s collective includes leading material scientists, physicists, physical chemists, mechanical scientists, which allowed covering all the fundamental and applied aspects of modern material science. The whole information block is divided into two volumes.

The first volume presents encyclopedic code of modern scientific views on physicochemical nature of solids, structure forming processes, materials behavior under the influence of external physical fields and chemical factors, as well as on inorganic materials analysis, research and diagnostics methods.

The second volume includes issues dedicated to the separate groups of materials and main production. This volume systematizes the main facts on alloys based on ferrous, non-ferrous, rare-earth, refractory, precious, radioactive metals, alkali elements; materials based on metallic compounds (borides, carbides, nitrides, silicides of transition materials and intermetallic compounds); materials based on non-metallic elements and their oxide and non-oxide compounds; glass and pyroceramics. Nanostructure and composite materials are paid special attention. This volume systematizes the facts on main inorganic materials production technologies, including metallurgical, CVD, powder, fibrous, hydrothermal, electrochemical, electrothermal, electron-beam, plasma and laser technologies, as well as materials joint technologies (welding and brazing) and high pressure technologies.

Fundamental approach to inorganic material science, stated systematically on high scientific level allows recommend this edition for scientists, engineers, post-graduates and students specialized in modern materials science.

10:00 Invited oral

The organization of international cooperation in the field of materials science

Leonid I. Chernyshev[1], Petro Smertenko[2], Jerzy Tokarski[3]

1. *Frantsevich Institute for Problems of Materials Science (IPMS), 3, Krzhizhanivsky Str., Kiev 03680, Ukraine* **2.** *EUREKA-UKRAINE, Kiev 03142, Ukraine* **3.** *EUREKA-POLAND, Warsaw 03333, Poland*

e-mail: chern@ipms.kiev.ua

Development of European Research Area (ERA) deals with some creative ideas:

- Enable researchers to move and interact seamlessly, benefit from world-class infrastructures and work with excellent networks of research institutions;

- Share, teach, value and use knowledge effectively for social, business and policy purposes;

- Optimise and open European, national and regional research programmes in order to support the best research throughout Europe and coordinate these programmes to address major challenges together;

- Develop strong links with partners around the world so that Europe benefits from the worldwide progress of knowledge, contributes to global development and takes a leading role in international initiatives to solve global issues.

The achievement of main innovation goals in ERA has to be supplied by various tools and mechanisms: first of all this is 7th Framework Program (FP7) and COST, EUREKA, European Technology Platform (ETP), Joint Technology Initiatives (JTI). Each of these programs has own tasks: for example, ETP is focused on technological directions which manage competitiveness of Europe and plays a key role in improvement of the coordination of scientific and technical priorities of EU with needs of industry. JTI follows mainly from ETP and is called to solve problems which have to be solved to achieve the planned purposes, but which can not be solved by existing tools.

Through its flexible and decentralised Network, EUREKA offers project partners rapid access to a wealth of knowledge, skills and expertise across Europe and facilitates access to national public and private funding schemes.

Individual, cluster and umbrella EUREKA projects cover practically all main scientific directions and promote collaboration between science and business.

New Eurostars Program, joint between EUREKA and FP7, is the first European funding and support programme to be specifically dedicated to SMEs and good example of synergy in ERA.

Coffee break

Tuesday morning, 16 September, 10:30
Main Hall

Parallel Session

Tuesday morning, 16 September, 11:00
Room 208

11:00 Oral

Microstructural evolution of reaction bonded boron carbide composites

Amir Weizman, Smuel Hayun, Helen Dilman, Moshe P. Dariel, Naum Frage

Ben-Gurion University of the Negev, P.O.Box 653, Beer-Sheva 84105, Israel

e-mail: amirwa@bgu.ac.il

The reaction bonding approach involves generally the infiltration of a compacted mixture of boron carbide and free carbon by liquid silicon. The reaction of molten silicon with boron carbide and free carbon particles leads to the formation of silicon carbide and the final fully dense composite consists of initial B_4C grains, newly formed $B_{12}(B,C,Si)_3$, SiC and residual Si. In the present communication, we describe a different approach for the fabrication of reaction bonded boron carbide. According to this approach, a preform, consisting of a mixture of multimodal boron carbide powders with various average particle sizes, is infiltrated with molten silicon. The preform, prior infiltration has a relatively high green density (75-80%), and the amount of the residual silicon in the final product is significantly lowered as compared to that obtained by the conventional approach. The SiC phase particles have a plate-like shape in the reaction bonded boron carbide prepared from carbon-free performs, in contrast to most SiC particles, which display a polygonal shape in the composite prepared by the conventional approach.. The reaction bonded boron carbide has a rim-core structure, which is formed in the course of a dissolution precipitation process. In samples fabricated from multi modal powder mixtures, most fine initial boron carbide particles have transformed into the new ternary $B_{12}(B,C,Si)_3$ phase, while the coarse particles are surrounded by the rim layer. A model of stoichiometric saturation, which takes into account the non-equilibrium conditions between solid and liquid solutions, was used in order to explain the microstructural evolution in the reaction bonded composites. The isothermal section at 1500^0C of the ternary B-C-Si phase diagram, calculated using the Thermocalc software, was used for predicting the chemical reactions and the equilibrium states in the course of the interaction between boron carbide and molten silicon.

11:15 Oral

The Max phases and kinking nonlinear elastic solids A newly identified class of solids

Michel W. Barsoum

Drexel University, 3141 Chestnut St, Philadelphia 19104, United States

e-mail: barsoumw@drexel.edu

The layered, hexagonal carbides and nitrides with the general formula: $M_{n+1}AX_n$, (MAX) where n = 1 to 3, M is an early transition metal, A is an A-group (mostly IIIA and IVA) element and X is either C and/or N combine some of the best attributes of metals and ceramics. Like metals, they are electrically and thermally conductive, most *readily machinable* (manual hack saw will suffice) not susceptible to thermal shock, plastic at high temperatures, and exceptionally damage tolerant. Like ceramics, they are elastically rigid, lightweight, and maintain their strengths to high temperatures. The ternaries Ti_3SiC_2 and Ti_2AlC are creep, fatigue and oxidation resistant. More recently we have also shown that the MAX phases are but a subset of solids that we termed kinking nonlinear elastic, KNE, because one of their important – and in many cases only - deformation mode is the formation of fully reversible, dislocation-based incipient kink bands, IKBs. The ramifications of these results are far-reaching. First, they identify the hysteretic mesoscopic units invoked to explain the behavior of nonlinear mesoscopic elastic solids in geology – that to date had remained a mystery – as incipient KBs. Second, they elucidate, for the first time, why graphite responds to stress the way it does; a 50 + year old problem. We further claim, and present compelling evidence, that most if not *all* solids with *c/a ratios* > 1.5 - which per force are plastically anisotropic – will deform by kinking. KNE solids include most layered solids, such as mica, $LiNbO_3$, Mg, Ti, Zn, Co, and other hexagonal metals, h-BN, GaN, MoS_2, as well as sapphire, among many others. Given the diversity and ubiquity of KNE solids it is clear that incipient IKBs play a much more important role in our daily life than has hitherto been appreciated.

11:30 Oral

Ceramic-polymer composites for medical application

Mikolaj Szafran[1], Gabriel Rokicki[1], Malgorzata Lewandowska[2]

1. *Warsaw University of Technology, Faculty of Chemistry, Koszykowa 75, Warszawa 00-662, Poland* **2.** *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland*

e-mail: szafran@ch.pw.edu.pl

Ceramic-polymer composites are widely used as dental materials and support for living cells in tissue engineering. However, they still have shortcomings limiting their application and need to be improved. In this study, a new synthesized urethane-methacrylic resin with low polymerization shrinkage and reduced oxygen inhibition was used as a component of a photocurable composite. Experimental samples were prepared from the unfilled resins by mixing with the silane-treated filler. Volumeric shrinkage and degree of conversion of the unfilled resins were examined by density measurements and FTIR spectroscopy. Filler containing samples were used for the microstructure analysis and microhardness tests. The results were compared with a commonly used Bis-GMA-based resin.

The results have shown that unfilled urethane-methacrylic resin exhibits significantly higher photopolymerization rate than the resin based on Bis-GMA. In addition, it consists of the monomers containing four methacrylic groups in a molecule and exhibits a very low polymerization shrinkage of 2,5% which is about 4 times lower than the shrinkage of a conventional Bis-GMA/TEGDMA system. The results indicate that urethane-methacrylic resin is a promising material that can be used as an alternative to Bis-GMA, mainly due to a relatively low polymerization shrinkage and low oxygen inhibition.

Polymer-ceramic composites for the tissue engineering based on a porous ceramic material consists of a porous ceramic of a mixture of hydroxyapatite and calcium phosphate, and the polymer phase, filling the pores of the ceramic material, consists of a biodegradable lactide-carbonate macromonomer which fills, to a variable degree, the pores of the ceramic base. Preliminary tests have shown that the calcium phosphate materials used are well tolerated by osteogenic human cells in *in vitro* cultures.

This work was financially supported by Ministry of Science and Higher Education: Project no. R 0802701

11:45 Oral

Preparation, properties and long-term behaviour of OCMC parts in industrial applications

Dieter Sporn, Walter Pritzkow, Reinhard Krueger, Arne Ruedinger

Fraunhofer ISC (ISC), Neunerplatz 2, Würzburg 97082, Germany

e-mail: sporn@isc.fraunhofer.de

Thin-walled OCMC parts can substitute metallic components very successfully in a number of applications where thermal loading and cycling as well as long term stability are the main issues for the choice of the suitable materials. Due to distinctly higher costs for OCMC parts the substitution of metallic parts is driven by measurable technical advantages like higher thermal stability, better behaviour under thermal cycling as well as distinctly longer life times of such components. Examples are burners, sintering aids, furnace equipment (hot zone) and hot-gas butterfly.

The OCMC parts reported here have been fabricated by using woven fiber materials like Nextel 610 that can be formed into the desired shape by using adjusted powder slurries. These slurries contain beside oxidic ceramic powders an inorganic binder which is derived by sol-gel precursors. The precursors exhibit supramolecular characteristics that allow adjusting the composition and the application conditions to the intended part fabrication as well. OCMC parts fabricated in this way show superior damage tolerance.

This paper covers the basics of the part fabrication by using the mentioned precursors and reports on the long-term behaviour of OCMC parts derived from this process.

12:00 Oral

On ways of development of new engineering ceramics

Sukyas Ordanyan[1], Vladimir Rumyantsev[2]

1. *StPSTI (STPSTI), Moskovsky, 26, Saint-Petersburg 190013, Russian Federation* **2.** *VIRIAL Ltd. (VIRIAL), Engelsa, 27, St-Petersburg 194156, Russian Federation*

e-mail: ceramic-department@yandex.ru

Any development of new ceramic materials with unique performance based on consolidation of nanosized powders could only succeed on condition of controlling the inevitable active re-precipitation processes during consolidation stage. A fairly effective way to control the grain growth and interphase formation is based on using the shielding effect of additional phases, introduced to obtain the desired parameters of the ceramic composition. Designing the heterophase ceramics one could estimate the phase compatibility either through thermodynamic calculations, or by using structural data of the component phases. The suggested classification of quasi-binary systems encompasses the co-existing refractory phases and defines the prospective 3- to 5-phase eutectics (over 500 systems). Using multi-phase sintered compositions guarantees to realize all the advantages of eutectic systems, such as lower sintering temperature and controlled evolution of the structure.

The VIRIAL Ltd. company gives practical implementation to the above ideas on potential of the multi-phase systems based on ultrafine or nanosized refractory components. A broad range of the high-performance composite systems (Me^dC-Me^dB_2, Me^dN-Me^dB_2, B_4C-Me^dB_2, SiC-Me^dB_2, AlN-Me^dN, Al_2O_3-ZrO_2, SiC-TiC-TiB_2, SiC-B_4C-TiB_2 etc.) were developed for most demanding applications, such as slide bearings and seal rings operating in corrosive and abrasive media, forming and cutting tools, and special high-temperature components. These high-performance products are manufactured commercially using the state-of-the-art machinery. Creative synergy between research and production results in high innovation tempo and development of new materials with maximally precise parameter combinations for specific technical applications.

Lunch break

Tuesday afternoon, 16 September, 12:30
Inner Courtyards

Parallel Session

Tuesday afternoon, 16 September, 14:00
Room 208

14:00 Invited oral

Features of phase transformations under low temperature synthesis of refractory compounds from mechanically activated powder mixtures

Iryna V. Uvarova

Institute for Problems of Materials Science, National Academy of Sciences of Ukraine, Krzizanovsky, Kyiv 38(044), Ukraine

e-mail: uvarova@ipms.kiev.ua

Decrease in the temperature of synthesis of refractory compounds can be achieved at the expense of acceleration of nuclei formation and diffusion processes via increasing the defectiveness of the structure of the interacting solids.

Different techniques for mechanical action on solid phase reagents which lead, on the one hand, to proceeding of mechanosynthesis reactions and, on the other hand, to decrease in the synthesis temperature and acceleration of all the process thanks to activation of diffusion processes in solid phases are considered in the present work.

In the case of proceeding of the mechanosynthesis reaction, under mechanical action formation of higher phases of refractory compounds with no intermediate products is preferable. As shown for a number of silicide and carbide systems, the mechanism of such reactions is interpreted in terms of acceleration of chemical interaction and formation of nuclei of the phase whose thermodynamic stability is determining under the process conditions.

Reduction in the tenseness (the mass ratio balls/powder) of processes of mechanical activation of reagents results only in increasing their specific surface area and defectiveness, which promotes a shift of the reaction of chemical interaction (in the case of further heat treatment) towards lower temperatures. The mechanism of these reactions is related to the determining role of diffusion processes.

Mechanical activation of a number of powder mixtures leads to activation of those reactions of solid solution formation that are not typical under usual conditions. This has been shown on the systems of solid solutions on the basis of titanium nitride in the Ti-Al-N system.

The decrease in the temperature of chemical interaction and possibility of production of refractory compounds with a particle size of about 100 nm are important results of intense mechanical action on reagents.

14:30 Oral

Gelcasting of ZTA composites using a new monomer: glycerol monoacrylate

Carolina Tallón[1], Maria Isabel Nieto[1], Rodrigo Moreno[1], Paulina Bednarek[2], Mikolaj Szafran[2], Tadeusz Mizerski[2]

1. *Consejo Superior de Investigaciones Cientfificas (ICV), Cº Valdelatas, SN, Madrid 2809, Spain* **2.** *Warsaw University of Technology, Faculty of Chemistry, Noakowskiego 3, Warszawa 00-664, Poland*

e-mail: rmoreno@icv.csic.es

Nanostructured materials with a nanosized dispersed phase have supposed a conceptual revolution in the field of ceramic-ceramic composites. The inclusion of a secondary phase, even in small quantities into a matrix allows enhancing the toughness and fracturing strength of the matrix. This is the case of the ZTA composites (zirconia-toughened alumina, ZTA) where the secondary phase of zirconia controls the matrix grain size and provides toughening through a phase transformation mechanism. In the present work, ZTA composites with 5vol% of nanosized, un-doped tetragonal ZrO_2 synthesized by freeze-drying have been prepared by an aqueous gelcasting process. Gelcasting was performed using a glycerol monoacrylate monomer synthesised in the laboratory, which allows obtaining near-net-shaped bodies with homogeneous microstructure without crosslinking agent. The stability of nanozirconia and submicrometric alumina was studied in terms of zeta potential and rheological measurements. The samples were characterized by SEM and density measurements, being the zirconia nanoparticles in the triple point between the alumina grains preventing exaggerated grain growth. Mechanical response was evaluated by indentantion tests. Composites prepared from bimodal suspensions containing nanometric and submicronic particles were studied in terms of rheological behaviour, density and microstructure and the results compared to those of the studied ZTA composites.

14:45 Oral

Fabrication of textured ceramics by colloidal processing in a high magnetic field

Yoshio Sakka

National Institute of Material Science (NIMS), Tsukuba, Japan

e-mail: SAKKA.Yoshio@nims.go.jp

The controlled development of texture is one of the ways for effectively improving properties of ceramics. We have demonstrated a new processing of textured ceramics with a feeble magnetic susceptibility by colloidal processing in a high magnetic field and subsequent heating. As colloidal processing, slip casting and electrophoretic deposition (EPD) have been conducted successfully. Requirements for obtaining textured ceramics by slip casting in a high magnetic field and sintering are as follows: (1) the particle should be single crystal and well dispersed, (2) crystal structure should be non-cubic to yield an anisotropic magnetic susceptibility, (3) magnetic energy should be larger than thermal motion energy, (4) the viscosity of the suspension should be low enough to rotate the particles with a low energy, and (5) grain growth is necessary to obtain a highly oriented structure especially when spherical particles are used. Crystalline-textured controlled laminated composites can be fabricated using EPD by varying the angle between the vectors of electric field and magnetic field. The colloidal processing in a high magnetic field confers several advantages and it is possible for this type of processing to be applied to other non-cubic ceramics, such as alumina, titania, zinc oxide, tin oxide, hydroxyapatite, aluminium nitride, silicon carbide, silicon nitride, etc.

15:00 Oral

Monosaccharides derivatives in gelcasting of ceramic powders

Mikolaj Szafran, Paulina Bednarek, Tadeusz Mizerski

Warsaw University of Technology, Faculty of Chemistry, Noakowskiego 3, Warszawa 00-664, Poland

e-mail: bednarek@ch.pw.edu.pl

High-quality, complex-shaped ceramic elements can be obtained by moulding techniques based on colloidal processes. Among these methods we can distinguish gelcasting, the method in which by means of an *in situ* polymerization, a macromolecular network is created to hold ceramic particles together. The key role in the process plays the suitable selections of an organic monomer which should be water soluble, cannot negatively influence rheological properties of ceramic slurry and must provide high mechanical strength of received green bodies. The monomer, which fulfils these requirements is acrylamide, but this compound is hazardous, and has probably cancerogenic action. In recent time acrylamide was replaced by other substances, e.g. 2-hydroxyethyl acrylate but the properties of received samples were not satisfactory. That is why new low-toxic monomers are still needful.

The interesting alternative for acrylic monomers can be compounds obtained on the basis on monosaccharides. Saccharides are water-soluble, non-toxic and due to the presence of many hydroxyl groups in a molecule, hydrogen bonds in a polymer network can be formed. As a result a cross-linked polymer network is received without adding any external cross-linking agent and obtained ceramic element is rigid enough. This fact allows reducing the quantity of added organic substances to the ceramic slurry.

The authors have synthesized monomers on the basis on glucose and fructose. One hydroxyl group in a molecule has been replaced by an acrylic group with double bond between carbons. Due to the presence of the double bond in a molecule, the compound after adding an initiator ia able to polymerize in a ceramic slurry. The monomers on the basis on monosaccharides are first of all environment friendly and can also provide high mechanical strength of received elements in the green state.

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Coffee break
Tuesday afternoon, 16 September, 15:30
Main Hall

Wednesday, 17 September

Parallel Session
Wednesday morning, 17 September, 9:00
Room 208

9:00 Invited oral

SPS fundamentals and application to manufacturing of ceramic-matrix nanocomposites

Andrey V. Ragulya

Institute for Problems of Materials Science, 3, Krzhizhanovsky, Kyiv 03142, Ukraine

e-mail: ragulya@ipms.kiev.ua

The spark plasma sintering (SPS) technique keeps the leading edge position among contemporary consolidation methods suitable for manufacturing of nanostructured materials. Conventional ceramic paradigm itself represents a combination of particulate technologies methods, which include powder synthesis stage, powder consolidation, sintering, and treatment, if necessary. This approach is quite universal, but it has a number of restrictions, mostly because of difficulties to achieve uniform component distribution in the bodies of multiphase materials. The nanocomposites represent the most promising class of bulk nanomaterials. Engineering of nanocomposites creates unlimited resources to prevent grain growth during consolidation and marry the best combination of structural and functional properties, however, their manufacturing is a challenge. Recently developed TiN-TiB_2, TiN-Si_3N_4, TiN-AlN, and other nanocomposites obtained by SPS techniques, their competitive mechanical properties will be illustrated. Numerous examples of experimental researches and characterizations of ceramic matrix nanocomposites obtained by both particle consolidation and polymer destruction methods under SPS conditions will be overviewed and potential applications of such materials described.

9:30 Oral

Spark Plasma Sintering Synthesis of Nanocrystalline Cobalt-Doped Titania

Manuela Stir[1], Radu Nicula[1], David Salamon[2], Zhijian Shen[2]

1. *EMPA Materials Research and Technology (EMPA), Feuerwerkerstr. 39, Thun 3602, Switzerland* **2.** *Department of Inorganic Chemistry, Svante Arrhenius väg 10, Stockholm SE-106 91, Sweden*

e-mail: manuela.stir@empa.ch

TiO2-based nanomaterials doped with transition metals, eg. Fe, Co, Mn etc., play an important role in modern applications like photocatalysis, magnetism or nanomedicine. We report on the synthesis of amorphous Co-doped TiO2 xerogels by solution-chemistry methods and their nanocrystallization. The structural changes of the solgel-derived nanomaterials were investigated by *in-situ* high-temperature powder diffraction using synchrotron radiation and by differential scanning calorimetry. The densification of Co-doped titania nanopowders to full density nanocrystalline bulk solids by spark plasma sintering is described in detail.

9:45 Oral

Correlation between applied pressure, properties and microstructure in pure ultrafine WC powder consolidated by Spark Plasma Sintering (SPS)

Salvatore Grasso[1,2], Yoshio Sakka[3], Giovanni Maizza[4]

1. *World Premier International Reserch Center Initiative on Materials Nanoarchitronics MANA (NIMS), 1-2-1 Sengen, Tukuba 305-0047, Japan* **2.** *Graduate School of Pure and Applied Sciences, University of Tsukuba, 1-2-1 Sengen, Tsukuba 305-0047, Japan* **3.** *National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba 305-0047, Japan* **4.** *Politecnico di Torino - Dipartimento di Scienze dei Materiali e Ingegneria Chimica, C.so Duca degli Abruzzi 24, Torino 10129, Italy*

e-mail: GRASSO.Salvatore@nims.go.jp

A combined experimental/numerical methodology is developed to fully consolidate pure ultrafine WC powder by means of Spark Plasma Sintering (SPS) operating under a current-control mode. The investigated applied pressure range from 5 to 80 MPa while the current intensity is held constant to 1400 A.

The developed SPS model employs a moving-mesh technique to account for the electro-thermal contact resistance change during shrinkage and punch sliding. The pressure dependence on the electro-thermal contact resistance is also taken into account by the model.

The experimental and numerical results clearly show the effects of pressure on the microstructure and hardness along the sample radius.

By increasing sintering pressure, complete densification was obtained reducing the peak temperature measured at die surface. By combining experimental and modeling results, a direct correlation among compact microstructure, homogeneity and sintering parameters, such as temperature and applied pressure, can be established.

10:00 Oral

Spark Plasma Sintering of Transparent Ceramics

Gilbert Fantozzi, Guillaume Bonnefont

e-mail: gilbert.fantozzi@insa-lyon.fr

Abstract

Elaboration of transparent polycrystalline ceramics is an important technological challenge because single crystals exhibit a high transparency but a low mechanical resistance. Polycrystalline ceramics have good mechanical properties. Nevertheless, in order to obtain a good transparency, the following objectives must be fulfilled:

- very low porosity (less than 0.05%) with a nanometer pore size
- for the non-cubic (birefringent) polycrystalline ceramics, the grain size must be lower than about 0.5 mm for visible light
- ceramics must be single phase materials and cannot be sintered with a liquid phase.

The tranparency needs to use very fine powders and specific sintering techniques. The nanopowders must be pure without the presence of strong agglomerates and can be doped in order to prevent grain growth. The most used sintering technique is the pressureless sintering followed by a hot isostatic pressing (HIP).

A new interesting technique can be also utilized: the spark plasma sintering (SPS).

The case of polycrystalline alumina will be particularly examined.

Commercial a-alumina nanopowder (BMA15, Baikowski Chimie, France) with a purity of 99.99%, an average particule size of about 170 nm and a surface area of 14 m2/g and doped a-alumina nanopowder with 50, 150 and 300 ppm of MgO were used.

The powders were sintered using a SPS equipment FCT HPD21 (Germany) in a graphite mold. Different temperature cycles (heating rates and sintering temperatures) have been studied.

Microstructure was observed on the fracture surface. The in-line transmission was measured with a spectrophotometer Jasco V670 as a function of the wavelength in the range 200-2500 nm.

The results are discussed as a function of the different cycles of temperature used during SPS and the effect of MgO doping is presented.

Coffee break

Wednesday morning, 17 September, 10:30
Main Hall

Parallel Session

Wednesday morning, 17 September, 11:00
Room 208

11:00 Invited oral

Nanocrystalline ceramics by spark plasma sintering of oxide nanopowders

Rachman Chaim[1], Claude Estournes[2], Zhijian Shen[3]

1. *Technion - Israel Institute of Technology, Dept. of Materials Engineering, Haifa 32000, Israel* **2.** *CIRIMAT, UMR CNRS 5085 (L2P-LCMIE), Toulouse, France* **3.** *Department of Inorganic Chemistry, Svante Arrhenius väg 10, Stockholm SE-106 91, Sweden*

e-mail: rchaim@technion.ac.il

Fully-dense bulk nanocrystalline ceramics may exhibit interesting physical properties that lack in their counterparts with conventional grain size. However, full densification of nanocrystalline ceramics is still a challenge due to the long term thermal processes. Spark plasma sintering (SPS) was used for superfast densification of ceramic nanopowders. Application of high-density dc current pulses and load lead to rapid densification of ceramic nanopowders compacts. However, significant gap exists between the technological and fabrication achievements to the fundamental understanding of the SPS mechanisms due to the complexity of the thermal, electrical and mechanical processes that may be involved. Several different mechanisms such as vaporization-solidification, plastic deformation, surface-, grain boundary-, and volume-diffusions were assumed for the sintering and densification during the SPS.

Nanopowders of MgO, YAG, Nd-YAG, and Y_2O_3 were densified using SPS at different temperature ranges, pressures and durations. Nanocrystalline MgO and YAG powders were densified to optical transparency at distinctly different homologous temperatures (0.3Tm for nc-MgO and 0.7Tm for nc-YAG). Dense Nd-YAG and Y_2O_3 specimens were translucent with micrometer and nanometer grain size, respectively. Analysis of the density and grain size evolution versus the SPS parameters (i.e. pressure, temperature, duration) showed that densification of these nanopowders proceed either by plastic deformation, grain-rotation coalescence and sliding, aided by softening of the particle surfaces or by accelerated surface diffusion. The active densification mechanism depends on the changes both in the mechanical and electrical properties of the ceramic with temperature.
Examples for the observed optical transparency and the low-temperature superplastic behavior will be presented and discussed with respect to the nanostructure character of these ceramics.

11:30 Oral

Influence of different technological conditions on the synthesis processes of TiN-TiB2 ceramic composite by spark plasma sintering method

Oleksander S. Petukhov, Igor V. Khobta, Andrey V. Ragulya

Institute for Problems of Materials Science, 3, Krzhizhanovsky, Kyiv 03142, Ukraine

e-mail: ragulya@ipms.kiev.ua

The powder mixtures TiH2+BN, TiH2+BN+TiN, TiH2+BN+B with ratios of components, corresponded to TiB2 content 20-80 wt.% in the final samples, were used as the raw materials. TiN – TiB2 ceramic composite (practically clean) with relative density 64-99 % were synthesized. The composite with TiB2 content 36-60 wt.% and properties: hardness HV=19,7-25,4 GPa (the load was P=100 g), fracture toughness K1C=5,4-5,8 MPa*m1/2 (P=20 kg) were obtained. High heating rate (42-50 °C/sec) and, consequently, simultaneous passage of dehydrogenation, synthesis and starting stage of densification leads to increasing of the properties of obtained samples with enhancement of TiB2 content. Increase of TiB2 content to 80 wt.% results in extreme heat generation, heating-up and failure of the graphite die as a result of intensification of reaction of self-propagating high-temperature synthesis between Ti and B under high heating rate and sufficient partial pressure of hydrogen. Low heating rate (2-4 °C/sec) leads to formation of the structural skeleton on initial stage of the sintering and, therefore, to final structure inhomogeneity in consequence of scin-effect. It results in increasing of obtained samples properties does not occur though considerable densification. Passing of reaction between Ti and B which has higher velocity leads to primary initial formation of TiB2 crystal lattice. Higher hardness of TiB2 (34 GPa) in comparison with TiN (25 GPa) by approximately equal melting points (3123-3220 K) results in hardness increase of formed skeleton in consequence of increasing of TiB2 content and, consequently, to decrease of density and mechanical properties of final samples.

11:45 Oral

Doping and structural features of the apatite-type lanthanum silicate in the La2O3–SiO2–Al2O3 and La2O3–SiO2–Fe2O3 systems

Tamara Kharlamova[1], Svetlana Pavlova[1], Vladislav A. Sadykov[1], Marina Chaikina[2], Tamara Krieger[1], Olga Lapina[1], Dzhalil Khabibulin[1], Arcady Ishchenco[1], Yurii Pavluchin[2], Christos Argirusis[3]

1. *Boreskov Institute of Catalysis (BIC), pr. akad. Lavrentieva, 5, Novosibirsk 630090, Russian Federation* **2.** *Institute for Solid State and Mechanical Chemistry of RAS, Novosibirsk 630090, Russian Federation* **3.** *Clausthal University of Technology, Department of Materials Science and Technology, Clausthal-Zellerfeld, Germany*

e-mail: kharlamova@catalysis.ru

Apatite-type lanthanum silicates (ATLS) are of interest as a new class of solid electrolytes with a high oxygen ion conductivity at the intermediate temperature region [1]. The flexibility of the apatite structure allows doping over a wide range of elements and compositions, providing modification of ATLS properties. However, doping possibilities for the lanthanum silicate can be limited depending on the element nature, while data on phase diagrams for such systems being scarce. This paper is devoted to the study of doping and structural features of the apatite in La_2O_3–SiO_2–Al_2O_3 and La_2O_3–SiO_2–Fe_2O_3 systems.

Samples prepared using mechanochemical activation were characterized by XRD, TEM, ^{29}Si and ^{27}Al MAS NMR, IR, Mössbauer and UV-Vis spectroscopy. The incorporation of dopants into the Si sites of the apatite structure was confirmed for all calcined samples. However, it was shown that there is a bi-phase domain in both La_2O_3–SiO_2–Al_2O_3 and La_2O_3–SiO_2–Fe_2O_3 phase diagrams at room temperature where apatite and $LaAlO_3$ or $LaFeO_3$ phases coexist, with a continuous, but limited range of solid solutions $La_{9.33+x/3+y}Si_{6-x}Me_xO_{26+3y/2}$ (Me = Al, Fe; x = 0–1.5, y = 0–0.67) with the apatite structure being formed. The limit of the Si substitution is defined by the sample stoichiometry. Thus, the content of $LaMeO_3$ for systems with the same Si/Me ratio decreases among the samples $La_{9.67}Si_5MeO_{26}$>$La_{9.83}Si_5MeO_{26.25}$>$La_{10}Si_5MeO_{26.5}$, the latter being a single-phase apatite. In turn the apatite stoichiometry determines some of its structural features. Thus, a local structure of Si was shown to depend on the amount of the cation vacancies in the apatite. The formation of [Si_2O_7] fragments in this structure [1] appears to be typical for systems with cation vacancies. The results on the study of the dopant local structure will be presented as well.

This work is supported by EC 6 Framework Program within MATSILC Project.

[1] E. Kendrick, et al. J. Mater. Chem. 17 (2007) 3104.

12:00 Oral

Two-Component Ceramic Injection Moulding (CIM) for Large-Scale Production for Railway Applications

Maciej Krystian, René Nagel

Austrian Research Centers Seibersdorf (ARCS), Seibersdorf A-2444, Austria

e-mail: maciej.krystian@arcs.ac.at

The two component Ceramic Injection Moulding (CIM) – known from two-coloured plastic parts – has been developed as a low cost and large series manufacturing technique for production of advanced complex shaped ceramic components for automotive and/or railway applications offering a high degree of structural and functional integrity. This manufacturing technique allows production of novel components with complex geometries within tight tolerances, short processing times, high degree of functionality and longer life cycles by combining two ceramic materials with different properties without additional joining steps.

The task required: adaptation of powder and powder blends properties (in regard to improved flowability); tailoring of ceramic feedstock properties (considering adjustment of simultaneous shrinking behaviour of couples of feedstocks during co-debinding and co-sintering); tool design; development of environmental-friendly debinding process of co-injected feedstocks; characterisation of green as well as sintered parts (including non-destructive testing) and – last but not least – implementation of simulation techniques of mould filling for a more flexible and cost-saving production.

Lunch break

Wednesday afternoon, 17 September, 12:30
Inner Courtyards

Parallel session

Wednesday afternoon, 17 September, 14:00
Room 208

14:00 Oral

Design principles and manufacturing approaches in carbide-carbon hetero-modulus ceramics

Igor L. Shabalin[1], Anna Biedunkiewicz[2], Urszula R. Gabriel[2]

1. *Salford University, Physics Department, Salford M5 4WT, United Kingdom* **2.** *Szczecin University of Technology, Institute of Materials Engineering, Szczecin 70-310, Poland*

e-mail: i.shabalin@salford.ac.uk

By means of the inclusion of *sp*^{2}-structured carbon phases with low Young's modulus, the properties of refractory/hard carbide ceramic matrix with high Young's modulus can be improved significantly. The application of those hetero-modulus ceramic composites is extremely effective at high temperatures. The behaviour and properties of the transition-metal carbide – carbon ceramics are mainly defined by the interface of the high-modulus matrix with covalent-bonded planes of graphite phase. The great difference in the coefficients of thermal expansion between the matrix and its anisotropic reinforcement leads to the formation of specific microstructure. The thermal shock resistance of the carbide-carbon ceramics is greatly improved in comparison with those for the single-phase carbides. This effect is observed due to the Cook – Gordon stopping crack mechanism, which is realized in carbide-carbon systems on the weak interface boundaries. The experience of recently discovered, novel temperature-pressure-dependent phenomenon, 'ridge effect' allows preparing of protective self-sintering scales on the surface of carbide-carbon ceramics to inhibit high-temperature corrosion/erosion of the material. The proposed design principles consist in searching the compositional ranges, which are met the requirements to both crack initiation and crack propagation thermal-shock-resistance criteria in particular case of exploitation of ceramics parts. The subsequent procedure resolves itself into selection of the better Pilling – Bedworth ratio for the composite to form effective coatings by means of pre-oxidizing technique. The optimization procedures can be realized only in the frame of corresponding concept of the manufacture. The previously developed methods for fabrication of carbide-carbon composite can be essentially improved due to the nanotechnological approach, in particular, advanced synthesis of carbides and application of different polymer and metallorganic precursors.

14:15 Oral

Fabrication of Ni - NiO composites from water based slurries

Mario Mora[2], Rodrigo Moreno[1], Antonio Javier Sanchez-Herencia[1]

1. *Consejo Superior de Investigaciones Cientificas ICV (ICV-CSIC), Kelsen nº5, Madrid 28049, Spain* **2.** *Instituto de Ciencia de Materiales de Aragon CSIC. Universidad de Zaragoza, Zaragoza 50018, Spain*

e-mail: ajsanchez@icv.csic.es

In order to fabricate tapes of NiO and Ni-NiO composites, water based slurries that employed mixtures of those powders are prepared with a solid content of 37 vol%. The compositional ratio of Ni-NiO vary from 100 to 40 % of Ni and 10 wt% of a latex emulsion is added as a binder in all the cases. Rheological characterization is performed in pure and binder containing slurries showing that viscosity of slurries increases with the NiO content. Green density of tapes decreases as the NiO relative content increases. Samples are sintered in air in order to fabricate NiO tapes or under flowing atmosphere to fabricate Ni-NiO composites. The 50Ni/50NiO slurry is selected to dipping experiment on traditional ceramic tiles in order to evaluate the capability to fabricate buffer coating for superconductors..

14:30 Oral

Characteristic of Al_2O_3 – Ni composites obtained by slip casting method.

Łukasz Wasilewski[1], Katarzyna Konopka[1], Magdalena Gizowska[2], Mikołaj Szafran[2]

1. *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland* **2.** *Warsaw University of Technology, Faculty of Chemistry, Noakowskiego 3, Warszawa 00-664, Poland*

e-mail: piescirogi@tlen.pl

The work deals with the study of functionally graded Al_2O_3 – Ni composites characterization. Functionally graded materials (FGM) show promising hypothesized applications such as joints between different types of materials, thermoelectric converters, graded surface coatings, graded solid oxide fuel cells, thermal barrier materials.

Al_2O_3 – Ni composites were prepared by slip casting method using powders of α-Al_2O_3 (of average particle diameter 0,4 μm and density of 3,93 g/cm^3) and nickel (of average particle diameter 2,13 μm and density of 8,9 g/cm^3). The gradient concentrations of Ni particles were obtained by gravity sedimentation of metal particles and by additional forcing the movement of Ni particles in magnetic field.

The microstructures of composites were characterised by scanning electron microscopy (SEM). Observations confirmed gradient concentration of Ni particles. The hardness test revealed the distribution of hardness in function of Ni particles gradient.

Acknowledgement:

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14:45 Oral

Phase relations and nanostructures in the oxide systems based on zirconia and hafnia with lanthanides

Olena R. Andriyevskaya

Frantsevich Institute for Problems of Materials Science (IPMS), 3, Krzhizhanivsky Str., Kiev 03680, Ukraine

e-mail: era@ipms.kiev.ua

Directly solidified ceramic eutectics and transformation toughened sintered ceramics based on stabilized zirconia and hafnia are considered advanced structural and functional ceramic materials. Binary and ternary ceramic alloys, containing hafnia, zirconia, yttria and lanthanides are crystallized forming the ultrafine structures, the grain size of which is determined by both the cooling rate and phase composition. Present work is about phase equilibria and nanostructures development resulting from the quenching of the melts and from the moderate temperature sintering.

Phase equilibria in the systems $HfO_2(ZrO_2)$-Y_2O_3-Ln_2O_3 (where Ln= La, Ce, Sm, Eu, Gd, Er) were studied in the wide range of temperatures (1100-2800 °C) and concentrations by experimental methods: X-ray diffraction, thermal analysis in air using a solar furnace at temperatures to 3000 °C, differential thermal analysis in He at temperatures to 2500 °C, microstructural and petrographic analyses, electron microscopy using melted and annealed samples and theoretical means: development of a mathematical models for the liquidus surfaces by a reduced polynomial method.

Isothermal sections of these phase diagrams at 1900, 1600, 1500, 1250, 1100 °C is created. No new phases were found. The crystallization of the alloys in the ZrO_2 (HfO_2)-Y_2O_3-Ln_2O_3 (where Ln= La, Eu, Er) systems was investigated using the data on the structure of the liquidus and solidus surfaces. The crystallization paths for the alloys and the schematic of the reactions are constructed. The equilibrium phase diagrams have been deduced. The temperature and composition of invariant phase - equilibria as well as interconnection between grain size, Ln_2O_3 content and the type polymorphous transformation were determined. The systems ZrO_2 (HfO_2)-Y_2O_3-Er_2O_3 are characterized by the formation of extended solid solutions based on F-ZrO_2(HfO_2), C- and H-Y_2O_3, Er_2O_3.

15:00 Oral

Phase diagrams of the systems Al_2O_3–ZrO_2–Ln(Y)$_2O_3$ as a scientific base for creating new high-temperature structural ceramics

Sergij M. Lakiza, Lidiya M. Lopato

Institute for Problems of Materials Science, National Academy of Sciences of Ukraine, Krzizanovsky, Kyiv 38(044), Ukraine

e-mail: sergij_lakiza@ukr.net

A search of heat-resistant materials with high strength and phase stability at temperatures above 1600 °C is actual taking into consideration the world energy and ecology crises. Up to this time there are no structural materials except directionally solidified oxide eutectics (DSE), which could be used in oxidizing environment and retain enough strength at such high temperatures.

They have many potentialities that the flexural and tensile strength are maintained right below the melting point temperature mainly due to fine phase interfaces, increased with decreasing of a characteristic dimension of the network microstructure without the reduction of creep resistance and plastically deformed over approximately up to 1550 °C. They also show a fairly good machinability and manufacturability of complex shape structural components in comparison with conventional sintered engineering ceramics.

However, low fracture toughness and thermal shock resistance originally resulted from the oxide/oxide composite are critical technical issues for a practical application.

For the further research of new eutectic composites it is still necessary to improve the materials reliability and durability. Binary to ternary and more eutectic composites are considered to be one of the possibilities to improve materials performances.
The systematic investigation of the Al_2O_3–ZrO_2–$Ln(Y)_2O_3$ phase diagrams revealed the formation of numerous alumina-rich ternary eutectics, which have similar gross composition, but consist of different set of phases. In these systems according to the participated lanthanide atom one can get three sets of ternary eutectics: $Al_2O_3/Ln_3Al_5O_{12}/ZrO_2$, $Al_2O_3/LnAlO_3/ ZrO_2$ and β-$Al_2O_3/LnAlO_3/ZrO_2$. This fact increases number of objects for directional solidification and allows choosing material with desirable set of properties for every specific utilization

Coffee break

Wednesday afternoon, 17 September, 15:30
Main Hall

Joint Poster Session 2

Wednesday afternoon, 17 September, 16:00
Main Hall

Thursday, 18 September

Parallel symposia

Thursday morning, 18 September, 9:00
Room 208

9:00 Oral

Epitaxial-like thin films of $La_5Ca_9Cu_{24}O_{41}$ grown on MgO and $SrTiO_3$ substrates using PLD.

Maria Pervolaraki[1], Ioannis Giapintzakis[1], Gabriel Socol[2], Nicolaie Stefan[2], Felix Sima[2], Carmen G. Ristoscu[2], Ion Mihailescu[2], Aurel M. Vlaicu[3], Romuald Saint-Martin[4], Alexandre Revcolevschi[4]

1. *University of Cyprus (UCY), 75 Kallipoleos Avenue, Nicosia 1678, Cyprus* **2.** *National Institute for Lasers, Plasma and Radiation Physics, 111 Atomistilor Street, Bucharest- Magurele 77125, Romania* **3.** *National Institute of Materials Physics, 105 Atomistilor Street, Bucharest- Magurele 77125, Romania* **4.** *Laboratoire de Physico-Chimie de l'Etat Solide, Université Paris-Sud, Orsay 91405, France*

e-mail: pervolaraki@ucy.ac.cy

Thermal management in electronic devices remains a challenge to this day. Materials exhibiting high thermal conductivity and still being electrical insulators are desired. Single crystals of low-dimensional quantum cuprate oxides have shown high magnetic thermal conductivity at room temperature predominately in one dimension [1]. Thin films of these materials are needed for various applications. To this end, we have been investigating the growth of $La_5Ca_9Cu_{24}O_{41}$ thin films on various substrates. In this work we will present results related to the fabrication, morphological and structural characterization of these films.

Epitaxial-like films of $La_5Ca_9Cu_{24}O_{41}$ were fabricated on MgO and $SrTiO_3$ single crystal substrates using pulsed laser deposition (PLD) at 248 nm. The target of the exotic complex oxide was ablated at a fluence of 2J/cm^2 and 10 Hz. The depositions took place at various substrate temperatures up to 800ºC and in oxygen atmosphere. The effect of substrate temperature on the quality of the thin films will be discussed.

[1] C. Hess, Eur. Phys. J. Special Topics 151, 73-83 (2007)

9:15 Oral

Y_2O_3 Thin Film Deposited by Two-step Process and Its Resistance to Halogen Plasma

Masashi Ishii, Naoki Ikeda, Daiju Tsuya, Kenji Sakurai

National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba 305-0047, Japan

e-mail: ISHII.Masashi@nims.go.jp

Y_2O_3 thin film as an inorganic plating compliant with RoHS regulations of chromium-containing materials is deposited by a two-step process, magnetron sputtering deposition of an yttrium metal and following oxidization. We discussed crystalline property and resistance to harsh environments of the films deposited by this method.

In the first magnetron sputtering deposition process, the Y metal was deposited with RF (Radio frequency) power of 30 W. The Ar process gas was used at the flow rate of 10 sccm (standard cubic centimeter per minute) and pressure in the process chamber during the deposition was fixed at 3 Pa. The substrate was (100)-oriented Si wafer. Immediately after the sputtering deposition for 30 min, the Y film was installed into a furnace and heated in the atmosphere for 30 min as the second oxidization process. From in-plane X-ray diffraction (XRD), we found that in-plane oriented Y_2O_3 was grown on the Si substrate and the (440) diffraction peak was intensified with increasing oxidization temperature up to 675°C. Above this temperature, the Y_2O_3 was translated to randomly orientated polycrystalline film. On the other hand, the deposited film using a single-step process with an Y_2O_3 target was amorphous in our experimental conditions.

We investigated resistance of the in-plane oriented Y_2O_3 film to halogen plasma. The plasma gas was CF_4 or SF_6. We compared the etching rate between the Si wafer and the Y_2O_3 film. The etching rate of Y_2O_3 and ratio to that of Si were 2 nm/min and 0.05 for CF_4, and $<$ 4 nm/min and $<$ 0.0056 for SF_6. The result indicates high resistance of the Y_2O_3 film to the halogen plasma, especially for SF_6; the Y_2O_3 film has a potential ability as a plating material to avoid erosion of an inside wall of semiconductor process chambers using halogen plasma.

This work is partly supported by Grant-in-Aid for Scientific Research (C) (19560029) from The Ministry of Education, Culture, Sports, Science and Technology, Japan.

9:30 Oral

Quenching green and enhancing red upconversion emissions of Er^{3+} by reducing tetragonality in Yb^{3+} co-doped ferroelectrics

Tung-Ching Huang, Wen-Feng Hsieh

Department of Photonics, Institute of Electro-Optical Engineering, National Chiao Tung Univ, Hsinchu 30050, Taiwan

e-mail: htc.eo92g@nctu.edu.tw

As increasing Yb^{3+} co-doped concentrations in 6 mol% Er^{3+} doped $PbTiO_3$, $BaTiO_3$, and $SrTiO_3$ polycrystalline powder samples, we have observed the room-temperature green upconversion (UC) emission at 550 nm being quenched by the simultaneously enhanced red UC emission at 660 nm under the 980-nm laser excitation. For codoping Yb^{3+} ions up to 6 mol% in $PbTiO_3$ and only Er^{3+} doped $PbTiO_3$ samples, which still possess relatively large tetragonality, the green UC emission is still much stronger than red one. In these cases, both the UC emissions are dominated by the two-photon process. But, as further increasing the Yb^{3+} ion concentration, the crystal structures tend to become cubic phase with enhancing red UC emission and almost diminishing in green emission. Since the pure $BaTiO_3$ crystal exhibits weaker tetragonality than $PbTiO_3$, the stronger red emission and weaker green one were expected at the lower codoped Yb^{3+} concentration in $BaTiO_3$ system than in $PbTiO_3$ one. The observed quench of green radiation accompanied with enhancement of red radiation should be due to the efficient energy back-transfer (EBT) process as reported by Chen, *et al.* by raising Yb^{3+} concentration [1]. The efficient EBT process requires not only level match of $^4S_{3/2}\rightarrow{}^4I_{13/2}$ in Er^{3+} and $^2F_{7/2}\rightarrow{}^2F_{5/2}$ in Yb^{3+} but also resonant match of the laser photon energy with the transitions of $^4I_{15/2}\rightarrow{}^4I_{11/2}$ and $^4I_{13/2}\rightarrow{}^4F_{9/2}$ in Er^{3+} as well as $^2F_{7/2}\rightarrow{}^2F_{5/2}$ in Yb^{3+}. As a result, declining tetragonality results in the centrosymmetric crystal field for high Yb^{3+}-ion concentration to achieve the level matches that is difficult to be fulfilled with asymmetric crystal field in ferroelectric phase.

[1] G. Chen, G. Somesfalean, Y. Liu, Z. Zhang, Q. Sun, and F. Wang, Phys. Rev. B **75**, 195204 (2007).

9:45 Oral

Application of Ti-Al-N MAX-phase for contacts to GaN

Michał A. Borysiewicz[1], Eliana Kamińska[1], Anna Piotrowska[1], Iwona Pasternak[1], Elzbieta Dynowska[2], Rafał Jakieła[2]

1. *Institute of Electron Technology (ITE), al. Lotników 32/46, Warszawa 02-668, Poland* **2.** *Polish Academy of Sciences, Institute of Physics, al. Lotników 32/46, Warszawa 02-668, Poland*

e-mail: mbory@ite.waw.pl

We report the results of studies on MAX phases [1,2] in the context of possible applications as thermally stable contact metallizations to GaN. The outstanding properties of these phases, such as good thermal and electrical conductivity, oxidation resistance, damage tolerance and thermal stability even at temperatures as high as 1000°C [2,3] as well as their hexagonal structure, make these materials promising for such applications.

The properties mentioned above are a result of the nanolaminate hexagonal structure of these compounds [1,2], which consist of: a transition metal (M), an element from group IIIA or IVA (A) and carbon or nitrogen (X). Monocrystalline MAX phase is made of MX monolayers intertwined with monoatomic A layers.

Taking into account the fact, that Ti/Al bilayer yields low resistivity ohmic contacts to n-GaN [4], our approach was to make contacts out of a Ti-Al-N MAX phase, which would improve the thermal stability of the contact system.

The conducted experiments involved: (1) depositing Ti/Al/TiN multilayers on n-GaN substrate with subsequent heat treatment in an N_2 or Ar flow in 600°C; (2) depositing Ti/Al multilayers on n-GaN substrate followed by heat treatment in a N_2 flow in 600°C. The resistivity of the metallization films was measured with a four-point probe and the ohmic contact characteristics were inferred from circular transmission line method. The samples' microstructure was characterised with High Resolution X-Ray Diffractometry and Secondary Ion Mass Spectrometry depth profiling.

This study was partially supported by the EC under the project "Materials for Robust Gallium Nitride" CP-IP 214610-2 MORGaN.

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10:00 Oral

Thermal conductivity measurement of a $La_5Ca_9Cu_{24}O_{41}$ thin film using the 3ω method.

Georgios I. Athanasopoulos, Efthymios C. Svoukis, Maria Pervolaraki, Ioannis Giapintzakis

University of Cyprus (UCY), Kallipoleos Avenue, Nicosia 1678, Cyprus

e-mail: kanenas33@hotmail.com

Through the last decades great effort has been put in the microelectronics industry on the fabrication of new devices always trying to reduce size while at the same time increasing performance and reliability. However, the increase of temperature on these devices is the main problem arising. Thus, thermal management and controlling of temperature on the devices are important issues. To address this problem, accurate thermal characterization of the materials been used is very important.

Materials like $La_5Ca_9Cu_{24}O_{41}$ have magnetic thermal conductivity (of the order of 100 W/mK at room temperature) as efficient as metallic heat conductors with the benefit of being electrically insulating. Furthermore $La_5Ca_9Cu_{24}O_{41}$ is highly anisotropic.

A possible strategy for heat dissipation is the use of a $La_5Ca_9Cu_{24}O_{41}$ thin film to guide the heat to a heat sink.

Traditional steady state methods used for thermal conductivity measurements cannot be employed on thin films due to their very small mass. A dynamic method (3ω) is therefore used.

We will present thermal conductivity measurements of a $La_5Ca_9Cu_{24}O_{41}$ thin film using the 3ω method.

Coffee break

Thursday morning, 18 September, 10:30
Main Hall

Parallel Session

Thursday morning, 18 September, 11:00
Room 208

11:00 Oral

Advanced nanoporous yttria-stabilized zirconia ceramics for luminescent oxygen sensors

Janusz D. Fidelus[1], Łukasz Zych[3], Donats Millers[2], Krisjanis Smits[2], Larisa Grigorjeva[2], Witold Łojkowski[1], Krzysztof Haberko[3]

1. *Polish Academy of Sciences, Institute of High Pressure Physics (UNIPRESS), Sokolowska 29/37, Warszawa 01-142, Poland* **2.** *Institute of Solid State Physics, University of Latvia, 8 Kengaraga, Riga LV-1063, Latvia* **3.** *AGH University of Science and Technology (AGH), al. Mickiewicza 30, Kraków 30-059, Poland*

e-mail: jdf@unipress.waw.pl

The discovered luminescence sensitivity for oxygen content in ZrO_2 and ZrO_2:Y nanopowders [1, 2] have recently become of great scientific and technological interest. There is possibility to use these materials in luminescence sensors. However the use of nanopowder for oxygen content detection meet technical difficulties. Therefore important is production of compact ZrO_2 material having luminescent properties similar to that known for nanopowders.

In the present work we discuss the results of physicochemical and luminescence investigations of yttria-stabilized zirconia nanopowders obtained by hydrothermal reaction, driven by microwave and nanoporous ceramics prepared from them.

The ceramics with Y_2O_3 contents of 3 and 8 mol % have been produced from a set of nanopowders and had open porosity within the range of 5 to 50 %. It is shown that the porosity of ceramics depend on technological process during filter-pressing followed by sintering. The porosity of ceramics provide well–developed surface thus the efficiency of processes at the surface (e.g. interaction with oxygen) could be high.

We followed luminescence properties for a number of sintered ceramics, annealed in the oxygen – nitrogen gas mixtures, with different partial pressures of oxygen. The luminescence of ceramics was compared with that of nanopowders used for ceramics sintering and annealed under the same conditions as ceramics. The differences in the luminescence spectra of those materials have been explained in connection to the number of defect types.

The work was supported by grant no. N N508 0851 33 of MNiSW granted for the years 2007 – 2009.

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11:15 Oral

Effect of inhomogeneities of nanostructural magnesium diboride and SiC adding on critical current density

Tatiana Prikhna[1], Artem Kozyrev[1], Wolfgang Gawalek[2], Yaroslav Savchuk[1], Mikhael Wendt[2], Nina Sergienko[1], Viktor Moshchil[1], Tobias Habisreuther[2], Ulrikh Dittrich[3], Sergey Dub[1], Vladimir Melnikov[1], Christa Schmidt[2], Doris Litzkendorf[2], Jan Dellith[2], Peter Nagorny[1]

1. *V. Bakul Institute for Superhard Materials NAS of Ukraine, 2, Autozavodska str., Kiev 04074, Ukraine* **2.** *Institut fuer Photonische Technologien (IPHT), Albert-Einstein-Strasse 9, Jena D07745, Germany* **3.** *Starck GmbH, Goslar 38642, Germany*

e-mail: kozyrev-a@list.ru

In materials synthesized from Mg and B taken in the magnesium diboride stoichiometry under high-pressure 2 GPa in 973 K -1373 K temperature range the inhomogeneities of size about 200 microns and below like as grains of magnesium dodecaborides and grains with higher oxygen concentration can be observed The larger amount and finer distribution of dodecaboride grains correlate with higher pinning force and higher critical current density. On the one hand, an increase of the synthesis temperature leads to a decrease of the amount of magnesium dodecaboride in the structure and on the other provokes the segregation of oxygen-enriched phase into the fine homogeneously dispersed grains, which can promote pining as well. This can explain the fact that as the synthesis temperature increases from 1073 K to 1323 K, two local maximums of critical currents at the beginning and the end of this temperature range can be observed.

The extremely high critical current densities were attained for the material with SiC added to the stoichiometric MgB_2 mixture of magnesium and amorphous boron with 0.66 % of oxygen when synthesized at 2 GPa, 1050 °C for 1 h: in zero magnetic field it reached 1.6×10^6A/cm^2 at 10 K and 1.24×10^6A/cm^2 at 20 K, was above 10^6 A/cm^2 in the fields up to 2 and 1 T at 10 and 20 K, respectively, and higher than 10^5 A/cm^2 in the fields up to 5 and 3.5 T at 10 and 20 K, respectively. The field of irreversibility at 20 KJ was higher than 8 Tand at 10 T in 10 T field the critical current density exceeded 1000 A/cm^2. By adding SiC in the amount of 10 wt % in the case of synthesis at 1050 °C (under 2 GPa) the critical current density of the material can be increased by a factor of 1.4-10 (in magnetic fields from 0 to 10 T at 10 K and in magnetic fields from 0 to 6 T at 20 K).

11:30 Oral

Radiation Defects in BCS-Superconductor MgB_2

Anatoliy Blinkin[1], Anna Blinkina[2], Valeriy Derevyanko[1], Anatoliy Dovbnya[1], Vitaliy Finkel[1], Ilya Shlyakhov[1], Tatyana Sukhareva[1]

1. *Kharkov Institute of Physics and Technology (KIPT), Akademiskaja 1, Kharkov 61108, Ukraine* **2.** *Kharkov National University, 4 Svoboda Sq., Kharkov 61077, Ukraine*

e-mail: blinkina@gmail.com

The purpose of the work is a study of the electron irradiation influence with the beam middle energy E ~ 10 MeV on the crystal structure, critical temperature T_c and the temperature dependence of the new BCS-superconductor MgB_2 resistance. In most researches the high doses of irradiation $(\sim 5\cdot10^{17} \le at \le \sim 5\cdot10^{19}\ \mathrm{cm}^{-2})$ were used. Thus the number of displacements per atom (*dpa*) can reach about 10, and T_c goes down from ~ 38 K to ~ 5 K.

Obviously, at the small irradiation doses the probability of flowing processes of point defects recombination is relatively small; in addition, the probability of point defects' appearance in sublattices of Mg and B in the elementary cell of MgB_2 can appear different. There is the potential possibility of studying the influence of disordering processes in different sublattices on MgB_2 properties in the normal and superconducting states.

We showed, that the intensities of the different diffraction lines are variously sensible to character of filling MgB_2 crystal lattice positions with the ions of Mg and B, and also with vacancies, that allows reliably to differentiate the features of crystal lattice imperfectness in the superconductor MgB_2. This circumstance opens prospects for the further study of two-gaps superconductivity nature.

On the initial stage of the irradiation ($0 \leq \Phi \cdot t \leq \sim 5 \cdot 10^{15}$ cm^{-2}) we observed strong growth of diffraction lines intensities relation (I_{110}/I_{100}) and reduction of T_c. The effect is connected with the formation of vacancies in Mg-sublattice. The decrease of I_{110}/I_{100} and T_c growth on the second stage of irradiation ($\sim 5 \cdot 10^{15} \leq \Phi \cdot t \leq \sim 1 \cdot 10^{16}$ cm^{-2}) can be bounded only with the process of the vacancies appearance in B-sublattice. And, finally, weak growth of I_{110}/I_{100} and insignificant decline of T_c on the third stage of irradiation ($\Phi \cdot t \geq \sim 1 \cdot 10^{16}$ cm^{-2}) can be provided by pending process of the simultaneous defects formation in two sublattices of the superconductor MgB_2 elementary cell.

11:45 Oral

The wettability by liquid metals and brazing processes for joining of functional perovskite ceramics

Tetiana Sydorenko, Yury V. Naidich, Oleksiy Durov

Institute for Problems in Materias Science (IPMS), 3, Krzhizhanivsky Str., Kiev 03680, Ukraine

e-mail: tvsid@ukr.net

Functional ceramic materials with especial electrophysical properties as barium titanate are attracting much interest for their application (capacitor dielectrics, resistors, thermal sensors, etc.). The strong contact of ceramic to metal is necessary in many applications. Research of interface interaction and wetting of functional $BaTiO_3$ ceramics by the melting metals was carried out. Regularity of capillary processes and control methods of them are established for 2 conditions of barium titanate: ferroelectric ($BaTiO_3$ stoichiometric compound) and semiconductor ($BaTiO_{3-x}$ structure with oxygen defect).

The wetting in the air of ferroelectric ceramics by Ag-Cu-O system was studied in this work. Furthermore, wetting processes of semiconducting $BaTiO_3$-ceramics by metals and alloys were studied in vacuum: 12 pure metals and some Ti-containing alloys (Cu-Sn-Ti, Cu-Ga-Ti, Ag-Cu-Ti). This investigation discovers that the majority of metals do not wet a surface of perovskite ceramics. Addition of chemically active component (Ti) to alloys leads to significant reduction in the contact angle for $BaTiO_3$. The microstructure of ceramics/metal contacting phases was researched.

The joining technology of $BaTiO_3$ ceramic with metals and method of coating plating with high adhesion were elaborated. The best methods of ceramic brazing and metallization base on using of active fillers in vacuum. So, standard Ag-Cu-Ti filler was used for $BaTiO_3$-ceramic metallization and the uniform coating was obtained. For some application metallization and brazing of ferroelectric $BaTiO_3$ may be preferable on the air. The metal-oxygen technology was used: mix of Ag and Cu (3 at. %) powders were painted on ceramic surface and samples were annealed at 890 °C on the air. In such conditions the solid silver powder and the eutectic liquid exists in Ag-Cu-O system. This liquid wets the ceramic and also provides the sintering of silver powder. Thus the uniform coating with strong adhesion to ceramic is forms.

11:45 Oral

Microwave sintering of electroless Ni plated SiC and Fe powders

Ahmet Yönetken, Ayhan Erol, Sabri Cevik

Afyon Kocatepe Universitesi, Afyonkarahisar 03200, Turkey

e-mail: yonetken68@hotmail.com

Ni-Fe matrix composites reinforced with SiC were produced by microwave sintering at various temperatures. A uniform nickel layer on SiC and Fe powders was deposited prior to sintering using electroless plating technique, allowing close surface contact. The formation of carbides between SiC and Fe powders is controlled through Ni layer existing on the starting powders. A composite consisting of a ceramic phase, SiC, within a matrix of Ni_3Fe and NiFe, was prepared within the temperature range 500°C-900°C under Ar shroud. Characterization of composites were carried out by XRD, SEM(Scanning Electron Microscope), compressive testing and hardness measurements were employed. Results suggest that the best properties as maximum tensile strength σ_{max} and hardness (HV) were obtained at 900°C and the microwave sintering of electroless Ni plated SiC and Fe powders is a promising technique to produce ceramic reinforced Nickel Fe composites.

12:00 Oral

The Mystery of the Great Pyramids of Egypt: A Partial Solution

Michel W. Barsoum, Alexander Moseson, Aaron Sakulich, Eva Jud

Drexel University, 3141 Chestnut St, Philadelphia 19104, United States

e-mail: barsoumw@drexel.edu

For about 4500 years, the mystery of how the Great Pyramids of Giza were built has endured. How did the Ancient Egyptians pull 70 ton granite slabs up an earthen ramp—without the benefit of wheels— 2/3 up the Great Pyramid? How did they carve granite, with pure copper? In some cases, adjacent blocks fit so well together that, even today, a human hair card cannot be inserted between them. Most important of all, to this day, Egyptologists have yet to explain how the tops of the pyramids were built. In this talk, we will present conclusive scientific evidence that a solution proposed over 20 years ago by a French materials scientist, J. Davidovits is partially correct and can answer some, but not all, the mysteries of one of the most impressive constructs of humankind. The historical, archeological, and technological implications of our conclusions to today's world are truly profound and will be touched upon.

Lunch break

Thursday afternoon, 18 September, 12:30
Inner Courtyards

Parallel Session

Thursday afternoon, 18 September, 14:00
Room 208

14:00 Oral

Characterization of nanoscale properties of the interfacial coatings on SiC reinforced fibers for CMC's

Natalya Baklanova

Institute for Solid State and Mechanical Chemistry of RAS, Novosibirsk 630090, Russian Federation

e-mail: baklanova@solid.nsc.ru

It is widely accepted that the mechanical behavior of high-temperature composite materials reinforced by SiC fibers is highly depend on the interphase between fibers and matrix. To replace the phenomenological understanding of adhesion, tribology and the interface/fracture mechanics by atomic-scale mechanisms it is necessary to investigate the nanoscopic nature of interphases. The purpose of this work is to develop and to characterize the interfacial coatings for SiC (Hi-Nicalon, Hi-Nicalon-S, Tyranno-SA) reinforced fibers for ceramic matrix composites. As interfacial coatings, the refractory oxides, including stabilized zirconia, for SiC fibers have been investigated. The surface chemistry, morphology, composition, topography, roughness, local mechanical and adhesive properties of interphases were evaluated by different analytical techniques, including SEM/EDS, TEM, XPS, XRD, AFM, micro Raman analysis. Direct apparent adhesion force mapping measurements on as-received and coated fibers were performed by AFM. The obtained results provide new insights into composite material mechanical performance.

14:15 Oral

On the estimation of defects containing materials using extended non-linear theory of elasticity

Oleksandr V. Vdovychenko, Valeriy V. Skorokhod, Mykhailo B. Shtern

Frantsevich Institute for Problems of Materials Science (IPMS), 3, Krzhizhanivsky Str., Kiev 03680, Ukraine

e-mail: ovdovychenko@yahoo.com

Ceramics/ metal matrix composites containing rigid inclusions and different kinds of damages are considered. The special attention is paid to contribution of cracks into overall response of ceramic/metal materials under the propagation of elastic waves. Based on micromechanical considerations a mathematical model of the mechanical behavior of studied materials is developed. Unlike the known models, the created one is sensitive to difference between contribution spherical and plane pores or cracks. As a result the overall response of the materials mentioned above is different for tension and compression. The dynamic behavior of these materials has been investigated in range of elastic consideration. The free oscillations of these materials were studied. The resonant frequency dependence on magnitude of oscillations that inhere to the given type of modeling materials was established. Obtained results were used to formulate a principally new method for the detection of defects in materials fabricated by ceramic technology and powder metallurgy. This technique makes possible to differ the contribution of volume pores and plane defects on the elastic properties of such materials. The method allows the estimation of the plane defects and makes possible to monitor and to control technological routes parameters for needed way of consolidation of metal/ceramics powder materials.

14:30 Oral

Modification of the composite by electron beem

Natalia Bukrina, Anna G. Knyazeva, Vladimir E. Ovcharenko

Institute of Stregth Physics and Materials Science of SB RAS, Tomsk, Russian Federation

e-mail: bookr@mail.ru

Surface modification of the composite have the feature, associating with the difference of the physical processes, running in the hard inclusions, in the matrix and on the interface. The experimental examinations indicate that at the impulse electron-beam treatment of the composite on the base of the TiC with NiCr- binder the non-equilibrium structurally phase state develop in the surface layer, supporting the change of the physical- mechanical properties of the surface layer. The kinetic regularities of the structurally non-equilibrium state formation in the surface layer of the metal-ceramic alloy during electron-beem treatment are determined by the parameters of the external action, the properties of the inclusions and matrix, and also of the character of the contact between them. The detailed experimental investigation of the non-equilibrium processes in the surface layers meets with the technical troubles. Therefore, the mathematic simulation plays the important role at the analysis of the non-equilibrium processes. The objective of present work consist in the computational investigation of the mathematical model of the surface modification of the composite. The model of the non-equilibrium surface layer formation during the electron-beam modification of the composite is suggested in this work. The features of the transport processes in the matrix and inclusions, and the interface character also are taken into consideration. The dynamics of particles solution action of in the matrix have been studied, the estimation of thermal stresses during electron-beem treatment have been carried out. For the first approximation, we use the known problems of thermoelasticity, including the exact analytical solutions for the estimation of thermal stresses for the material in different particular cases. It was shown that the character of the diffusion zone formation varies near by the vicinity of the particles, located on the different distance from the surface under treated.

Coffee break

Thursday afternoon, 18 September, 15:30
Main Hall

Friday, 19 September

E-MRS & EPDIC Joint Plenary Session

Friday morning, 19 September, 9:00

Coffee break

Friday morning, 19 September, 10:30
Main Hall

Parallel Session

Friday morning, 19 September, 11:00
Room 208

11:00 Invited oral

Reliability of oxide matrix composites

Zbigniew Pędzich

AGH University of Science and Technology, Faculty of Materials Science and Ceramics (AGH UST), Mickiewicza 30, Kraków 30-059, Poland

e-mail: pedzich@agh.edu.pl

The work presents results of investigations on reliability of sintered particulate composites with alumina or zirconia matrix. These oxides are basic structural materials widely applied in engineering.

The reliability analysis were made in two aspects – the resistance on subcritical crack growth

and dispersion of bending strength in meaning of the Weibull statistic.

Generally, the investigations result showed that manufacturing of composites on the base of mentioned oxides could profitably influence mechanical properties. However, potential reliability improvement wasn't obvious, and its scale could change in very wide range.

The potential property improvement could be particularly significant in composite systems with alumina matrix. The scale of property improvement in zirconia matrix composites was limited (when compared with results for alumina matrix).

The scale of property improvement mainly depended on kind, amount and dispersion of strengthening phase. The change of these parameters was effective in differentiation such composite parameters as: the matrix grain size (the Zener effect), the inclusion agglomeration ratio or the interphase boundary state. The mentioned factors influenced potential size and size distribution of critical flaws what determined the Weibull statistic of composites.

One couldn't omit important role of residual stresses in composites. These stresses are generating by the mismatch of thermal expansion coefficients of constituent phases in composites. Locally, the value of these stresses could be significant, comparable with the bending strength of investigated materials. Such stresses, their value and character (tension or compression) were also very important for resistance on subcritical crack growth.

But, this feature was mainly influenced by the presence of a new category of grain boundaries – the interphase boundaries. They substantially changed the way of degradation of grain boundaries under subcritical loading.

11:30 Oral

The effective Poisson ratio of two-phase composites

Willi Pabst, Eva Gregorová

Institute of Chemical Technology (VSCHT), Technicka 5, Prague 16628, Czech Republic

e-mail: pabstw@vscht.cz

The effective Poisson ratio of three-dimensional two-phase composites is discussed from the theoretical point of view. It is shown that – in contrast to porous materials – the Voigt-Reuss and Hashin-Shtrikman (or Walpole) bounds for the bulk and shear modulus impose certain restrictions beyond the general condition that the Poisson ratio must be in the range between – 1 and + 0.5. Here, the conditions for auxetic behavior (occurrence of negative Poisson ratios) are investigated. It is found, that a two-phase composite of non-auxetic phases (i.e. phases with phase bulk moduli higher than the phase shear moduli) may be auxetic, when the phase contrast (ratio of the phase bulk and shear moduli) is sufficiently high. In particular, it is shown that even composites with two phases of the same Poisson ratio (i.e. the same bulk-to-shear modulus ratio) can have a negative effective Poisson ratio (i.e. exhibit auxetic behavior) when the phase contrast is higher than 3.8 for anisotropic materials or higher than 8.6 for isotropic materials. For a given set of phase bulk and shear moduli the minimum Poisson ratio of the composite and the corresponding composition can be predicted, and this information may be exploited in materials design to produce auxetic materials. Examples of actually or potentially auxetic material combinations are given, together with the minimum Poisson ratio that can be achieved in these systems. The special case of porous materials (extreme case with infinite phase contrast) is briefly discussed as well, together with the microstructural features to achieve auxetic behavior (reentrant-corner, node-fibril and rotating-hinge microstructures). On the other hand, when the phase contrast is small, such as in densely sintered ceramics (e.g. pore-free alumina-zirconia composites), auxetic behavior principally cannot be achieved, and in these cases the effective Poisson ratio is well predicted by simple relations, including the mixture-rule approximation.

12:00 Invited oral

Estimation of crystallographic defects density in ceramics from ESEM/EBSD data

Krzysztof Sztwiertnia[1], Marek A. Faryna[1], Henryk Tomaszewski[2]

1. *Polish Academy of Sciences, Institute of Metallurgy and Materials Sciences (IMIM PAN), Reymonta 25, Kraków 30-059, Poland*
2. *Institute of Electronic Materials Technology (ITME), Wólczyńska 133, Warszawa 01-919, Poland*

e-mail: nmfaryna@imim-pan.krakow.pl

Several properties of materials depend, to a large extent, on the character and distribution of crystallographic defects. This paper proposes a method to estimate the density of these defects at defined points of the sample, based on quantitative Electron BackScatter Diffraction (EBSD) data analysis in Environmental Scanning Electron Microscope (ESEM). The principle of the method is based on the effect of the diffraction lines broadening at each point where the local density of defects rises. The work presents a few examples of analysis of alumina and zirconia ceramics, which surfaces were deformed by shoot pining. The method appears easy to be for implementation, provided that several conditions, discussed in the paper, are met.

Lunch break

Friday afternoon, 19 September, 12:30
Inner Courtyards

Abstracts

in author alphabetical order

Invited oral

Some Facts about Mechanical Properties of CMC

Roman Pampuch

AGH University of Science and Technology, Department of Ceramics Technology (AGH), Kraków, Poland

e-mail: roman.pampuch@neostrada.pl

It has been shown that, similarly, to monolithic ceramics, a great collection of data for particulate CMC present statistrically significant linear relationship between fracture toughness and bending strength. Up to a formation of particle clusters (often coinciding with the percolation threshold) three types of property changes with the volume fraction of dispersed particles is found. Namely, the increase of fracture toughness alone without strength changes (found usually on dispersion of borides in various matrices), the simultaneous increase of toughness and strangth (typical for alumina-zirconia composites), and the strenght increase with no significant changes of fracture toughness (example, aluinina-silicon carbide CMC) . The occurrence of these cases may be rationalized by considering residual stress fields in the composites.

Posters

Monday, 15 September

Joint Poster Session 1

Monday & Wednesday
Monday afternoon, 15 September, 16:00
Main Hall

16:00 Poster I01

Gelcasting in moulding of ceramic powders with application of new monomers

Paulina Bednarek, Mikolaj Szafran, Tadeusz Mizerski

Warsaw University of Technology, Faculty of Chemistry, Noakowskiego 3, Warszawa 00-664, Poland

e-mail: bednarek@ch.pw.edu.pl

In fabrication of ceramic elements widely applied methods are still injection moulding and slip casting, but both techniques have serious limitations. In order to overcome these limitations the colloidal processes are investigated. One of the extensively studied forming method is gelcasting, which combines conventional moulding from slips with polymer chemistry. Gelcasting process allows obtaining high-quality, complex-shaped ceramic elements by means of an *in situ* polymerization, through which a macromolecular network is created to hold ceramic particles together.

The key role in the process plays selection of a suitable monomer, which is able to provide high mechanical strength of a gelled part. The applied monomers must perform a series of conditions: they must be water soluble, non-toxic and high mechanical properties must be achieved by as low as possible concentration of a monomer in a ceramic slurry.

For many years commonly applied monomer in gelcasting method was acrylamide, which has probably cancerogenic action, therefore recently acrylic monomers, such as 2-hydroxyethyl acrylate started replacing hazardous acrylamide.

The research made by authors concentrate on the synthesis and application of new water-soluble and non-toxic monomers on the basis of monosaccharides. The presence of many hydroxyl groups in a monomer molecule allows forming hydrogen bonds in a polymer network. As a result a cross-linked polymer network is received and no external cross-linking agent is necessary to obtain a rigid ceramic part. This fact allows reducing the quantity of added organic substances to the ceramic slurry and the amount of gases released to the atmosphere during polymer burnout.

This work was partially financially supported by Faculty of Chemistry Warsaw University of Technology: Project no. 504G/1020/0787

16:00 Poster I02

Investigation of compaction of diatoms by die pressing and slip casting method

Katarzyna Konopka[1], Mikołaj Szafran[2], Ewa Bobryk[2], Anna Danelska[2]

1. *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland* **2.** *Warsaw University of Technology, Faculty of Chemistry, Noakowskiego 3, Warszawa 00-664, Poland*

e-mail: kako@inmat.pw.edu.pl

Our introductory investigations were carried out on molding and sintering of diatomite materials. Two different types of diatomite material were used for this purpose – crystalline diatoms (specific surface BET = 1,52 m^2/g) and amorphous diatoms (specific surface BET = 8,76 m^2/g). The aim of this research was to elaborate a suitable method for obtaining dense sinters with preserved nanoporosity, which is typical for such materials. Two methods of molding were applied –die pressing at the pressure ranges 25 – 50 MPa with usage of different binders and a slip casting in gypsum mold with an array of various deflocculants and organic binders employed. Sophisticated and extraordinarily diversified forms of powder particles are not conducive to its densification. Slip casting made from diatoms reveals significant thixotropy and sedimentation. Moreover, there are also difficulties with powders molding, especially concerning amorphous diatoms. Open porosity and the rate of density were measured for the samples, which were sintered in the temperature range from 1000 to 1400ºC. The microstructure of aforesaid samples was analyzed by Scanning Electron Microscope.

This work was financially supported by Ministry of Science and Higher Education:Project no. N507438834

16:00 Poster I03

Ceramic Composites With SiC Matrix Produced By Liquid Silicon Infiltration Process For Frictional Applications

Victor I. Kulik[1], Alexey S. Nilov[1], Anatoliy P. Garshin[2], Vadim Savich[3], Nikolay A. Shipitsa[3], Alexandr P. Ilyuschenko[3], Alexandr A. Dmitrovich[3]

1. *Baltic State Technical University (BSTU), 1st Krasnoarmeyskaya st. 1, Saint-Petersburg 190005, Russian Federation* **2.** *St.-Petersburg State Polytechnical University, Saint-Petersburg 194064, Russian Federation* **3.** *Research institute of powder metallurgy, Platonova 41, Minsk 220071, Belarus*

e-mail: victor.i.kulik@gmail.com

The present work is on production of silicon carbide-based ceramic matrix composites (CMC) reinforced with carbon fibers, the so called C_f/SiC-composites. Because of the extreme hardness and high abrasion resistance of SiC such CMCs belong to the most promising advanced materials for frictional applications. In particular C_f/SiC-composites-based brake disks and pads for passenger cars have been developed in the last few years. An efficient way to obtain C_f/SiC-composites is a methods based on Liquid Silicon Infiltration (LSI) process. In this work the production of the C_f/SiC-composite involved forming the C_f-reinforced plastic preforms from chopped carbon fibre and phenolic resin, carbonization of the perform to produce C_f-reinforced coke matrix (C_f/C-composite) with subsequent perform siliconizing by silicon melt. The phenolic resin contained powdered carbon, silicon carbide and other fillers. Different CMC samples were produced with varying composition and ratio of initial components. The obtained CMC samples were characterized for their residual porosity, composition, microstructure, mechanical and tribotechnical prameters. Mechanical tests were used to determine the flexural strength and fracture toughness of the CMCs. Tribotechnical parameters (coefficient of friction and wear) were measured on the inertial stands which allow carrying out tests of frictional materials by the “plane-plane” scheme in conditions maximally close to real friction centres (frictional coupling, braces, clutches and etc.). Tribotechnical tests of C_f/SiC-composite have been carried out in combination with different riders. The correlation between the initial composition of the composite and its microstructure, physical-mechanical and tribotechnical properties is found and discussed.

16:00 Poster I04

Experimental And Theoretical Study of CVI Process Production of Composites With SiC Matrix From Methylsilane

Victor I. Kulik[1], Mark S. Ramm[2], Alexey V. Kulik[1], Yuri V. Zagashvili[1], Natalia L. Vetkina[1], Andrey M. Abysov[3], Eugene A. Bogatchev[4], Anton V. Lakhin[4], Anatoliy N. Timofeev[4]

1. *Baltic State Technical University (BSTU), 1st Krasnoarmeyskaya st. 1, Saint-Petersburg 190005, Russian Federation* **2.** *Reseach-and-production company Ceracom Ltd, Saint-Petersburg 190005, Russian Federation* **3.** *Saint-Petersburg State Technological Institute, Saint-Petersburg 190013, Russian Federation* **4.** *JSC Kompozit, Korolev 141070, Russian Federation*

e-mail: victor.i.kulik@gmail.com

Chemical Vapor Infiltration (CVI) is one of the most promising methods for production of high-quality CMCs. To fabricate CMC with SiC matrix, different precursors are currently used. Methylsilane (CH_3SiH_3) is now considered as an alternative to haloid precursors. Principal advantages of methylsilane (MS) are: (1) environmental safety of the process due to absence of chlorine and chemical stability of MS at room temperature; (2) lowering of the process temperature down to 650-800 °C, which allows densification of preforms made from nonrefractory metals and low-temperature ceramics. One of the most important problems in CVI research is finding the optimal technological parameters providing minimal infiltration time and required quality. A possible way of solving these problems is in combination of experimental study and numerical simulations. In the present work, 1D modelling of isothermal CVI for MS precursor was used to describe phenomena in the porous preform. Porous medium of such preform includes many pore systems with different scales. The mathematical model of the preform densification included description of gas mixture transport inside these pore systems, SiC deposition kinetics, and evolution of porous medium. Species transport is simulated accounting for diffusion and convection (including phase transition-induced convection). In this work, we analysed the influence of the CVI operating conditions on distributions of species concentrations and pressure along the preform thickness during the process as well as on the process duration, average residual porosity and distribution in the preform of the residual porosity. Besides, the present work reports on the experimental research of such preforms densification by isothermal CVI. Experimental process was studied at different temperatures. The obtained CMC samples were characterized for their composition, microstructure and residual porosity. Computational results are compared with experimental observations.

16:00 Poster I05

Modeling and Automation of Pressing Processes in Powder Metallurgy

Viktor Lyashenko[1], Mykhaylo V. Zagirnyak[1], Tetyana Hryhorova[1], Damijan Miljavec[2]

1. *Kremenchuk State Polytechnical University, Kremenchuk, Ukraine*
2. *University of Ljubljana, faculty of mathematics and physics (FMF), Jadranska 19, Ljubljana 1000, Slovenia*

e-mail: gasta1@yandex.ru

Modeling of hot-pressing processes of metal powder materials together with organic plasticizer is considered. The balance equation of substance in a container during the pressing process has been chosen as a mathematical model. In this case, pressure applied to the powder in the container during the pressing process is the reason for concentration change. A thermal conductivity equation has been solved together with balance equation of substance. The joint solution for the balance equation and the thermal conductivity equation with relevant edge conditions has been found. As the equations are non-linear, their joint solution is made by a numerical method. An algorithm which provides getting a solution of as high accuracy as it is desired has been made. A control system of hot-pressing process taking two stages has been developed. At the first stage an insignificant thickening of metal powder, till a compact product is formed, and diffusion of the plasticizer around grains edges take place. At the second stage the product being pressed is thickened till it forms a solid composite. During the pressing process temperature and pressure control is performed with corresponding sensors. Pressing is carried out in automatic mode according to algorithm pre-developed on the basis of equations solution. Pressing of soft magnetic material based on iron has been made. The X-ray spectrum analysis of specimens of obtained soft magnetic composites showed that the electric isolation layer is spread uniformly across the grain surface and magnetic loss is low, when these composites are used in electric devices.

16:00 Poster I07

Layer by Layer Laser Synthesis of 3D Ceramic MEMS from Oxide Powder Mixtures.

Igor V. Shishkovsky[1], Yuri G. Morozov[2], Maxim V. Kuznetsov[2]

1. *P.N. Lebedev Physics Institute of RAS, Samara branch, Novo-Sadovaja st. 221, Samara 443011, Russian Federation* **2.** *Institute of Structural Macrokinetics and Materials Science, Russian Academy of Sciences, Chernogolovka 142432, Russian Federation*

e-mail: shiv@fian.smr.ru

The experimental researches of possibility of layer-by layer laser synthesis of 3D ceramic MEMS via the SLS of powder exothermal mixtures traditionally used in technology of SHSare described. In our researches it was accomplished firstly possibility of overlapping of SLS and SHS processes. It haveallowed to receive not only stronger material copies of 3D items of the complexshape, but also to expand the functional characteristics of these three-dimensional objects at the expense of synthesis of new porous phases (piezo- ceramics, ferrites, high-temperature superconductivity etc.). Moreover, the external laser influence is not come only to an additional thermal heating of a reaction mixture. We are considering that the uses of laser radiation approach is very promising, as one of ways of implementation of such resonant condition.

At the stage of computer modeling at the CAD/CAE level, there are open perspectives of subsequent reproduction of smart 3D structures via SLS. These materials can find their application in the aerospace, chemical, and nuclear power industry. In this case, an SHS reaction is only initiated within a spot of focused laser beam that is scanned over the surface of a powder mixture until formation of a desired computer-designed configuration. At present study, our experimental results by SLS have been described for the following SHS oxide systems:

· mixture of oxides for synthesis of ceramics: TiO_2 + ZrO_2 + PbO, $Al(Al_2O_3)$ + $Zr(ZrO_2)$;

· mixture of oxides for synthesis of ferrites: BaO_2 + Fe_2O_3 + Cr_2O_3 + Fe, Li_2CO_3+ Fe_2O_3+Cr_2O_3+Fe.

· high-temperature superconductivity oxide ceramics $YBa_2Cu_3O_7$, $SrFe_{12}O_{19}$.

Optimization of the process of 2D and 3D computer-aided prototyping is discussed with emphasis on synthesis of 3D parts. It was emphasized, that PZT and ferrites systems are more perspective for synthesis of functionally graded tools and MEMS.

16:00 Poster I08

Ceramic composites from nanostructured powders

Tatyana M. Ulyanova, Krutko Ni, Titova Lu, Paemurd Eu

Institute of General and Inorganic Chemistry of NAS of Belarus (IGIC), Surganov str., 9, Minsk 220072, Belarus

e-mail: ulya@igic.bas-net.by

It is known at temperatures above 1500^0C the triple solid solutions of zirconia stabilized by alkali-earth metals have been degraded. These phenomena reduce the strength properties of ceramics. It was logical to assume an increase of physical-mechanical properties of the composite materials prepared from nanostructured refractory oxides powders.

The present work is devoted to research of interaction of oxide nanostructured powders in the triple systems Al_2O_3-ZrO_2-MgO and Al_2O_3-ZrO_2-Y_2O_3, and an influence of composition and production method on structure and properties of composite refractory ceramics.

For preparation of composites two methods were used. In the first way earlire prepared three-component nanostructured fibers were crushed, graded on fractions and were formed by a static pressure. On the second way three-component powders were prepared by sedimentation of gel hydroxide of aluminium with simultaneous introduction in gel the synthesized fibrous nanostructured powders partially stabilized (MgO) zirconia. The samples were pressed and annealed in oxidizing atmosphere at the temperatures from 100 up to 1600^0C. Then structure and physical-mechanical properties of ceramic samples were investigated. Due to high dispersity and reactivity of nanostructured powders at the 550-600^0C from metal oxides the triple solid solutions were formed which strengthened the composite. Density annealed at the 1600^0C ceramic samples of partially stabilized zirconia (PSZ) and composite powder of 80 % PSZ : 20 % Al_2O_3 amounted 5,96 and 5,54 g/cm^3, it's value went down up to 4,2 g/cm^3 with increasing in content Al_2O_3 to 80 mas. %. The open porosity did not exceed 0,2 – 0,4 %. The fibrous oxide three-component powders can be used as fillers for composites and dense ceramics.

16:00 Poster I09

Water-thinnable poly(urethanecarbamide) dispersions in die pressing of alumina

Paweł Wiśniewski[1], Janusz Kozakiewicz[2], Anita Koncka-Foland[2], Mikołaj Szafran[1], Gabriel Rokicki[1]

1. *Warsaw University of Technology, Faculty of Chemistry, Noakowskiego 3, Warszawa 00-664, Poland* **2.** *Industrial Chemistry Research Institute (ICRI), Rydygiera 8, Warszawa 01-793, Poland*

e-mail: pawelwi@ch.pw.edu.pl

In ceramics technology, different polymeric binders with various chemical structure are applied for different molding methods. A narrow range of water-soluble organic binders, such as poly(vinyl alcohol) and poly(oxyethylene glycol) are most often used in die pressing method. The samples obtained with these binders mentioned are characterized by a relative small density and small mechanical strength before and after sintering.An organic binder is very important additive in the dry pressing process of ceramic powders. It must attend many demands such as miscibility with ceramic powder, low toxicity, low burnout residue, sufficient suitable glass transition temperature, must assure high green density, suitable green strength etc.In the die pressing the most important problem is to determine the binder system providing high mechanical green strength and high green density. The green density depends on granules packing and it determines the final density after sintering.Such polymeric dispersions should, at their minimal amount, cause a decrease the friction forces between the ceramic powder particles and between the ceramics powder particles and matrix, providing a high mechanical strength of green samples. The content of organic binders should not exceed 0.5-3% wt.% with respect to alumina powder.Due to small numbers of accessible water-thinnable polymeric binders studies have been undertaken on the application in the ceramics technology of specially synthesized poly(urethanecarbamide) binders characterized by different chemical structure, contained oligooxosilanediol in their composition.The purpose of this work was to study the effect of new water-thinnable dispersions on the thickening ability of ceramic granulates obtained by them; density, Weibull modulus, mechanical strength of green and sintered samples obtained by die pressing method.

The work was supported by the Polish Ministry of Science and Higher Education No 3 T09B 022 29

16:00 Poster I10

Synthesis of pyrochlore-free $Pb(Ni_{1/3}Nb_{2/3}O_3)$-$PbTiO_3$ powders and ceramics via an organics-assisted solid state reaction

Yin Ye[1], Li M. Zhou[1], Hai Tao Huang[2]

1. *Department of Mechanical Engineering, The Hong Kong Polytechnic University, Hung Hum, Kowloon, Hong Kong none, Hong Kong* **2.** *Department of Applied Physics, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong 00852, Hong Kong*

e-mail: yeyinthu@gmail.com

By introducing organic species into the raw oxide powders before ball milling, pure perovskite $(1-x)Pb(Ni_{1/3}Nb_{2/3})O_3$–$xPbTiO_3$ (PNN-PT) powers and ceramics with the morphotropic phase boundary (MPB) composition at x=0.36 (0.64PNN-0.36PT) have been successfully synthesized via organics-assisted solid state reaction. Organics, like ethylene glycol, polyethylene glycol, ethylene glycol butyl ether and triethylene glycol dimethyl ether, are adopted. In order to examine the effect of additive organics, PNN-PT powders and ceramics are aslo prepared via conventional solid state reaction for comparison. The XRD results display that the introduction of the above organics facilitates the formation of the perovskite phase. The TG/DSC analysis demonstrates that the decomposition of additive organics is delayed by the connections between PbO and organics. FT-IR also indicates that there are interactions between PbO and additive organics. We propose that interactions between PbO and oxygen atoms in the organic chains favor the formation of the perovskite phase. Consequently, pure perovskite phase has been attained in PNN-PT powders with the assistance of organics. In contrast, pyrochlore phases still remain in PNN-PT powders prepared by conventional solid state reaction. The dielectric and piezoelectric properties of PNN-PT ceramics have been measured. It is shown that PNN-PT ceramics prepared via organics-assisted route, exhibit excellent electrical performance, which is higher than that of PNN-PT ceramics prepared via conventional solid state reaction.

16:00 Poster I11

Molten salt synthesis and characterization of $Bi_4Ti_3O_{12}$ crystals

Teresa Zaremba

Silesian University of Technology, Department of Inorganic Chemistry and Technology, ul. Krzywoustego 6, Gliwice 44-100, Poland

e-mail: teresa.zaremba@polsl.pl

Molten salt synthesis (MSS) is one of the important methods of preparing ceramic powders. Molten salts are used as a reaction aid to prepare complex oxides from their constituent oxides. Particulate materials with shape anisotropy are prepared by this technique and used as starting materials for grain-oriented ceramics.

The purpose of the work is to investigate the formation of $Bi_4Ti_3O_{12}$ using the molten salt method. The conventional method requires a high calcination temperature, usually leading to particle coarsening and aggregation of the $Bi_4Ti_3O_{12}$ powders. Ferroelectric $Bi_4Ti_3O_{12}$ is a suitable material for applications at high temperature transducers, capacitors and sensors.

In the present study, the influence of parameters of synthesis (temperature, time) and salt contents on morphology and size of $Bi_4Ti_3O_{12}$ crystals were investigated. Two kinds of eutectic salt mixtures, 0.5 NaCl + 0.5 KCl or 0.742 Na_2SO_4 + 0.258 K_2SO_4 were used as the flux. Eutectic temperatures are 650ºC and 831ºC for the chloride and sulfate fluxes, respectively. Mechanically mixed $Bi_2O_3 – TiO_2$ mixture was used as the starting material.

The mixtures of the precursors and salts were placed in a sealed alumina crucibles and heated at temperatures ranging from 700 to 1100ºC for a desired time period. The product obtained was washed with hot water several times until no trace of anion was detected by $AgNO_3$ or $Ba(NO_3)_2$ aqueous solution. The dried product was examined by XRD analysis. The particle morphology was examined by scanning electron microscopy (SEM).

It has been found, that formation of $Bi_4Ti_3O_{12}$ was accelerated by the presence of molten salts. In both fluxes aggregated particles were obtained. Finally discrete plate-like particles were formed, on heating for longer periods or at higher temperatures. These results suggest that the molten salt method is useful not only for producing ultra-fine powders with anisotropy, but also for controlling the aggregation states of the powders.

16:00 Poster I12

Morphology control of $K_{0.5}Bi_{0.5}TiO_3$ and $Na_{0.5}Bi_{0.5}TiO_3$ ferroelectric ceramic powders by molten salt synthesis

Teresa Zaremba

Silesian University of Technology, Department of Inorganic Chemistry and Technology, ul. Krzywoustego 6, Gliwice 44-100, Poland

e-mail: teresa.zaremba@polsl.pl

Lead oxide based ferroelectric and piezoelectric ceramics, represented by lead zirconate titanate (PZT), are widely used for piezoelectric actuators, sensors and transducers. However, volatilization of toxic PbO during high-temperature sintering causes environmental pollution. Therefore, it is necessary to develop environment – friendly lead-free piezoelectric ceramics.

Sodium bismuth titanate $Na_{0.5}Bi_{0.5}TiO_3$ (NBT) and potassium bismuth titanate $K_{0.5}Bi_{0.5}TiO_3$ (KBT) are very useful candidates of lead-free piezoelectric ceramics. NBT and KBT powders are traditionally prepared by solid-state reaction via the calcinations of metal oxide or carbonate powders.

The goal of the present work was to investigate the formation of NBT and KBT at low temperatures and at short times using the molten salt method. The first stage of the study related to obtaining NBT and KBT using Bi_2O_3, TiO_2, Na_2CO_3 and K_2CO_3 as starting raw materials. The second stage included obtaining NBT and KBT from intermediate binary compound $Bi_4Ti_3O_{12}$ and TiO_2, Na_2CO_3 and K_2CO_3, respectively. The precursors were mixed with a mechanically driven agate mortar and pestle for 1h. The mole fractions of NaCl and KCl were equal. Equal weight mixtures of salts and precursors were used. The mixed powders were heated to temperatures of 800 to 1000ºC in a covered alumina crucibles for the desired time. After thermal treatment the salts were remove by washing with deionized water several times. The morphology of the powders obtained was examined by SEM. Phases present were determined by XRD.

It has been found, that molten salt synthesiss of NBT and KBT is one low-temperature route which has been of considerable interest. It allows melt-solid reactions which are much faster due to small diffusion distances and higher mobility of oxides in the melt. The powder particles with an anisotropic shape were prepared by using a starting precursor $Bi_4Ti_3O_{12}$ with an anisotropic shape.

16:00 Poster I13

Investigations on synthesis and microstructure of potassium titanates

Teresa Zaremba, Dagmara Garczorz

Silesian University of Technology, Department of Inorganic Chemistry and Technology, ul. Krzywoustego 6, Gliwice 44-100, Poland

e-mail: teresa.zaremba@polsl.pl

The crystal structure and properties of potassium titanates, $K_2Ti_nO_{2n+1}$ (n = 1-8), are dependent on the value of n. Characteristic of potassium titanates with high potassium content is the existence of a layer structure, and they show a distinctive intercalation ability and catalytic activity. However, in the case of potassium titanates with a low potassium content, they have a tunnel structure and exhibit high thermal insulating ability and chemical stability.

Potassium titanates fibers and whiskers with high mechanical properties and thermal resistance are interesting for industrial applicatons as new and promising fillers for polymer and Al-based alloy composites.

Among the whiskers, potassium titanate whiskers have several benefits compared with other ceramic whiskers. One of the most desirable features is the low cost of the whiskers itself.

In the first stage of the present work, $K_2Ti_4O_9$ and $K_2Ti_6O_{13}$ whiskers were synthesized by the calcination and slow-cooling method under specific conditions. Powder XRD analysis was used to study the formation of potassium titanates. The charaterization of the whiskers was carried out by means SEM.

In the second stage polycrystalline samples of $K_2Ti_4O_9$ and $K_2Ti_6O_{13}$ were prepared by heating a mixtures of K_2CO_3 and TiO_2 at 850ºC for 1h. The powder products obtained from the thermal treatment were used to produce potassium titanate ceramics. Tabletes were prepared in green state with a static pressure, 10 or 50 MPa, respectively. The sintering temperature was selected considering the temperature resistance of potassium titanates (1000-1200ºC). Absorbability, open porosity and apparent density of the tablets after sintering were determined by Archimedes method.

As a result, a sintered body of $K_2Ti_4O_9$ or $K_2Ti_6O_{13}$ with porous and fibrous textures was prepared. It is expected that the sintered body having such a texture would be suitable for the application of fibre-reinforced plastic and metal.

16:00 Poster I14

Effect of carboxyl group in monosaccharide ring on viscosity of nanometric alumina suspension

Paweł Falkowski[1], Mikolaj Szafran[1], Andrzej Temeriusz[2]

1. *Warsaw University of Technology, Faculty of Chemistry, Noakowskiego 3, Warszawa 00-664, Poland* **2.** *Warsaw University, Faculty of Chemistry, Pasteura 1, Warszawa 02-093, Poland*

e-mail: falkowski@ch.pw.edu.pl

In the last few years many different methods of synthesis and characterization of nanopowders were developed. Unfortunately, there are still no good and efficient methods of moldings of nanopowders. One of the major problems is high tendency of nanopowders to agglomeration. This effect causes that it is difficult to obtain materials with nanostructure after sintering. Therefore the molding methods which allow reducing the agglomeration and giving homogeneity in green bodies and after sintering are searched for.

It is possible to reduce agglomeration of nanopowders through introduction of dispersing agents into ceramic suspension in slip cast method. Previous researches showed that addition of monosaccharides is very effective in reducing the viscosity of suspensions of nanometric alumina particles. The monosaccharides as processing additives have a number of advantages. They are nontoxic, soluble in water, readily available and inexpensive.

The viscosity of suspension with various monosaccharides differ widely Because the monosaccharides differ from each other only in location of substituent groups in space the observing diversity of properties is the result of differences in chemical structures of hexose.

The deflocculating properties of monosaccharides can be increase by substitution of carboxyl group into monosaccharide ring. It may be due to the deprotonation/protonation processes that occur in alumina suspensions with addition of acid derivative. It is also possible that higher amount of H^+ ions introduced with acid can change a double electric layer. The substituted carboxyl groups may change the structure of sugar molecule and influence on adsorption of monosaccharides onto nanopowder alumina particles.

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16:00 Poster I15

Layered Molybdenum and Tungsten Dichalcogenides nanosized powders

Nataliia Konig[1], Leonid Kulikov[1], Lev Akselrud[2], Volodymyr Davydov[2]

1. *Frantsevich Institute for Problems of Materials Science (IPMS), 3, Krzhizhanivsky Str., Kiev 03680, Ukraine* **2.** *Franko Lviv National University, 6, Cyril and Mefodiy Str., Lviv 79005, Ukraine*

e-mail: sem_kob@ipms.kiev.ua

Layered Molybdenum and Tungsten Dichalcogenides nanotechnologies open wide prospects for multifunctional nanomaterials design: solid, radiation-resistant nanolubricants, antifriction composite nanomaterials for space and ground based operation conditions (hydrogen atmosphere and medical facilities including); nanolubricant additives to industrial machine oils and greases for their tribotechnical parameters improvement; nanomaterials for energy converters; nanocatalysts, photocatalysis; nanomaterials as super shock absorbers at very high pressures**.**

Developed laboratory nanotechnologies enable to synthesize the nanocrystalline $2H\text{-}MCh_2$ (M=Mo, W; Ch=S, Se) homogeneous powders ($2H\text{-}MoS_2$ structure type characteristic for micron powders). The average sizes of anisotropic nanoparticles are adjusted in wide ranges effectively: $2H\text{-}MoS_2$ – $d_{[013]}$=2.7(2)–4.7(2) nm, $d_{[110]}$=8.5(4)–53(3) nm; $2H\text{-}WS_2$ – $d_{[013]}$=2.7(2)–8.0(5) nm, $d_{[110]}$=7.9(4)–123(8) nm; $2H\text{-}MoSe_2$ – $d_{[013]}$=5.2(3)–44(3) nm, $d_{[110]}$=25.4(1.6)–50(3) nm; $2H\text{-}WSe_2$ – $d_{[013]}$=4.5(3)–33(2) nm, $d_{[110]}$=18.7(1.2)–82(5) nm (for [013] and [110] crystallographic directions accordingly). Annealing temperatures have a dominating influence on anisotropic nanoparticles growth. Real layered $2H\text{-}WS_2$ and $2H\text{-}MoS_2$ nanostructures are characterized by different levels of atomic disordering. Realization of disordering processes was carried out by powerful ultrasonic action in different liquid mediums. Thus $2H\text{-}WS_2$ nanostructures are characterized by higher stability in disordering processes in comparison with $2H\text{-}MoS_2$ nanostructures.

Extremely small sizes of anisotropic nanoparticles (~1 nm for [013] direction), possible topochemical intercalation reactions (by hydrogen, different metals, organic compounds), disordering processes of real layered nanostructures can change essentially structural-sensitive physical properties of layered $2H\text{-}MCh_2$ (M=Mo, W; Ch=S, Se) nanosized powders that can be used effectively for above multipurpose nanomaterials design.

16:00 Poster I16

Mechanochemical synthesis and some properties of barium titanate nanooparticles

Volodymyr Sydorchuk[1], Svitlana Khalameida[1], Valeriy Zazhigalov[1], Borys Gorelov[2], Oksana Kotenok[2], Stanislav Makhno[2]

1. *Institute of Sorption and Problems of Endoecology NAS of Ukraine, 13 Gen Naumova Str., Kyiv 03164, Ukraine* **2.** *Institute of Surface Chemistry NAS of Ukraine, 17 General Naumov, Kyiv 03164, Ukraine*

e-mail: bilychi@online.com.ua

In the present work the barium titanate (BT) fabricated via mechanochemical treatment (MChT) have been investigated. Powders consisting of BT nanoparticles were synthesized by decomposition of barium titanyl oxalate BTO (BT-ox) and interaction of BaO and TiO2 (BT-o) during MChT for 5-10 h in air. In addition, the matrix samples of BT nanoparticles were prepared by means of BTO thermal decomposition in silica pores. It was shown (XRD data) that nanoparticles of pure tetragonal BaTiO3 were obtained. They have the specific surface area SSA 20-70 m2/g and crystallite size D 10-30 nm. The BT-o particles demonstrate the paraelectric – ferroelectric phase transition at 132oC (DSC data). The real ε1 and imaginery ε2 permittivity of BT-ox were about 4-5 and 0.5-1.5 accordingly and for BT-o ε1=18 and ε2= 6 in the temperature interval of 25-170oC. After annealing at 650oC which is accompanied by the mass loss the permittivity of both samples lowers and at 800-850oC the ε1 and ε2 increase to values about 14-17 and 1-2 in BT-ox and ε1 =26, ε2 =10-12 in BT-o. Moreover, the BT-ox particles display the phase transition at about 120-130oC. The annealing at 1100oC do not change essentially the permittivity and transition temperature of both samples. The BT-ox/SiO2 (25 % w/w BT) composite has SSA 140 m2/g, pore volume V=0.77 cm3/g and D~12 nm. Heating at 850 - 1100oC does not influence on D while the SSA and V slightly decrease. The milled BT-o possesses the photocatalytic activity while the BT-ox is photocatalytically non-active. However, in BT-ox annealed at 600-800˚C the destruction of safranin T with the rate constant Kd = 4-5•10-5 s-1 under UV-irradiation for power 30 W enhances (in BT-o Kd is 4-8•10-5 s-1). On the contrary, the annealing of BT-o leads to the loss of the photocatalytic activity. Thus, the mechanochemical treatment allows to obtain the ferroelectric particles of BT with ε1 = 18-26 for 8-12 GHz and change their photocatalitical properties.

16:00 Poster I17

Synthesis of submicron $SrFe_{12-x}Al_xO_{19}$ particles with very high coercitivity

Lev A. Trusov, Dmitry D. Zaitsev, Pavel E. Kazin

M.V. Lomonosov Moscow State University, Vorobyevy gory, Moscow 119992, Russian Federation

e-mail: doz.trusov@gmail.com

Magnetically hard M-type hexaferrites ($AFe_{12}O_{19}$, A = Ba, Sr) are oxide solids which play the dominant role on the permanent-magnet market due to their high magnetocrystalline anisotropy, chemical stability and low cost.

Monodomain submicron hexaferrite particles have excellent hard magnetic properties. One of the most efficient methods of their synthesis is crystallization of oxide glass precursor, e.g. in the SrO-Fe_2O_3-B_2O_3 system. This technique allows wide variation in chemical composition and thermal treatment conditions, thus particle size and, consequently, magnetic properties of the material can be controlled. Also the improvement of hexaferrite properties can be achieved by substitution of iron ions by aluminum. The glass crystallization is very suitable way to obtain aluminum doped monodomain hexaferrite particles at relatively low temperatures.

This work is concerned with synthesis of fine strontium hexaferrite particles by crystallization of glasses in the SrO-Fe_2O_3-Al_2O_3-B_2O_3 system.

The glasses were prepared by rapid quenching of initial reagents melt ($SrCO_3$, Fe_2O_3, Al_2O_3, H_3BO_3) between two steel rollers. The glass-ceramic samples were formed during heat treatment of glasses at 650-950 °C and fine hexaferrite powders were derived by dissolving of glass ceramics. The materials obtained were characterized by x-ray diffraction, electron microscopy and magnetic measurements.

The glass-ceramic materials based on $SrFe_{12-x}Al_xO_{19}$ exhibit very high coercivity values up to 10.18 Oe. The substitution rate x in the record sample equals to 1.3. The hexaferrite powder obtained from this glass-ceramic sample has the saturation magnetization value of 49.6 emu/g and corresponding coercivity. Crystal structure of the powder was refined by Rietveld method and distribution of Al atoms on Fe sites was determined. Al atoms occupy 41% of 2a sites, 14% of 12k sites and 5% of 4e(1/2) sites, while 4f sites are not affected.

16:00 Poster I18

Microstructural and mechanical characterization of zirconia based composite

Mariusz Andrzejczuk[1], Malgorzata Lewandowska[1], Tomaz Kosmac[2], Krzysztof J. Kurzydlowski[1]

1. *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland* **2.** *Josef Stefan Institute, Jamova 39, Ljubljana 1001, Slovenia*

e-mail: mandrzejczuk@inmat.pw.edu.pl

In present work, we report on a new zirconia-based ceramic composite that was obtained by infiltration of biscuit-sintered Y-TZP blanks with a pre-ceramic polysilazane-derived precursor and subsequent thermal treatment. Two grades of zirconia powder (TZ-3YSB-E - Coarse and TZ-3YB-E - Fine) with different crystallite size and surface area were used. A series of porous 3Y-TZP ceramics with an open porosity of maximum 37% were produced by dry pressing and biscuit-sintering at 1125-1300^{o}C in air. The porous samples were infiltrated and then subjected to a thermal treatment at a temperature of 1000^{o}C in air.

The influence of infiltration process on mechanical properties of composites was determined. TEM and SEM observation were carried out to characterize the microstructure. The mechanical properties (flexural strength, hardness and elastic modulus) were measured. The correlation between microstructural features and mechanical properties of infiltrated zirconia ceramic was discussed.

16:00 Poster I19

Mechanical behavior of NiO-10Sc1CeSZ ceramics in high-temperature hydrogen environment

Bogdan Vasyliv[2], Iegor Brodnikovskyi[1], Oleksandr Pasenko[2], Orest Ostash[3], Oleksandr Vasylyev[1]

1. *Institute for Problems of Materials Science, 3, Krzhizhanovsky, Kyiv 03142, Ukraine* **2.** *Karpenko Physico-Mechanical Institute of the National Academy of Sciences of Ukraine (PMI), 5 Naukova str., Lviv 79601, Ukraine* **3.** *Ukrainian State Chemical-technology University (USCTU), 8 Gagarin Ave., Dnepropetrovsk 49005, Ukraine*

e-mail: bregor@ya.ru

Long-term operation of the solid oxide fuel cell (SOFC) depends strongly on reliability of its components. In the case of SOFCs incorporating Ni-ScCeSZ anodes, hydrogen reduction of NiO usually takes place during the first service cycle of operation or conditioning. Initial reduction causes changes in the chemistry, microstructure and properties of the Ni-ZrO_2 anode material, which in turn induce mechanical stresses in the cell.

The biaxial strength and elastic properties of unreduced (NiO–ScCeSZ) and reduced (Ni–ScCeSZ) anode were studied. Biaxial strength was determined by the biaxial flexure test ball-on-ball method at ambient temperature in air. Several specimens were tested in hydrogen atmosphere at 600 °C too. It was found considerable deterioration in mechanical behavior of Ni-ScCeSZ anodes after hydrogen reduction comparing to initial state. Biaxial strength of anode samples decrease from 100 MPa in air at ambient temperature to ~20 MPa after reduction in hydrogen atmosphere at 600 °C.

Additionally, in-plane biaxial strength was determined in hydrogen atmosphere at 600 °C using concentric ring-on-ring test. Displacement of the specimens under constant load and their electric conductivity during full testing time (up to 5 hours) were measured and recorded using PC analog-digital device. As a result compliance-time and conductivity-time dependences for the specimens were plotted as a function of their reduction in hydrogen.

Experimental results showed that respectively to changes in the chemical composition of Ni- ScCeSZ anode materials during reduction, the compliance of the anode specimens and their electric conductivity changes as well. It was found considerable deterioration in mechanical behavior of Ni- ScCeSZ anodes after hydrogen reduction comparing to initial state.

16:00 Poster I20

Evaluation of residual stress in PZT films produced by laser ablation using X-Ray Diffraction and Raman spectroscopy

Sofia A. Rodrigues, Anabela G. Rolo, Anatoli A. Khodorov, Mario Pereira, Maria J. Gomes

University of Minho (UM), Campus de Gualtar, Braga 4710057, Portugal

e-mail: mjesus@fisica.uminho.pt

Lead Zirconate Titanate (PZT) films were deposited on $Pt/TiO_2/SiO_2/Si$ substrates by Pulsed Laser Deposition (PLD) technique, using a Nd:YAG laser with a source pulse wavelength of 1064 nm and duration of 5-7 ns delivering an energy of 320 mJ per pulse. The film growth was performed in O_2 atmosphere (0,40 mbar) while the substrate was heated at 600ºC by a quartz lamp. Starting from ceramic targets based on PZT compositions and containing 5% mol. of excess of PbO to compensate the lead evaporation during heat treatment, the films with different compositions Zr/Ti 55/45, 65/35 and 92/8 were successfully grown.

The residual stresses in the PZT films were studied using Raman spectroscopy and X-ray diffraction techniques. Based on lattice parameters and the elastic constants of PZT the stress in the films was estimated from XRD measurements using the calculated d-spacing in the stressed and unstressed states. The results revealed the presence of compressive stress in PZT with composition 55/45 and tensile stress in the others. On the other hand, analysing the shift of Raman phonon frequency in the A1(TO3) and E(LO3) vibration modes the stresses in this films were also estimated. The residual stresses extracted from the A1(TO3) mode are consistent with those extracted from the E(LO3) mode as well as with the stresses calculated from x-ray diffraction data.

16:00 Poster I21

Effective properties of ceramic matrix composites

Eva Gregorová, Willi Pabst

Institute of Chemical Technology (VSCHT), Technicka 5, Prague 16628, Czech Republic

e-mail: eva.gregorova@vscht.cz

Micromechanical theories of effective properties (elastic constants, thermal and electric conductivity, permittivity) are summarized for isotropic and transversely isotropic ceramic matrix composites (with isometric particulate fillers, aligned continuous fibers, platelets or short fibers, either randomly or preferentially oriented). In particular, the one-point (Wiener-Paul) and two-point (Hashin-Shtrikman) bounds for isotropic composites are given and compared with published literature data (with oxide and non-oxide ceramic matrices). It is shown that for small phase contrast (ratio of the phase properties) the Hashin-Shtrikman bounds give a good estimate of the effective property, while for large phase contrasts the effective properties typically exhibit an S-shaped curve in dependence of the second-phase volume fraction, being close to the upper Hashin-Shtrikman bound when the phase with the higher property value is the matrix phase and vice versa. In the extreme case of porous ceramics (where the inclusion phase are vacuous voids) the transition between the two regimes degenerates to a percolation threshold, while the non-linear self-consistent effective medium approximation (Bruggeman model) reduces to the linear approximation (dilute or non-interaction approximation) in this case. Literature data are shown for alumina-zirconia composites and fiber- or platelet-reinforced ceramics.

Acknowledgement:*This study was part of the project “Porous ceramics, ceramic composites and nanoceramics“ (Grant No. IAA401250703), supported by the Grant Agency of the Academy of Sciences of the Czech Republic.*

16:00 Poster I22

Mechanical properties of functional alumina/polyurethane biocomposite

Zbigniew Jaegermann[1], Anna Boczkowska[2], Agata Domańska[2], Sławomir Michałowski[1]

1. *Institute of Glass, Ceramics, Refractory and Construction Materials (ISC), Postepu 9, Warszawa 02-676, Poland* **2.** *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland*

e-mail: bioceramika@neostrada.pl

The purpose of the research consists in obtaining and testing gradient ceramics/polymer biocomposite. It could be used for design and future production of small joints endoprosthesis parts. The material should fulfill at least three functions which determine the usefulness of prosthesis: load bearing function, fastening and stabilizing endoprosthesis to the bone and tribologic function allowing mating with another parts of the joint or prosthesis.

Samples of alumina foams were formed by polymeric sponge method using structural sponges of different pore per inch density. During the mapping process of alumina foams a 3D structure of interconnected posts was built. Structures of different size of spaces between posts and differing total porosity can be obtained by the selection of polyurethane sponges types.

Degradable polyurethanes based on poly(e-caprolactone)diol and 4,4`-diisocyanate dicycloheksymethane were made. As chain extenders two different agents were used: ethylene glycol (EG) and water. Advantage of the polymer made from water as a chain extender is its long pot-life and low viscosity before curing as well as very good physical and mechanical properties in comparison to polymer made from EG as a chain extender. The alumina/polymer composite is characterized by much higher compressive strength than alumina foam itself. The compressive strength of the composite depends on the polymer composition used for the infiltration of alumina foams.

Polyurethanes characterized by good wear resistance, based on 4,4`-diisocyanate dicycloheksymethane and polytetramethylene ether glycol (PTMEG) were also prepared.

Results show that it is possible to obtain functional alumina/polyurethane composite, which could fulfill requirements for the material used for manufacturing of joint endoprosthesis parts.

This work is financed by Polish Ministry of Science and Higher Education (grant nr 3 T08D 03129)

16:00 Poster I23

Mesoporous silica thin film with ordered lamellar structure with properties for hard-coating and low-k materials

Young-Uk Kwon, Ki-Rim Lee

Sungkyunkwan University (SKKU), 300, Chunchun-Dong, Jangan-Gu, Suwon 440-746, Korea, South

e-mail: ywkwon@skku.edu

We report the synthesis of silica thin films with an unusual structure and unusual physical properties arising from the structure. The thin films were synthesized by sol-gel chemistry with a neutral surfactant as the structure-directing agent followed by controlled aging and calcination. The glazing angle X-ray diffraction, transmittance X-ray diffraction, transmission electron microscopy, scanning electron microscopy data all indicated that these films had lamellar structures with modulated silica density with alternating high density layers and low density layers. The thicknesses of the high density and low density layers could be controlled to 4.8-7.5 nm and 1.7-2.5 nm, respectably, by adjusting the concentrations of reagents and catalysts in the coating sol-gel solutions. Nanoindentation measurement data on these films produced 2-3 GPa for the hardness and 20-40 GPa for the Young's modulus, which are unusually high for pure silica films. Typical sol-gel silica films have 0.2-0.3 GPa of hardness and 5-10 GPa of Young's modulus. More surprisingly, these films showed very low dielectric constants of 1.2-1.7. All these unusual physical properties, which are highly desirable for low-k materials for the next generation of semiconductor industry, can be explained with the lamellar structures in the nanometer length scale of our films. In this presentation, the formation mechanism and details of the characterization data of our silica films will be presented.

16:00 Poster I25

Phase development and properties of high-temperature ceramic in the system mullite-ZrO_2

Gaida Sedmale, Ingunda Sperberga, Janis Grabis, Alexey Hmelov

Riga Technical University, Miera 34, Riga, Latvia

e-mail: gsedmale@ktf.rtu.lv

Mullite-zirconia ceramics were explored by different prepared powders. Conventional and hydrothemal treatment methods of starting components, characteristics of synthesised powders and their influence on sintering rates, phase composition and properties of mullite-zirconia ceramics were studied and compared. Compositions of Al_2O_3 $_{(gamma)}$,$SiO_2.nH_2O$, ZrO_2 mon. and Y_2O_3 for conventional and of $Al(NO_3).9H_2O$, SiO_2-aeroc, $ZrOO(NO_3).2H_2O$ and $Y(NO_3).6H_2O$ for hydrothermal preparing of starting powders were used to fulfil the mullite stoichiometric composition. The pressed samples were sintered at temperatures from 1000 to 1500^{0}C. The effect of hydrothermal preparing process on grain size (average 50-150nm) of sintered samples is emphasized.

It is shown that densification is largely affected by milling time by conventional, as well hydrothermal preparing. XRD and SEM examinations showed the differences in mullite and ZrO_2 (tetr.) crystalline phases formed starting from 1300^{0}C from conventional powders. In comparision with previously mentioned samples from hydrothermally prepared powders had a higher tendency to form a mullite phase, starting already from 1000^{0}C.

Bending strenght and pressure resistance measurements for samples from conventionally prepared powders showed that these values are remarkably influenced by milling time - for the maximum time (24h) the pressure resistance for at 1400^{0}C sintered samples reached 280-300 MPa, bending strenght - 70-75 MPa.

16:00 Poster I26

Influence of ceramic inclusions on structure and properties of composite materials on the basis of metals

Mikalai Shypitsa, Anatoly Dmitrovitch

Research institute of powder metallurgy, Platonova 41, Minsk 220071, Belarus

e-mail: shipitsa@tut.by

Object of investigation is frictional materials on the base of metals with ceramic inclusions (silicon carbide, alumina, nitride of aluminum and some others). The samples for tests are manufactured by standard methods of powder metallurgy

In work mechanical properties (hardness, impact strength, coefficient of friction, wear) of composite materials were investigated. Structures of these materials are resulted.

Tests have shown that mechanical properties insignificantly depend on hardness of inclusions. Properties of materials are defined by mechanisms of interaction of inclusions with a metals.

16:00 Poster I27

WC-6%Co composites sintered by the reactive Pulse Plasma Sintering method.

Dariusz Siemiaszko[1], Andrzej Michalski[2], Marcin Rosinski[2]

1. *Military University of Technology, Faculty of Advanced Technology and Chemistry, Kaliskiego 2, Warszawa 00-908, Poland*
2. *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland*

e-mail: dsiemiaszko@wat.edu.pl

The paper presents the results of examinations of tungsten carbide sinters produced of a mixture of tungsten, carbon and cobalt powders using the Pulse Plasma Sintering method. With the use of the powder mixture, the WC-Co composites were produced during a single technological process. The structure of the sinters was examined microscopically and their phase compositions, chemical compositions, hardness and densities were determined. The carbides sintered by the reactive PPS method (from W, C and Co powders) have a higher hardness (2130 HV30) than the conventional method (1660 HV30). The stress intensity coefficient KIC (11.9 MPam-0.5) was similar to carbide sintered conventionally.

16:00 Poster I28

Machining of the advanced MMC and CMC composites

Włodzimierz S. Wilk, Barbara Staniewicz-Brudnik, Lucyna R. Jaworska

Institute of Advanced Manufacturing Technology (IOS), Wrocławska 37A, Kraków 30-011, Poland

e-mail: wwilk@ios.krakow.pl

Modern Metal Matrix Composites (*MMC's*) and Ceramic Matrix Composites (*CMC's*) for automotive and aviation applications will be discussed. The research works of CMC Composites manufacturing in the Institute of Advanced Manufacturing Technology, will be described.

The selection of tools, machine tools, conditions and parameters of machining aluminium composite castings with ceramic preforms of Al_2O_3 in AlSi9Mg alloy, formed by pressure squeeze infiltration, which imitates the piston head of internal combustion engine, will be described. The important role at the cast composite machining have cut-off processes (the castings gating system cutting-off, cutting-out and slicing the samples for investigation, grinding the final samples for the tensile tests, cutting-through of the worn parts at the recycling processes).

The results of carried out machining tests of aluminium composites reinforced with Al_2O_3 and Si_3N_4 particulates, will be given. The characteristic of the diamond grinding wheels, made in the Institute of Advanced Manufacturing Technology for this task, will be given. The basic problem of machining MMC's and CMC's composite materials is intensive edge's wear, induced by hard ceramic phases with high abrasive properties. Only use of tools with diamond edges and diamond grinding wheels have resulted in long edges lives and short machining times, for such composites.

16:00 Poster I29

Sprayed targets from zinc oxide with additives of rare-earth compound for obtaining of multipurpose touch microsystems

Vladimir Koleshko[2], Shauchonak A. Alex[1,2], Anatoly Gulai[2]

1. *Research institute of powder metallurgy, Platonova 41, Minsk 220071, Belarus* **2.** *Belarussian National Technical University (BNTU), F. Skariny, 65, Minsk 220027, Belarus*

e-mail: alexshev56@mail.ru

Synthesis of piezoelectric materials used for production of thin-film nanostructures on superficial acoustic waves is one of perspective scientific and technical directions on creation of multipurpose sensor controls. They are sensitive to various physical and chemical influences. In this connection piezo active materials of sprayed targets on a basis of micro-nanopowders of zinc oxide with additives of rare-earth elements and their compound (oxides, fluorides, hydrides) are developed. Use of nanosize and submicron powders allows to lower sintering temperature, to activate processes of sintering and to receive high density (above 98 %) fine-grained (0,5-2,0 μm) targets. The fine-grained structure of a material target promotes stabilization of process parameters of their vacuum spraying and obtaining of piezoelectric touch microsystems. Introduction of microadditives of rare-earth compound in concentration of 0,1-5,0 % leads to increase of electro-acoustic properties of piezoelectric thin films, in particular their factor of electromechanical communication. Moreover, microadditives substantially define influence of physical and chemical actions on geometrical, electric and elastic properties of a sensitive piezoelectric layer of a microsensor control on PEAHENS. With use of the developed targets multilayered structures for excitation of superficial waves are received, and also multipurpose touch microsystems of the control of temperature, pressure, structure of gas environments are created.

16:00 Poster I30

Formation and study of luminescence ceramics based on polycrystalline calcium fluorapatite doped with europium ions

Nataliya V. Babayevskaya[1], Oleksandra S. Kryzhanovska[1], Yuriy N. Savin[1], Alexander V. Tolmachev[1], Pavel V. Mateychenko[1], Tatyana G. Deineka[1], Zoya I. Kolupaeva[2]

1. *Institute for Single Crystals NAS of Ukraine (ISC), 60 Lenin Ave., Kharkov 61001, Ukraine* **2.** *National Technical University"Kharkov Polytechnical Institute", 21 Frunze str., Kharkov 61002, Ukraine*

e-mail: Babayevskaya@isc.kharkov.ua

At present materials science the ceramics based on apatite-like compound doped with REE have been extensively studied for use as phosphors and laser materials. Monophasic polycrystalline FAP and FAP:Eu^{3+} were obtained using the precipitation from aqueous solution method. As-obtained samples were compacted in tablets at 660 MPa and were sintered in oxygen atmosphere 600 – 1200 ^{o}C. XRD analysis showed that no additional phase are observed. The increase of sintering temperature leads to growth of nanocrystalline blocks size (L) – from 42 nm to 54 nm. It was observed that ceramic density arise up to 1100 ^{o}C – ρ_{rel}= 84.67 % and decrease at 1200 ^{o}C – ρ_{rel}=19.1 %. The ceramics porosity reaches maximum value at ρ_{rel}= 74.06 %. The optimal sintering temperature (t=1100 ^{o}C), at which the intensive luminescence of Eu^{3+} in FAP structure is observed, was found.

16:00 Poster I31

Ceramic $BaZn_{1/3}Ta_{2/3}O_3$ for microwave applications

Ciceron A. Berbecaru[1], Horia V. Alexandru[1], Andrei Ioachim[2], Mariana I. Toacsan, Liviu Nedelcu[2], Gabriel Banciu, Rodica Ramer[2], Ecaterina Andronescu[3], Sorin Jinga[3], Cornelia Jinga[3]

1. *University of Bucharest, Faculty of Physics, Bucharest-Magurele p.o.box mg-11, Bucharest 76900, Romania* **2.** *National Institute of Materials Physics (NIMP), Atomistilor 105 bis, Bucharest 077125, Romania* **3.** *University Politehnica of Bucharest, Polizu 1-7, Bucharest, Romania*

e-mail: berbecaru2ciceron@yahoo.com

The $BaZn_{1/3}Ta_{2/3}O_3$ is a member of the new perovskit oxide generation, widely used in high frequency domain. Their high permittivity 28-30, low losses and an excellent thermal stability on a large temperature scale, make them suitable for microwave applications. The ceramics are obtained by solid state reaction. Samples were sintered in air at 1550, 1600 and 1650 ^{o}C temperature range for 2 hours, followed by 10 h annealing at 1410 ^{o}C, to improve the material's properties, [1, 2, 3]. Scanning Electron Microscopy, X-ray diffraction and Energy Dispersive **X**-ray analysis were performed to investigate the morphology and the structure of the ceramics. A secondary phase and the unit cell distortion were found from XRD data. The sintering temperature promotes a long-range order with a 2:1 ratio of Ta and Zn cations on the octahedral positions of the perovskite structure. A HIOKI 3522 LCR bridge was used to investigate the dielectric parameters of the BZT ceramics on 45 Hz ¸ 5 MHz frequency range, in conjunction with the Quatro Cryosystem on the temperature range -150 / +150 ^{o}C. A high stability of the permittivity was noticed. The dielectric properties measured in the microwave range were correlated with morphological and structural properties. The Hakki-Coleman method was employed to measure the dielectric constant of the samples. Typical values of 28 at 6 GHz were found and less than 6 ppm/deg positive temperature coefficient of the resonance frequency. To improve the microwave parameters of BZT (i.e. Q x f > 100,000 GHz), sintering temperatures greater than 1600 ^{o}C and annealing time higher than 10h were required.

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16:00 Poster I32

Structure, magnetic and dielectric properties of $Bi_5Ti_3FeO_{15}$ multiferroic ceramics after high energy ball milling and free sintering process.

Grzegorz Dercz[1], Jolanta Rymarczyk[2], Krystian Prusik[1], Aneta Hanc[1], Lucjan Pająk[1], Jan Ilczuk[2]

1. *University of Silesia, Institute of Material Science, Bankowa 12, Katowice 40-007, Poland* **2.** *University of Silesia, Department of Material Science, Żeromskiego 3, Sosnowiec 41-200, Poland*

e-mail: gdercz@op.pl

The $Bi_5Ti_3FeO_{15}$ ceramic belongs to ferroelectromagnetics characterized by presence of simultaneous magnetic and ferroelectric ordering. This class of materials exhibits a spontaneous magnetization and polarization that can be switched by an applied magnetic and electric field, respectively.

The $Bi_5Ti_3FeO_{15}$ (BTF) multiferroic ceramic can be applied during construction of different electronic devices of new generation. This type of ceramics is promising owing to the possibility of their applications as different types of memory elements.

In this paper the structural, magnetic and dielectric properties of the multiferroic ceramics $Bi_5Ti_3FeO_{15}$ are presented.

The test material was prepared in two stages. In the first stage it was obtained as a result of the reaction in the solid phase synthesis from the mixture of the bismuth (Bi_2O_3), titanium (TiO_2) and iron (Fe_2O_3) simple oxides. Polycrystalline precursor material (mixture of Bi_2O_3, TiO_2 and Fe_2O_3 powders) was milled by high-energy vibratory mill for 1, 3, 5 and 10 hours. The second stage free sintering synthesis reaction was conducted at 800ºC temperature in 5 h time.

The X-ray diffraction methods were applied for the structure characterization of the studied samples. The parameters of diffraction line profiles were determined by PRO-FIT Toraya procedure. The crystallite sizes and lattice distortions were analyzed using Williamson-Hall method. The values of lattice parameters determined by Rietveld method. Investigations of hyperfine interactions in the studied materials were carried out by Mössbauer spectroscopy. The powder morphology was analyzed by scanning electron microscopy (SEM) and transmission electron microscopy (TEM) techniques. Thermal dependence of dielectric permittivity was studied. Hysteresis loop was observed and magnetic properties of multiferroic ceramics were investigated.

16:00 Poster I33

Plasma treatment of plasma sprayed HA coatings.

Agata K. Dudek

Częstochowa University of Technology, Institute of Materials Ingineering, Armii Krajowej 19, Częstochowa 42-200, Poland

e-mail: dudek@mim.pcz.czest.pl

Hydroxyapatite had been confirmed to be bioactive since it was first made in the 1970's. The artificial synthetic material had been used as an important biomaterial for numerous medical applications, such as ortopedical and dental implants. HAp possesses low mechanical strength and fracture toughness which is an obstacle to its applications.

A suitable method for improving the mechanical properties is based on the synthesis of composites made oh HAp and other phases (i.e. ZrO_2). Zirconia which has the characteristics of high strength and stress-induced phase transformation toughening, has been used to improve the strength of brittle materials. ZrO_2 ceramics are a bioinert material [2-4].

Spherical HAp powder were added to 8%wt. yttrium partially stabilized zirconia powder (YSZ) and 20% wt.Y_2O_3 and coated on the titanium substrate. Plasma treatment was conducted on plasma sprayed hydroxyapatite (HA) coatings. Various plasma parameters were investigated. The study examines the use of a plasma to enhance the coating HA, HA+ ZrO_2+Y_2O_3. The crystalline phases of the HAp and HAp+ZrO_2 coatings were analyzed by X-ray diffractometry.

16:00 Poster I34

Ionic conductivity in the CeO_2-Sm_2O_3-MO (M = Ca, Ba, Sr,) system

Magdalena M. Dudek

AGH University of Science and Technology, Faculty of Materials Science and Ceramics (AGH UST), Mickiewicza 30, Kraków 30-059, Poland

e-mail: potoczek@agh.edu.pl

Rare earth-doped ceria (RDC) has higher values of ionic conductivity than fully yttria-stabilized zirconia (8YSZ), in the temperature range of 600-800^{o}C. The main drawback of CeO_2-based electrolytes is the increased electronic conduction under low oxygen partial pressure, that is accompanied by the reduction of Ce^{4+} to Ce^{3+}. It has been reported that reduction of ceria-based materials can be neglected at lower temperatures, around 600-700^{o}C. However, such low temperatures are not suitable for singly doped-ceria operations, as SOFC¢s electrolyte material has a high resistance. One possible way to improve their electrical conductivity is through structural modification of ceria solid solution.

The aim of this work was to examine how codoping small quantities of MO (M = Ca, Ba, Sr) in $Ce_{1-x}Sm_xO_2$ solid solutions influenced the electrical and mechanical properties of ceria-based materials The sol-gel method was used to prepare CeO_2-based powders. Transmission electron microscopy was used to observe morphology of powders. Phase composition and lattice parameters were examined with XRD diffraction analysis. Scanning electron microscopy was used to observe a microstructure of samples. Electrical properties were studied by a.c impedance spectroscopy in the temperature range of 200-800^{o}C. In order to determine the oxide ion transfer number, the EMF of oxygen concentration cell was measured. For different Sm_2O_3-CeO_2-MO (M

= Ba, Sr, Ca) compositions the relation between structure, microstructure, electrical properties are presented and discussed.

16:00 Poster I36

Oxygen-ion conducting ceramic materials based on perovskite $Sr_3Bi_2O_6$

Maria V. Golikova, Vladimir V. Pankov, Leanid V. Makhnach

Belarusian State University (BSU), F. Skaryna av. 4, Minsk 220050, Belarus

e-mail: marusia-gol@tut.by

To discover new ceramic materials with oxygen-ion conductivity the Sr-Bi-Ni-O system was investigated. By solid-phase synthesis from nitrates two perovskite-like phases ($Sr_3Bi_{1,1}Ni_{0,9}O_{6\pm\delta}$. and $Sr_3Bi_{0,6}Ni_{1,4}O_{6\pm\delta}$) were synthesized and the optimal synthesis conditions were determined. Indicating of X-ray patterns of these compounds was carried out. It was determined that $Sr_3Bi_{1,1}Ni_{0,9}O_{6\pm\delta}$ was insulator at room temperature, $Sr_3Bi_{0,6}Ni_{1,4}O_{6\pm\delta}$ was conductor. The temperature dependence of specific resistance of $Sr_3Bi_{0,6}Ni_{1,4}O_{6\pm\delta}$ was defined. The processes of oxygen isolation and absorption of $Sr_3Bi_{0,6}Ni_{1,4}O_{6-\delta}$ during heating and cooling were investigated.

16:00 Poster I37

ZnO ceramic sintering and luminescence properties

Larisa Grigorjeva[1], Donats Millers[1], Krisjanis Smits[1], Witold Łojkowski[2], Janusz D. Fidelus[2], Krzysztof Bieńkowski[2], Tadeusz Chudoba[2], Claude J. Monty[3]

1. *Institute of Solid State Physics, University of Latvia, 8 Kengaraga, Riga LV-1063, Latvia* **2.** *Polish Academy of Sciences, High Pressure Research Center (UNIPRESS), Sokolowska 29/37, Warszawa 01-142, Poland* **3.** *CNRS laboratoire Procedes, Materiaux et Energie solaire (PROMES), BP5 Odeillo, Font-Romeu 66120, France*

e-mail: lgrig@latnet.lv

The ZnO is well known luminescent material and its properties have been intensively studied due to the progress in preparation of nanostructured material. ZnO crystal luminescence satisfies the requirements to special characteristics of fast scintillators: high light output in subnanosecond time, low afterglow, high density and radiation resistance, suitable emission wavelength. However the crystal cost is very high. ZnO ceramic was known as varistor material. At the same time the ZnO ceramic will be applied as a material for fast scintillator. The goal of present study is the developing of the nanoparticle preparation technology and the ceramic sintering process (especially for obtaining transparent ceramic) as well as to understand the scintillation process in ZnO nanopowders and ceramics.

Simple high temperature sintering (14000C, 1-3 min) and high pressure low temperature sintering (8GPa, 3500C, 5 min) were used for ceramic preparation. The grains of obtained ceramics were ~1 µm and 100 nm, accordingly.

The SEM, XRD and time-resolved luminescence methods were used for obtained ceramic testing.

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16:00 Poster I38

Excitation transfer in zirconia nanocrystals and ceramics

Donats Millers[1], Larisa Grigorjeva[1], Krisjanis Smits[1], Janusz D. Fidelus[2], Agnieszka Opalińska[2,3], Witold Łojkowski[2]

1. *Institute of Solid State Physics, University of Latvia, 8 Kengaraga, Riga LV-1063, Latvia* **2.** *Polish Academy of Sciences, Institute of High Pressure Physics (UNIPRESS), Sokolowska 29/37, Warszawa 01-142, Poland* **3.** *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland*

e-mail: dmillers@latnet.lv

The electronic excitations (charge carriers, excitons) in zirconia are mobile at room temperature. Therefore the energy and/or charge transfer take place and final stages of these processes are either the excitation trapping at crystalline lattice imperfections, either the self-trapping (excitation self-localization in the initially perfect lattice). The both cases could result in creation of excited state and this excited state is origin of luminescence. Hence, the study of time – resolved luminescence provide information of excitation transfer processes. The pure and rare earth doped zirconia nanocrystals as well as ceramics were studied by time resolved luminescence methods under 3 kinds of excitation: nitrogen laser (337 nm) pulses, YAG:Nd laser (532 nm and 266 nm) second and forth harmonic pulses, electron beam (270 kV, 10^{12} el/cm^2 per pulse) pulses. The laser beam excitation is within band gap and therefore lattice defects and dopands were excited. Electron beam excitation creates the electrons and holes mainly in host lattice. The defects concentration in oxygen sub-lattice was changed via zirconia annealing at different oxygen partial pressure. The increase of defects concentration in oxygen sub-lattice causes the increase of luminescence intensity under excitation within band gap region, whereas the intensity of luminescence was suppressed if band carriers were created. It is suggested the defects in oxygen sub-lattice acts as efficient traps for charge carriers, but they are not a radiative recombination centers. The processes were similar in free-standing nanocrystals and nanostructured ceramics. The dopands introduced allowed to study the electronic excitation trasfer process from host to the dopand via comparision of result of dopand direct excitation with that of host band-to-band excitation.

The work was partly supported by grants 05.1720 of LCS and no. N N508 0851 33 of MNiSW granted for the years 2007 – 2009

16:00 Poster I39

Luminescence and temperature dependency of β-SiAlON phosphor

Youn-Gon Park, Jeong Ho Ryu, Hyong Sik Won, Sang Hyun Kim, Hideo Suzuki, Chul Soo Yoon

Samsung Electro Mechanics Co, 314, Meatan 3-Dong, Suwon 443-743, Korea, South

e-mail: calvin.park@samsung.com

In recent times, rare-earth-doped oxynitride or nitride compounds have been reported to be photoluminescent and may then serve as new phosphors because of their good thermal and chemical stabilities. In this study, β-SiAlON:Eu2+ oxynitride phosphors with compositions of Eu2+xSi6-zAlzOzN8-z were successfully prepared using GPS (gas pressured sintering) process. The phase purity, microstructure, luminescent and thermal quenching properties for the prepared β-SiAlON:Eu2+ phosphors were investigated in detail. The obtained β-

SiAlON:Eu2+ phosphors had a rod-like morphology with a uniform size of 3-5 μm in length and 0.5-1 μm in diameter. The β-SiAlON:Eu2+ phosphors absorbed UV-visible spectral region, and showed a single intense broadband emission in visible range. The effects of the Eu2+ doping concentration (x) and Si/Al ratio (z) on the optical properties for the β-SiAlON:Eu2+ were discussed under consideration of concentration quenching and nephelauxetic effect. The temperature dependence on photoluminescence (PL) properties was investigated from 25 to 275 °C, and the activation energies (ΔE) for thermal quenching of the prepared β-SiAlON:Eu2+ were determined by Arrhenius fitting. The experimental results clearly indicates that the prepared β-SiAlON:Eu2+ phosphors have great potentials as a down-conversion green phosphor for white light emitting diodes (LEDs) utilizing near UV or blue LEDs as the primary light source.

16:00 Poster I40

Synthesis and luminescent properties of Ca-α-SiAlON:Eu^{2+} phosphors

Youn-Gon Park, Jeong Ho Ryu, Hyong Sik Won, Sang Hyun Kim, Hideo Suzuki, Chul Soo Yoon

Samsung Electro Mechanics Co, 314, Meatan 3-Dong, Suwon 443-743, Korea, South

e-mail: calvin.park@samsung.com

The white LEDs (light-emitting diodes) comprised of a blue LED chip and YAG:Ce^{3+} yellow phosphor are promising new-generation light source which can replace conventional incandescent and fluorescent lamps due to their reliability and low energy consumption. However, these white LEDs are not applicable for indoor lighting purpose due to their less red luminescence and relatively lower color rendering index value. In recent days, rare-earth-doped oxynitride or nitride compounds have been reported to be photoluminescent and may then serve as new phosphors with good thermal and chemical stabilities because the higher formal charge of N^{3-} compared with O^{2-} and the nephelauxetic effect induced by the difference in electro-negativity of nitrogen with oxygen would lead to larger ligand-field splitting of the 5d levels and the center of gravity of the 5d states at lower energy as shown in Fig. 1. In this work, Ca-α-SiAlON:Eu^{2+} based yellow oxynitride micro-crystals were prepared using GPS (gas pressured sintering) method. The crystallinity and particle morphology of the prepared micro-crystals were characterized. The temperature dependence of luminescence properties was investigated from 25 to 275 °C. The Stokes shift and zero-phonon line was calculated mathematically and estimated from the spectral data. The prepared Ca-α-SiAlON: Eu^{2+} showed superior thermal quenching properties compared to a commercially used YAG:Ce^{3+}. In addition, the activation energies (ΔE) for thermal quenching of the prepared Ca-α-SiAlON:Eu^{2+} phosphors were determined by Arrhenius fitting.

16:00 Poster I41

Eu Luminescence in zirconia nanocrystals

Krisjanis Smits[1], Donats Millers[1], Larisa Grigorjeva[1], Anatolijs Sarakovskis[1], Agnieszka Opalińska[2], Janusz D. Fidelus[2], Witold Łojkowski[2]

1. *Institute of Solid State Physics, University of Latvia, 8 Kengaraga, Riga LV-1063, Latvia* **2.** *Polish Academy of Sciences, Institute of High Pressure Physics (UNIPRESS), Sokolowska 29/37, Warszawa 01-142, Poland*

e-mail: smits@cfi.lu.lv

The time – resolved luminescence of Eu^{3+} in a pure and Yttria – stabilized zirconia nanocrystals was studied. For luminescence excitation different excitation sources was used: tunable pulsed solid state laser NT342/3UV (pulse duration ~4 ns) from Ekspla (210-355nm; 420-2300nm) with Andor SR-303i-B spectrometer and YAG laser 4-th harmonic (pulse duration ~2 ns) with MDR3 grating monohromator, PMT and photon counting board for time resolution measurements. The size and phase was characterized with BET and XRD (Diffractometer X'Pert Pro MPD).

The zirconia nanocrystals were produced by the microwave driven hydrothermal method. The luminescence spectra shows typical (592nm- $^5D_0$ – $^7F_1$ and 613nm- $^5D_0$ – $^7F_2$) Eu^{3+} bands. With increase of europium concentration luminescence from host defects decreases, but Eu^{3+} luminescence increases. This indicates the energy transfer from host to dopant.

The increase of Eu concentration led to the appearance of additional $^5D_0 - {}^7F_2$ (electric dipole) luminescence band. It was showed this band is due to change of nanocrystal structure. The observed splitting as well as the decay kinetics of luminescence gave a strong witness that the Eu^{3+} in ZrO$_2$ is incorporated in two different symmetry sites. The XRD spectrum confirms that with increase of Eu concentration tetragonal phase appears. The $^5D_0$ – $^7F_2$ transitions in the monoclinic and tetragonal phase zirconia have slightly different energies and this was confirmed by the luminescence excitation spectra – the monoclinic and tetragonal phases have different excitation spectra.

The work was partly supported by grants 05.0026 of LCS and no. N N508 0851 33 of MNiSW granted for the years 2007 – 2009

16:00 Poster I42

Synthesis and properties of a (La,Sr)MnO$_{3-x}$ -based magnetoresistive composites from borate glasses.

Alexander V. Vasiliev[1,2], Dmitry D. Zaitsev[1], Pavel E. Kazin[2]

1. *Faculty of Materials Science, Moscow State University, Lenin Hills, Moscow 119992, Russian Federation* **2.** *Chemistry Department, Moscow State University, Leninskie Gory, 1-3, Moscow 119992, Russian Federation*

e-mail: a.vasiliev@inorg.chem.msu.ru

Materials based on doped rare-earth manganites can significantly change their electrical resistance in an applied magnetic field. This is the so-called colossal magnetoresistance effect. These materials can be used in different magnetoresistive sensors and devices, such as ultrahigh-density read heads for magnetic memory, metal detectors, compasses, linear and angular position sensors, temperature detectors, and bolometers.

The colossal magnetoresistance effect is observed in manganite crystallites. A way to increase the total magnetoresistance of such materials is to obtain composites with thin dielectric films between conductive ferromagnetic particles; in this case, the tunnel magnetoresistance effect occurs.

The amorphous precursors was synthesized by preliminarily annealing a mechanical mixture of manganese(III) and lanthanum(III) oxides, boric acid, and strontium carbonate of the nominal compositions La0.67Sr0.33MnO3 + xSrB2O4 (x=0,32; 0,56; 0,86; 1,00; 1,10; 1,30; 1,59; 1,95) at 800°C. Then, the precursor was pressed into pellets 1 cm in diameter, which were melted with an arc burner. The melt was quenched between copper plates. The glasslike samples thus prepared were annealed at 850 - 1000°C for 2 or 24 h.

X-ray powder diffraction showed that the glassceramic samples contain mainly two crystalline phases (La,Sr)MnO3 and SrB2O4.

The field dependence of the sample resistivity was measured by the standard four-probe technique at 77 K and 297 K. The negative magnetoresistance was as large as 14,4% at 80 kA/m, 77K and 6,2% at 40 kA/m, 297K. It is worth noting that a low electrical resistance (tens of ohms) and the magnetoresistance effect were observed at a relatively small manganite content. This is likely due to the microstructure features of the sample, in which the interpenetration of the manganite and borate phases ensures good percolation.

16:00 Poster I43

Transparent cobalt-doped magnesium aluminate ceramics for Q-switch applications – powder preparation and sintering

Anna Wajler, Henryk Tomaszewski, Helena Węglarz

Institute of Electronic Materials Technology (ITME), Warszawa 01919, Poland

e-mail: anna.wajler@itme.edu.pl

One of the most important applications of the oxide crystals doped with Co^{2+} is passive Q-switching of solid-state lasers operating in the near-infrared region of 1.3-1.6 μm. Passive Q-switches generate high power laser pulses without the use of electro-optic Q-switches, which results in reducing the package size and eliminating high-voltage powder supply. Co^{2+}-doped magnesium aluminate (Co^{2+}: $MgAl_2O_4$) crystal is used as a media for Q-switch of e.g. 1.32 μm and 1.44 μm Nd:YAG lasers, 1.32 μm iodine lasers and 1.54 μm erbium glass lasers. Due to relatively lower costs, faster and easier preparation by ceramic technology it would be interesting to use transparent polycrystalline Co^{2+}: $MgAl_2O_4$ instead of single crystals.

In this work a series of Co-doped $MgAl_2O_4$ powders (0.1at.% to 4at.%) and undoped $MgAl_2O_4$ powders were prepared by co-precipitation and calcination. Precursors obtained after precipitation and calcined powders were examined by XRD and SEM. The powders were sintered by vacuum sintering and hot pressing (HP). In the second case LiF was used as sintering aid. Both ceramics were of density close to theoretical, but only HP-made were transparent. As found, the main reason of light scattering, as proved by XRD and SEM, were presence of residual porosity and nanograins of cobalt oxide (in the case of higher cobalt content) on spinel grain boundaries.

16:00 Poster I44

Transparent Nd:YAG ceramics sintered from nanometric powders- effect of co-precipitation temperature on powder sinterability

Helena Węglarz, Anna Wajler, Henryk Tomaszewski, Zdzislaw M. Librant, Tadeusz Łukasiewicz

Institute of Electronic Materials Technology (ITME), Wólczyńska 133, Warszawa 01-919, Poland

e-mail: anna.wajler@itme.edu.pl

Neodymium doped yttrium aluminum garnet (Nd:YAG) is one of the best known and widely used laser materials. Last years showed a big interest in preparation of Nd:YAG ceramics, instead of single crystals. There is a number of reasons, why production of Nd:YAG ceramics can be attractive alternative to Czochralski grown crystals. Reduction of manufacturing time, lower costs or larger size components belong to one of these. Nd:YAG ceramics can be prepared by two methods: reactive sintering of appropriate oxides and sintering of Nd:YAG powders. The second method offers some advantages, like smaller grain size or higher uniformity of material, but at the same time it appears to be more difficult.

The aim of the presented work was to prepare transparent ceramics using Nd:YAG nanopowder prepared by co-precipitation and calcination followed by vacuum sintering. Co-precipitation was conducted using yttrium, aluminum and neodymium nitrates (4N) and ammonium carbonate as precipitant. Reaction temperature was set on 10^{o}C, 20^{o}C, 50^{o}C and 70^{o}C. As occured only in the case of powder from the highest co-precipitation temperature transparent ceramics was obtained. Detailed studies of phase composition of powders and its precursors, microscopic observations of powders, precursors and ceramics as well as mercury porosimeter measurements of pressed samples were performed to explain the reasons of observed differences.

16:00 Poster I45

Characteristics of Sm-doped $BiFeO_3$ ceramics prepared by a modified solid-state-reaction method

Yingbang Yao, Yanmin Zhang, Ching Yee Lam, Chee Leung Mak, Kin Hung Wong

Department of Applied Physics, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong 00852, Hong Kong

e-mail: yaoyingbang@126.com

Sm-doped $BiFeO_3$ have been prepared by a modified solid-state-reaction method, of which a much faster heating and cooling rates during the sintering stage were employed. The doping level was from 1mol%, 3mol%, 5mol%, to 8mol%. Different processing parameters, such as sintering temperature and annealing temperature, have been optimized to get high quality samples. Based on the results from the dielectric loss studies, the optimum sintering and annealing temperatures were found to be 825^{o}C and 300^{o}C respectively. With increasing Sm doping level, the dielectric loss was increased, probably due to the larger number of pores, as observed by the scanning electron microscopy. Leakage-free P-E hysteresis loops in square shape were observed in all samples. The remnant polarization (Pr) was maximized in the 5mol%-doped sample, which showed a Pr value of as high as 35uC/cm^2. Furthermore, remnant magnetization was observed after Sm doping and the 8mol%-doped sample possessed the largest remnant magnetization of 0.007emu/g. On the basis of our studies, the modified solid-state-reaction method was proved to be an effective method for the preparation of high quality BFO ceramics and the Sm dopant can greatly improve the ferroelectric and magnetic properties.

16:00 Poster I46

Optical ceramics based on cubic refractory oxides via vacuum sintering

Tatyana G. Deineka, Miron Kosmyna, Boris Nazarenko, Vyacheslav M. Puzikov, Zoya P. Sergienko, Alexey N. Shekhovtsov, Alexander V. Tolmachev, Elena A. Vovk, Oleg M. Vovk, Roman P. Yavetskiy

Institute for Single Crystals NAS of Ukraine (ISC), 60 Lenin Ave., Kharkov 61001, Ukraine

e-mail: yavetskiy@isc.kharkov.ua

Nowadays optical ceramics based on cubic materials is considered as a new class of laser or scintillation hosts. It possess excellent optical properties, improved functional characteristics and better mechanical properties compared to single crystals with the same compositions.

Utilization of nanopowders as starting materials allows one to obtain ceramics with full density at relatively low temperatures. Many techniques have been adapted to consolidate highly sinterable nanopowders in a bulk medium, including hot pressing, solid state reaction method, and high-pressure low temperature sintering. We report some recent results on consolidation of Lu_2O_3 and $Y_3Al_5O_{12}$ nanopowders to form transparent ceramics by vacuum sintering.

Lu_2O_3 and $Y_3Al_5O_{12}$ nanopowders with suitable particle size and morphology have been obtained by co-precipitation method. The phase evolution of precursors depending on calcination temperature has been studied using DTA and XPA methods. The morphology of calcinated powders has been studied using TEM. The optimal calcination temperature of precursors to obtain well dispersed powders with average size of 40-60 nm was determined to be T=1100 °C. The sintering ability of Lu_2O_3 and $Y_3Al_5O_{12}$ nanopowders depending on the obtaining conditions has been studied using constant rate of heating sintering.

Compaction of nanopowders has been carried out using cold isostatical or uniaxial pressure at P=200-400 MPa. Vacuum sintering was performed using vacuum furnace at T=1750-1850 °C for 10 hours. It has been shown that sintered transparent ceramics based on Lu_2O_3 or $Y_3Al_5O_{12}$ possess near pore-free structure, vacuum density, grain size up to 50 mkm and linear transmission coefficient up to 60 % for the 1 mm thick specimen. Main luminescent properties of rare earth doped Lu_2O_3, $Y_3Al_5O_{12}$ ceramics for scintillation applications have been determined. The ways to improve the optical transmission of obtained transparent ceramics will also be discussed.

16:00 Poster I47

Joining of SiC to steel using SiC_f/Cu composite.

Wiesława Olesińska, Marcin Chmielewski, Dariusz Kaliński, Katarzyna Z. Pietrzak

Institute of Electronic Materials Technology (ITME), Wólczyńska 133, Warszawa 01-919, Poland

e-mail: olesin-w@sp.itme.edu.pl

Silicon carbide materials, which show very high thermal conductivity, may form interesting applicative compositions when combined with metals of similar properties, such as e.g. copper. Layered Si-C materials and also volumetric composites (also containing SiC fibers) are of special interest. It is however difficult to join these materials, since silicon carbide is not wetted by copper, and since SiC may be decomposed as a result of its reacting with the elements of high chemical activity introduced into copper. Therefore, the process of bonding of these materials should involve the formation of a 'barrier layer' on their surface, such that will bind the decomposition products, restrict the diffusion of active components into the ceramic and ensure its good wettability by liquid copper. The most advantageous active additives able to hamper the decomposition of SiC should enable MeSiC compounds to be synthesized.

The present study was concerned with the wettability of sintered SiC and graphite surfaces by copper and its alloys, and how this wettability is changed when these surfaces were modified with active metals, such as Mn, Ti, Cr and Al. The metals were deposited using the sputtering method and powder metallurgy.

Certain properties of the SiC_f composites produced by the diffusion welding of fibers, plated galvanically with copper, and by pressing a copper powder with the fibers are discussed. The paper also describes the diffusion phenomena that take place in the interface layers of a SiC-Cu/SiC_f composite-steel joint.

16:00 Poster I48

Separation of oil impurities from oil in water emulsions enhance by modified surface of silica filters

Krzysztof Perkowski, Mikołaj Szafran, Janusz Sokołowski

Warsaw University of Technology, Faculty of Chemistry, Noakowskiego 3, Warszawa 00-664, Poland

e-mail: kperkowski@ch.pw.edu.pl

The main aim of the present studies was to develop a method for production of porous ceramic materials capable of separating oil contaminants from highly dispersed oil/water emulsions containing organic particles having dimensions of the order of 1 mm. The pore size of ceramic filtration discs should be at least 100 times as large as the diameter of organic particles separated. The process of separation of oil-water emulsions will be realized in a system with closed liquid flow circuit. The treatment of emulsions will involve the use of ultrasonic waves for increasing the concentration of oil phase in the permeate. Porous ceramic filters used in the process were subjected to modifications aiming at an increase of filtration surface affinity to the oil phase, as well at initiation of local coagulation of oil particles at the filter surface.

Measurements of zeta potential of oil-water emulsion have shown univocally that they are featured by negative electrokinetic potential throughout the whole pH range. Separations of highly dispersed o/w emulsions are carried out in alkaline solutions of pH 8-10. For this reason the filtration discs should have a positive electrokinetic potential that would neutralize the surface charge of oil particles. That would reduce the electrostatic repulsion forces between organic particles thus enabling the coagulation process. It appeared, however, that electrokinetic potential of the sinter of a blend of silicon dioxide with addition of a high temperature binder is negative at pH region 8-10. For obtaining positive values of zeta potential it is necessary to deposit of NiO, MgO or CuO films on quartz sand filtration discs after sintering can shift the electrokinetic potential toward positive values. Literature data show that certain oxides such as NiO or MgO have positive zeta potential in the pH range 8-10.

The work was sponsored by the Ministry of Science and Higher Education in the frame of grants No. 1 T09B 058 30 and N508 008 32/0581

16:00 Poster I49

Protective properties of composite oxide coatings deposited by sol-gel method

Bożena Pietrzyk, Sebastian Miszczak, Zbigniew Gawroński

Technical University of Lodz, Institute of Materials Science and Engineering, 1/15 Stefanowskiego, Łódź 90-924, Poland

e-mail: bozena.pietrzyk@p.lodz.pl

The corrosion resistance of metals can be improved by means of the protective coatings. Recently, besides unary coatings also composite coatings have been investigated.

In this work, composite, sandwich type, Al_2O_3 - TiO_2 coatings were deposited on X2CrNi18-9 and 21CrMoV5 steels by the sol-gel method. TiO_2 and Al_2O_3 soles were prepared using titanium(IV) butoxide and aluminium isopropoxide, respectively. The coatings were annealed at the temperature of 500 and 800^{o}C.

The morphology of coatings was analyzed by SEM. Their protective properties were investigated in the range of electrochemical and high-temperature corrosion. Electrochemical tests were carried out in the

Ringer solution. High-temperature corrosion tests were carried out by the measurement of surrosion. The adhesion of coatings was evaluated using the scratch-test method.

It was found that composite oxide sol-gel coatings increased the resistance of investigated steels in the range of electrochemical and high-temperature corrosion and revealed the good adhesion to the steel substrates.

16:00 Poster I50

Effect of carbon interlayer on the protective properties of hydroxyapatite coating deposited on 316L stainless steel by sol-gel method

Bożena Pietrzyk[1], Jakub Gawroński[1], Tadeusz Błaszczyk[2]

1. *Technical University of Lodz, Institute of Materials Science and Engineering, 1/15 Stefanowskiego, Łódź 90-924, Poland* **2.** *University of Łódź, Department of General and Inorganic Chemistry, Narutowicza 68, Łódź 90-136, Poland*

e-mail: bozena.pietrzyk@p.lodz.pl

Hydroxyapatite (HAP) coatings were deposited on 316L stainless steel by the sol-gel method. The same technique was used also for deposition HAP coatings onto stainless steel substrates coated previously with carbon film by RF PACVD method. The HAP coatings were annealed in air at the temperature of 500°C and 700°C. Their morphology, chemical and crystalline structure were characterized using scanning electron microscopy , energy dispersive x-ray spectroscopy, Fourier transform infrared spectroscopy and X-ray diffraction. The protective properties of the coatings were investigated by means of electrochemical tests which were carried out in Tyrode's solution.

It was found that both carbon and HAP coating improved corrosion resistance of stainless steel substrate. Protective properties of composite carbon-HAP coating depended on the temperature of heat treatment. The composite coating annealed at 500°C revealed better protective properties than that treated at 700°C.

16:00 Poster I51

Investigation of contact interaction of metal melts and non metal materials by high temperature X-ray diffraction method

Tetiana Sydorenko, Oleksiy Durov, Miroslav V. Karpets, Vitaliy Krasovskyy

Institute for Problems in Materias Science (IPMS), 3, Krzhizhanivsky Str., Kiev 03680, Ukraine

e-mail: tvsid@ukr.net

The using of high temperature X-ray diffraction for in situ investigation of processes in liquid metal – solid non metal material systems. The mix of corresponding powders is used as experimental sample. The method was tested for alumina - Ag-Cu-Ti system. The formation of titanium monoxide was observed at high temperature, these results confirms the generally accepted theory. Barium titanate - Cu-Ti and calcium fluoride - Cu-Ti systems were also studied.

16:00 Poster I52

On cation segregation to the grain boundaries and creep response in zirconia-based ceramics

Santiago De Bernardi-Martín[1], Eugenio Zapata-Solvas[1], Francisco J. Guzman-Vazquez[2], Julio Gomez-Herrero[2], Diego Gómez-García[1], Arturo Domínguez-Rodríguez[1]

1. *Universidad de Sevilla (USE), Sevilla 41012, Spain* **2.** *Dept. Fisica Materia Condensada, Universidad Autonoma Madrid, Cantoblanco, Madrid 28049, Spain*

e-mail: debernardi@us.es

Segregation of aliovalent cations to the grain boundaries is reported to play a key role on the high-temperature plasticity of yttria-doped zirconia polycrystals. The role of such segregation on yttria-doped zirconia nanocrystals is still an open question. In order to go further into this problem, a systematic study of the high-temperature plasticity of ceria-doped zirconia polycrystals and nanocrystals has been carried out. Segregation of cerium cations to the grain boundaries should play no role regarding the mechanical behaviour due to the isovalency of zirconium and cerium. Therefore, this is an optimal system to explore the intrinsic behaviour of zirconia ceramics, segregation effects being removed. Preliminary results as well systematic tendencies will be confronted to the existing models in literature.

16:00 Poster I53

Hydrothermal Synthesis of $ZnAl_2O_4$ Spinel

Tomasz Strachowski[1,2], Daniel Sibera[3], Adam Presz[1], Roman Jędrzejewski[4], Jan Mizeracki[1], Witold Łojkowski[1], Urszula Narkiewicz[3]

1. *Polish Academy of Sciences, Institute of High Pressure Physics (UNIPRESS), Sokolowska 29/37, Warszawa 01-142, Poland* **2.** *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland* **3.** *Szczecin University of Technology, Institute of Chemical and Environment Engineering, Szczecin 70-322, Poland* **4.** *Szczecin University of Technology (SZUT), Pułaskiego 10, Szczecin 70-322, Poland*

e-mail: tomasz@unipress.waw.pl

Nanometric zinc aluminate ($ZnAl_2O_4$) of spinel structure was obtained by hydrothermal method using microwave reactor and stop-flow reactor. As the synthesis precursor were used aqueous solution of $Zn(NO_3)_2*6H_2O$ and $Al(NO_3)_3*9H_2O$ salts mixture. During preparation of salts solution, were kept such proportions that Al:Zn molar ratio was 2:1. For the precipitation of hydroxides from the solution, 2 M aqueous solution of KOH were used. During the synthesis process, were used the metal hydroxides suspension in the matrix solution. The aim of this work it was the comparsion of synthesis products from two types of reactors when the parameters of the process: pressure, temperature and reaction time, were kept this same. Achieved products were characterized using XRD analysis, surface area measurement by BET method and density. Morphology were observed using scanning microscope SEM.

Abstracts

in author alphabetical order

Poster

Electronic structure and thermodynamical properties of the multiphased Cr-Si

Iryna V. Uvarova

Institute for Problems of Materials Science, National Academy of Sciences of Ukraine, Krzizanovsky, Kyiv 38(044), Ukraine

e-mail: uvarova@ipms.kiev.ua

Poster

Development of methods for rapid biochemical control over the effect of iron based nanopowders on human organizm

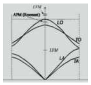
Iryna V. Uvarova, Nataly V. Boshytska, Olena A. Ivashchenko

Institute for Problems of Materials Science, National Academy of Sciences of Ukraine, Krzizanovsky, Kyiv 38(044), Ukraine

e-mail: uvarova@ipms.kiev.ua

New Opportunities and Challenges in Material Research using Phononon and Vibrational Spectra

Symposium J



Welcome

Welcome

In the last two decades research in area of lattice dynamic of solids were developed important methods of characterization playing a pivotal role in characterization of advanced materials at various dimensional and temporal scales. The growing interest and high technological relevance of the vibrational spectra research have been justified by using of new experimental instruments as Fourier spectroscopy and new light sources in infrared region as synchrotron radiation opened in several great facilities both in Europe and worldwide.

This E-MRS symposium is aimed to:

Firstly, we would like to highlight the trends and advances in the techniques of optical metrology in far-infrared region for monocrystals (mainly solid solutions), thin film materials, nanowires and nanotubes. Secondly, we will address the application of such techniques to the study of real local crystalline structure (character of basic cells distribution in lattice and quantitative analyses of defects and impurities) in these materials.

As manufacturing processes become more complicated, it is imperative to employ in-situ metrology; this is particularly true in the microelectronics and micro-systems industry, such as compound semiconductor electronics, photonics, MEMS and sensors.

The current trends in optical metrology mainly concern Fourier spectroscopy and Raman spectroscopy applied to micro- and nanostructures: infrared microscopy and Raman microscopy. Both related techniques (Fourier and Raman) have gained considerable interest in the last decade and are currently involved in the characterization of nanomaterials. In this symposium, these methods will be discussed with particular attention paid to their application, as well as their limitations and complementarities. The participants of Symposium J as well as of another Symposia are kindly welcome to discuss over mentioned problems.

Organisers

Organizers

Dr. Eugen Sheregii

University of Rzeszow, Rejtana 16a, 35-210 Rzeszow, Poland

e-mail: sheregii@univ.rzeszow.pl

Dr. Wojcech Gębicki

Warsaw Technical University

Koszykowa 75, 00-662 Warsaw, Poland

e-mail: wojtg@if.pw.edu.pl

Dr. Yurij Azhniuk

Institute of Electron Physics Ukrainian National Academy of Sciences.

Universitetska St. 21 , 88017 Uzhgorod, Ukraine.

e-mail:yu.azhniuk@gmail.com

Proceedings

Proceedings

The Contributions of Symposium will be published in special issue of phys. stat. sol. (c) part of contributions (of original character) in phys. stat. sol. (b).

Programme

Monday, 15 September

Opening & Plenary Session

Czochralski Award Ceremony
Monday morning, 15 September, 10:00
Small Hall (237)

Lunch break

Monday afternoon, 15 September, 12:30
Inner Courtyards

Phonons in Materials Research

Monday afternoon, 15 September, 14:00
Room 309
Chair: Prof. E.M. Sheregii

14:00 Invited oral

Ab initiocalculations of phonons and other properties of materials

Krzysztof Parlinski

Polish Academy of Sciences, Institute of Nuclear Physics (IFJ PAN), Radzikowskiego 152, Kraków 31-342, Poland Pedagogical University, Institute of Technics, Podchorążych 2, Kraków 30-084, Poland

e-mail: krzysztof.parlinski@ifj.edu.pl

The phonon dispersion curves, and phonon density of states, can be calculated with a standard *ab initio* and the direct method [1] codes.

The procedure, originally applied to pure bulk crystals only, has been extended to study defected crystals, surfaces, adsorbed atoms on the surface, multilayers, etc. The classical phonon dispersion curves and phonon density of state are now calculated routinely. Since the calculations provide not only the phonon frequencies, but also the polarization vectors, one can find the intensity of coherent and incoherent neutron and x-ray scattering to carry on comparisons to the measurements.

Present computer clusters allow to treat quite complex systems. In recent years an interest to strong electron correlation systems has been increased. Along this line the ab initio codes were supplemented by modulus capable to treat such systems. Numerous calculations show that even simple approach which includes local Coulomb interaction energy U reproduces quite well the phonon properties. The materials $PuCoGa_5$, Fe_3O_4 are examples of such systems. Magnetic properties of constituent atoms are another factor which frequently influences the phonon frequencies.

Temperature dependence of many quantities can be described by the quasiharmonic approximation. In particular, this approach allowed to establish the pressure-temperature phase diagram of AlN, Mg_2SiO_4, CaF_2. Ab initio phonon calculations can be performed on two-dimensional systems like graphene, multilayers and surfaces. Specially surfaces covered by monolayers of other compound are interesting to consider due to the appearance of stresses and their influences on the phonon spectra.

References

[1] http://wolf.ifj.edu.pl/phonon/

14:45 Invited oral

Unification of the phonon mode behavior in semiconductor alloys via a simple percolation concept

Olivier Pagès

Université Paul Verlaine, Laboratoire de Physique des Milieux Denses (LPMD), 1 Bd. Arago, Metz 57000, France

e-mail: pages@univ-metz.fr

The usual paradigm to describe long wavelength phonons in $AB_{1-x}C_x$ semiconductor alloys is the virtual crystal approximation (VCA), corresponding to local averaging of alloy disorder. With this, bonds of like species are immersed into the same VCA-like continuum and thus contribute to a unique phonon mode (1-bond→1-mode, macroscopic insight). In fact three sub-types are distinguished: (i) pure 1-bond→1-mode, (ii) mixed-mode, and exceptionally (iii) modified 2-mode. Types (i) and (ii) are accounted for by the modified-random-element-isodisplacement (MREI) model from Chang and Mitra. A theoretical criterion was worked out by Elliott within the coherent potential approximation (CPA) to distinguish between those two types, which has finalized the picture.

However, careful analysis of the vibration spectra in the literature reveals that, in fact, even the leading alloys in each class, i.e. InGaAs (i), ZnTeSe (ii) and InGaP (iii) do not fit into the MREI-VCA/Elliott-CPA classification. Our view is that the VCA misses the essence of the phonon behavior in alloys. As phonons relate directly to the bond force constant, i.e. to a *local* property, we infer that their understanding requires insight into the (B,C)-topologies, which comes to the percolation site theory. In fact, we show that unified understanding of the phonon mode behavior of the representative alloys we discuss can be achieved via a percolation model (1-bond→2-mode, mesoscopic insight) that views an alloy as a composite of the B-rich and C-rich regions, not as a continuum (VCA). The percolation model is a sort of sophistication to the mesoscopic scale of the MREI model, that operates at the macroscopic scale. The basic parameters are estimated via a simple *ab initio* protocol.

This reveals that phonons have the quite unique privilege to provide natural insight into the alloy disorder at the unusual mesoscopic scale. In particular this is much promising for the study of long-range ordering/anticlustering effects.

Coffee break

Monday afternoon, 15 September, 15:30
Main Hall

Joint Poster Session 1

The 1D Phonons, Lattice Dynamics, Electron-phonon coupling
Monday afternoon, 15 September, 16:00
Main Hall

Tuesday, 16 September

Joint session with Symposium A

Viabrational modes in nanotubes
Tuesday morning, 16 September, 9:00
Room 315
Chair: Prof. K. Parlinski

9:00 Invited oral

Vibrational modes in suspended carbon nanotubes probed by transport measurements

Herre S. Van der Zant

e-mail: h.s.j.vanderzant@tudelft.nl

Single-walled carbon nanotubes (SWNTs) are promising building blocks for nano-electromechanical systems because they have a low mass, are easily scalable through their length and have a high Young's modulus of 1.25 TPa, which is almost an order of magnitude higher than that of silicon. At room temperature, we have used a suspended, semiconducting carbon nanotube as a frequency mixer to detect its own mechanical motion. In the range of 200 MHz, a single gate-dependent resonance is observed, which we attribute to the bending mode vibration of suspended carbon nanotubes [1]. A continuum model [2] describes the gate-dependence of the resonance frequency very well and the analysis shows that the nanotube can be tuned from a regime without strain to a regime where it behaves as a vibrating string under tension. At low temperatures, the suspended nanotubes act as quantum dots. Vibrational modes then become visible as harmonic excitation spectra in single-electron tunneling. Phonon-assisted tunneling mediated by (long-wavelength) longitudinal vibration modes has been observed [3] and comparison with a Franck-Condon model indicates a rather strong electron-phonon coupling factor of order unity. Issues that are currently investigated include mechanisms for electron-vibron coupling, mechanical relaxation, mechanical modes in higher-order tunneling and "distortion blockade of current" in ultra-short (< 100 nm) nanotube segments.

[1] B. Witkamp, M. Poot and H.S.J. van der Zant, Nano Lett. **6** (2006) 2904.

[2] S. Sapmaz, Ya. M. Blanter, L. Gurevich, and H.S.J. van der Zant, Phys. Rev. B. **67** (2003) 235414.

[3] S. Sapmaz, P. Jarillo-Herrero, Ya. M. Blanter, C. Dekker and H.S.J. van der Zant, Phys. Rev. Lett. **96** (2006) 026801.

EMAIL: h.s.j.vanderzant@tudelft.nl

9:45	Invited oral

Quantum tunneling through moving nanoobjects

Konstantin Kikoin

Tel Aviv University (TAU), Ramat Aviv, Tel Aviv 69787, Israel

e-mail: konstk@post.tau.ac.il

Among many possibilities provided by nanotechnologies one of the most challenging is the possibility of study quantum tunneling through nanoobject moving in space by means of nanomechanical or electrostatic forces or due to excitation of vibration eigenmodes. We discuss various aspects of quantum tunneling through molecules and/or quantum dots in Kondo resonance regime. Kondo anomalies in tunnel conductance of molecular complexes may be induced by phonon absorption and emission assisting single-electron tunneling [1]. Kondo shuttling through double quantum dots arises due to specific dynamical symmetry of spin multiplets characterizing magnetic state of these nanoobjects [2]. This dynamical symmetry allows also conversion of time-dependent charge input signal applied to the gate into Kondo response in tunnel conductance [3]. All these effects may be described by means of the Anderson model applied to molecular complexes or double quantum dots in a contact with metallic electrodes with time-dependent tunneling between various components of nanodevice.

[1] K. Kikoin, M.N. Kiselev, M.R. Wegewijs, Phys. Rev. Lett. **96**, 176801 (2006)

[2] M.N. Kiselev, K. Kikoin, R.I. Shekhter, and V.M. Vinokur, Phys. Rev. B **74**, 233403 (4) (2006)

[3] M.N. Kiselev, K. Kikoin, J. Richert, arXiv:0803.2676

Coffee break

Tuesday morning, 16 September, 10:30
Main Hall

Joint session with Symposium A

Tuesday morning, 16 September, 11:00
Room 315

11:00	Invited oral

The widths of phonons

Manuel Cardona

Max-Planck-Institut FKF, Heisenbergstr. 1, Stuttgart D70569, Germany

e-mail: M.Cardona@fkf.mpg.de

Most information on the width of phonons in crystals has been obtained by laser Raman spectroscopy: The resolution usually available in INS, and more recently in Inelastic X-ray Scattering, is too poor to yield precise results on phonon widths. Recently, phonon width data have also been obtained by coherent phonon techniques (in the time domain) and by neutron echo experiments, but these methods apply only to phonons of relatively low frequency. Theoretically, the phonon widths are described as the imaginary part of a self-energy, its real part representing a phonon shift beyond the harmonic approximation. The self energy is temperature dependent, a fact that accounts for an increase in width with increasing temperature. The shift usually corresponds to a softening with increasing temperature, although the opposite is sometimes found. The mechanisms involved in this self- energy are either anharmonic interactions (e.g. decay into two phonons) and electron-phonon interactions (in the case of metals and semiconductors).

Several typical and also unusual experimental results involving semiconductors and high Tc superconductors will be discussed together with their theoretical interpretation on the bases mantioned above.

11:45	Invited oral

Raman-Mie scattering from spherical microparticles

Wolfgang Kiefer

Institut für Physikalische Chemie, Am Hubland, Würzburg 97074, Germany

e-mail: wolfgang.kiefer@mail.uni-wuerzburg.de

Spherical particles in the size range of micrometers are excellent resonators for visible light. The elastically (Mie) as well as inelastically (Raman) scattered light is significantly dominated by this property, which leads to so-called morphology dependent resonances (MDRs) in both types of light scattering mechanisms.

The lecture first describes the various ways of trapping single microparticles free in space. Then, applications of combined Raman/Mie scattering from single microdroplets are discussed. This includes evaporation studies, phase transitions, acid/base reactions and polymerization in a single microdroplet. Finally, stimulated Raman scattering from and femtosecond pulse excitation experiments on single microdroplets are described. To interpret the observed femtosecond-Mie spectra, a time-dependent Mie-theory had to be developed.

The work presented had been performed in the author's former laboratories by my former co-workers M. Lankers, J. Musick, J. Popp, V.E. Roman, O. Sbanski, K. Schaschek, S. Schlücker, T. Siebert, and M. Trunk to whom I am most thankful.

Lunch break

Tuesday afternoon, 16 September, 12:30
Inner Courtyards

Parallel Session

Phonons in nanotubes and nanoparticles
Tuesday afternoon, 16 September, 14:00
Room 309
Chair: Prof. Van der Zant

14:00 Oral

Light polarized resonant Raman spectra from individual carbon nanotubes

Jarosław Judek[1,2], David Brunel[2], Thierry Mélin[2], Leszek Adamowicz[1], Wojtek Gebicki[1]

1. *Warsaw University of Technology, Faculty of Physics, Koszykowa 75, Warszawa 00-662, Poland* **2.** *Institut d'Electronique, de Microélectronique et de Nanotechnologie (IEMN), cité scientifique, Lille 59655, France*

e-mail: jerryj@if.pw.edu.pl

There exist literature controversy concerning Raman scattering mechanism from carbon nanotubes. Namely, in the same nanotube the E_{2g} peak in the Y(XX)Y configuration can be stronger than the A_1 peak in the Y(ZZ)Y configuration, what is in disagreement with the depolarization effect.[1] In order to study this issue a detailed polarization dependent resonant Raman spectra from spatially isolated semiconducting single-, double- and multiwalled carbon nanotubes were measured and analysed. Angular variation of intensities for RBM, oTO, IFM, D, G, M and G' bands - in the case of SWNT and for RBM, G and G' band - in the case of DWNT and MWNT was analyzed. All intensities follow the function which is square product of $\cos(\varphi)\cos(\theta)$, where φ and θ are the angles between incident and scattered light polarizations, and the nanotube axis, respectively. Such polarization dependence of Raman spectra implies a diagonal Raman tensor. Weak quantitative changes in the G bands were observed, what suggests different subbands transitions $E_{\mu}^{v} \rightarrow E_{\mu'}^{c}$. On the above basis we suggest a presence of a Raman scattering mechanism, that could lead to the diagonal Raman scattering matrix. Possible explanation of these effects is discussed.

[1] "Advances in single nanotube spectroscopy: Raman spectra from cross-polarized light and chirality dependence of Raman frequencies", A. Jorio et al. Carbon 42 (2004) 1067-1069

14:25 Oral

Whispering modes gallery in nanotubular crystals as origin of high-Tc superconductivity, tera-hertz transducer and photo-acousto-electronic super-resonance effect

Vladimir Pokropivny

Frantsevich Institute for Problems of Materials Science (IPMS), 3, Krzhizhanivsky Str., Kiev 03680, Ukraine

e-mail: pokr@ipms.kiev.ua

Unique properties of carbon and noncarbon nanotubes in reality stem from their nanosize and cylindrical form making them the quantum nanocylinders, in which all the electronic, hypersonic, and electromagnetic waves belonging to the gallery of whispering modes was shown jointly to circulate. Low attenuation and high frequency are the peculiar features of these waves that is capable to enhance strongly the electron-phonon, electron-photon, and phonon-photon interactions. IR and Raman spectra of single-walled BN nanotubes were calculated by ab-initio RHF/6G-31 method. Ordered arrays of nanotubes and nanotubular crystals was shown to form the ideal media for: 1) the room-temperature superconductivity (V.V. Pokropivny. *Int.J.Nanotechnology*. **1**, 77 (2004)); 2) the novel physical phenomenon, the photo-acousto-electronic super-resonance (V.V. Pokropivny. *Mat.Sci. & Eng. C*. **25**, 771 (2005)); 3) the new piezo-acousto-electric transducer of hypersound in extremely high-frequency tera-hertz range (V.V. Pokropivny, et al. *PhysicaE: LowDim.Struct*. **37**, 283 (2007)). Physical background of these phenomena was surveyed.

14:50 Oral

Opportunities in Studying Materials with Developed Mesostructure using Vibration Spectra

Yuriy G. Bezimyanniy

Institute for Problems in Materias Science (IPMS), 3, Krzhizhanivsky Str., Kiev 03680, Ukraine

e-mail: bezimyni@i.com.ua

Vibration spectra are conventionally applied in studying properties of materials at different hierarchic levels. At microlevel, an example of such an application is analysis of vibration parameters of the material lattice. At macrolevel, vibrations of the material sample are used as a unified system. Naturally, in each of the above cases the vibrations occur at characteristic frequencies in significantly separated parts of spectra and carry completely different information on the material or items produced form this material.

At present materials with certain specified properties have found wide application. Creating an adequate complex inner structure of material when other levels may exist between the micro- and the macrolevels often forms these properties. The more complex material structure is, the larger number of parameters is required to describe the state of this material. The presence of developed mesostructure increases the volume of information necessary to represent the state of the material and makes the procedure of data securing from vibration spectra more complex.

The sensitivity of different parts in a vibration spectrum to the properties of the material with a larger number of hierarchic levels has been analyzed within the framework of known model approaches. The conditions and recommendations that allow the acquisition of information on the material properties at different hierarchic levels have been developed. The results of the theoretical analysis have been supported by experimental studies on the multiphase heterogeneous materials that are distinct by their composition, structure and properties and produced by the methods of powder metallurgy, namely, powder and fiber materials and their composites, ceramics, high-porous-cellular materials.

15:10 Oral

Surface phonons in $CdS_{1-x}Se_x$ semiconductor nanoparticles embedded in dielectric media

Yuriy Azhniuk[1], Yuriy I. Hutych[1], Vasyl V. Lopushansky[1], Alexander G. Milekhin[2], Alexander V. Gomonnai, Dietrich RT Zahn[3]

1. *Institute of Electron Physics, Ukr. Nat. Acad. Sci., Universytetska Str., Uzhhorod 88017, Ukraine* **2.** *Institute of Semiconductor Physics SB RAS, Lavrentjeva 13, Novosibirsk 630090, Russian Federation* **3.** *Technische Universitdt Chemnitz, Institut fur Physik, Chemnitz D-09107, Germany*

e-mail: azhn@ukrpost.net

Phonon spectra of $CdS_{1-x}Se_x$ semiconductor nanocrystals, embedded in dielectric media, have been extensively studied due to their broad applications resulting from confinement-related features in the optical spectra. Among the effects, playing an important role in the phonon spectra of nanometer-sized systems, the most significant are phonon confinement, compositional and size dispersion of nanocrystals within the ensemble, as well as a marked contribution of surface phonons due to the high surface-to-volume ratio.In spite of a considerable number of studies, the available data concerning the surface phonons in

$CdS_{1-x}Se_x$ nanocrystals are incomplete and often contradictory. The surface phonon chracteristics have been reported only for a limited interval of x, and the obtained experimental data are insufficient to discuss their consistency with theoretical predictions. There are also contradictory views on the dependence of the surface phonon frequencies in $CdS_{1-x}Se_x$ on the nanocrystal size. No special studies have been devoted to resonance behaviour of surface phonons in II-VI nanocrystals.

Here we report on the studies of surface phonons in $CdS_{1-x}Se_x$ nanocrystals embedded in dielectric media (borosilicate glass, gelatin, polyacrylamide, polyvinyl alcohol) for a broad range of the nanocrystal size and compositions by resonant Raman scattering. The measurements were performed using a Dilor XY 800 triple monochromator with a CCD camera with excitation by Ar+ and Kr+ laser light, tuned from 457.9 to 676.4 nm. The measurements were performed at room temperature.

Dependences of surface phonon parameters on the nanocrystal composition and size are analyzed. For CdS and CdSe nanocrystals a special attention is paid to the dependence of the surface phonon characteristics on the host medium type, the experimental results being compared with the relevant calculations. A strong dependence of the surface phonon frequency and halfwidth on the Raman excitation energy is observed.

Coffee break

Tuesday afternoon, 16 September, 15:30
Main Hall

Parallel Session

Phonons in Quantum Dots
Tuesday afternoon, 16 September, 16:00
Room 309
Chair: Dr. W. Gębicki

16:00 Invited oral

Phonons in InAs Quantum Dot Structures

Alexander G. Milekhin[1], Alexander I. Toropov[1], Dietrich RT Zahn[2]

1. *Institute of Semiconductor Physics SB RAS, Lavrentjeva 13, Novosibirsk 630090, Russian Federation* **2.** *Technische Universitdt Chemnitz, Institut fur Physik, Chemnitz D-09107, Germany*

e-mail: milekhin@thermo.isp.nsc.ru

We present a Raman study of the phonon spectra of periodical structures with (In,Ga)As QDs in (Al,Ga)As matrix as well as AlAs QDs embedded in InAs.

The nanostructures studied were grown by molecular beam epitaxy in the Stranski-Krastanov growth mode on (001)-oriented GaAs substrates.

Low frequency resonant Raman scattering by acoustic phonons was observed in the QD structures. The periodic oscillations seen in the Raman spectra are well described by the elastic continuum model.

Raman scattering by confined TO and LO phonons was observed in both in InAs and AlAs QDs. Optical phonons of QDs are strongly affected by both strain and confinement. The Raman study reveals a two-mode behavior of optical phonons in the whole composition range for both InGaAs QDs and the AlGaAs matrix.

With increasing excitation energy (from 1.8 to 2.4 eV) a red shift of InAs and GaAs-like LO phonons in InGaAs QDs is observed which is explained by selective resonant Raman scattering.

Interface InAs- and GaAs-like phonons as well as AlAs- and GaAs-like phonons were observed in InGaAs QDs and the AlGaAs matrix, respectively. Their frequency positions were analyzed as a function of the alloy content within the dielectric continuum model. The positions of IF phonons in the QD structures observed in the experiment agree well with calculated ones assuming the QDs have a shape of oblate ellipsoids.

In the vicinity with E_0 resonance in QDs, up to third-order scattering is observed, involving both pure overtones of the first-order InAs, GaAs and AlAs optical and interface phonons and combination of phonons from the materials. Possible mechanisms of these processes are discussed.

16:45 Invited oral

Interdiffusion Processes in Self-Organization of Quantum Dot Nanostructures: Raman Scattering and AFM-Investigtion

Mykhailo Valakh

Institute of Semiconductor Physics NAS Ukraine, Kyiv, Ukraine

e-mail: valakh@isp.kiev.ua

It is intended to discuss in this report the results obtained by author and his colleagues for different types of semiconductor nanostructures (Ge/Si, II-VI, III-V) by means of Raman Scattering accompanied by AFM, PL and High-Resolution X-Ray Diffraction. The possible deviation of the observed growth mechanism from a classical Stranski-Krastnov model will be discussed. This deviation was established to be due to the effect of the giant atomic interdiffusion. It is related not only to the anomalously strong surface diffusion of atoms, but is also stimulated by the large strain gradients in QDs and adjacent regions. The interdiffusion changes the growth kinetics and shape of the QDs.

The peculiarities of the interdiffusion in colloidal core-shell QDs are discussed for different combinations of core and shell materials ($E_g^{core} < E_g^{shell}$ and vice versa).

At last, the problem of the spatial lateral ordering of the QDs in multilayer structures is discussed. By the example of InGaAs/GaAs heterosystem it is shown that the very important condition for lateral ordering is the anisotropy of strain fields in the GaAs buffer layers. In multilayer structures a stepwise (from lower to higher layers) enhancement of the strain anisotropy takes place. This results in the anisotropic surface atomic migration and the formation of laterally ordered island chains or even quantum wires. It is important for application that both dots and wires have high size homogeneity.

Wednesday, 17 September

Parallel Session

Phonons in Quantum Wells and Quantum Wires
Wednesday morning, 17 September, 9:00
Room 309
Chair: Dr. Y. Azhniuk

9:00 Invited oral

Raman spectroscopy of ZnTe-based nanowires grown by MBE *

Wojciech Szuszkiewicz[1], Jean-Francois Morhange[2], Elżbieta Janik[1], Wojciech Zaleszczyk[1], Grzegorz Karczewski[1], Tomasz Wojtowicz[1]

1. *Polish Academy of Sciences, Institute of Physics, al. Lotników 32/46, Warszawa 02-668, Poland* **2.** *Institut des nanosciences de Paris (INSP), 140 rue de Lourmel, Paris 75015, France*

e-mail: szusz@ifpan.edu.pl

ZnTe and $Zn_{1-x}Mn_xTe$ nanowires (NWs) with a mixed crystal composition up to $x = 0.6$, grown on GaAs substrates by catalytically enhanced molecular beam epitaxy (MBE), have been investigated by Raman scattering. As it has been demonstrated previously [1,2], in the whole composition range the NWs crystallize in the zinc-blende structure with their axis (<111> direction) aligned along the <111> direction of the GaAs substrate, independently of the crystallographic orientation of this substrate. Their diameters vary in the range from 30 to 70 nm, and their typical length is 1000 nm.

Raman scattering was achieved in resonant condition with the excitation energy close to the direct energy gap of the material. The accumulation of Raman spectra was possible because of weak enough intensity of luminescence near this energy. The intensity of Raman signal was such that it was possible to observe up to three phonon replicas (2LO and 3LO) even on a single NW. The dependence of the Raman spectra on the Mn composition shows the typical behavior of bulk $Zn_{1-x}Mn_xTe$ alloy, which confirm the incorporation of Mn^{2+} ions on the cation substitutional sites of the ZnTe matrix of the NWs. For the composition range $x < 0.2$ the high crystalline quality of the investigated mixed crystal NWs, characterized by the width of the observed Raman structures, is comparable to that corresponding to pure ZnTe NWs [1,2]. The crystalline quality of NWs slightly degrades when the Mn content rises above 20%. This degradation can be attributed to an increasing number of defects or stacking faults in the mixed crystal NWs with higher compositions.

[1] E. Janik et al., *Appl. Phys. Lett.***89**, 133114 (2006).

[2] E. Janik et al., *Nanotechnology***18,** 475606 (2007).

* The research was partially supported by the Ministry of Science and Higher Education (Poland) through grants No N507 030 31/0735 and N515 015 32/0997, and by the Foundation for Polish Science through subsidy 12/2007.

9:50 Oral

Raman Spectroscopy of boron-doped silicon nanowires

Marcin Marczak[1,2], Emmanuelle Pichonat[3], Wojciech Gębicki[1], Thierry Mélin[2], Djamila Hourlier[2]

1. *Warsaw University of Technology, Faculty of Physics, Koszykowa 75, Warszawa 00-662, Poland* **2.** *Institut d'Electronique de Microelectronique et de Nanotechnologie, UMR CNRS 8520 (IEMN), BP 60069 - Cité scientifique-avenue Poincaré, Villeneuve d'Ascq 59652 Cedex, France* **3.** *Laboratoire de Spectrochimie Infrarouge et Raman, Université des Sciences et Technologies de Lil (LASIR), Bâtiment C5, Villeneuve d'Ascq 59655, France*

e-mail: mm@if.pw.edu.pl

We report the results of a Raman scattering study of an array of well aligned and individual isolated boron doped silicon nanowires (B-SiNW). Nanowires were grown by VLS utilizing CVD (Chemical Vapor Deposition) technique. Different excitation wavelengths were used (514nm and 632nm) to check the heating effects and the dependence of the Raman spectra on the excitation laser line. An asymmetric broadening and a shift of the LO-TO Raman band ($520cm^{-1}$) and boron feature at $620cm^{-1}$ have been observed in all analyzed samples. The asymmetry and shift are the result of the phonons interactions with the continuum of filled electron states, where increased number of free carriers are provided by boron doping.. Our data can be well fitted with a Fano-shape line, with the asymmetry parameter $q<4$. This indicates that the free carriers' concentration exceeds 10^{19} cm^{-3} [1]. Another factor that influence the silicon peak position is a sample laser heating. A nanowire perpendicular to the surface has been measured in function of a laser spot distant from the surface. A shift of $1\text{-}2cm^{-1}$ is visible.

[1] Cardeira *et al.* Phys. Rev. B 8, 4734 (1973)

10:10 Oral

Magnetophonon resonance in double quantum wells

Dariusz Płoch, Michał Marchewka, Mariusz J. Woźny, Eugen M. Sheregii

University of Rzeszow, Institute of Physics, Rejtana 16, Rzeszów 35-310, Poland

e-mail: dploch@univ.rzeszow.pl

Presence of some number of different phonon modes is common feature of lattices in ternary as well as quaternary solid solutions and in structures with double (DQW) and multi quantum wells (MQW). This peculiarity is rearranged on electron transport in such systems as diversification of electron-phonon interaction and is appeared in Magnetophonon Resonance (MPR) [1] as additional series of peaks what was observed in CdHgTe [2,3], ZnCdHgTe [4] and MnCdHgTe [5]. In case of MPR in MQW and super-lattices except additional series [6] was observed the subtle structure of peaks too [7]. In this paper are presented and analyze new data of MPR obtained in strong pulse magnetic fields for DQWs based on the GaAs/AlGaAs and InGaAs/InAlAs hetero-structures [8]. The analysis is based on correct calculation of the Landau level energies in QWs and on the conception of deformed tetrahedral basic cells of phonon spectra in solid solutions [9]. The subtle structure of the MPR peaks is explained without participation of the interface phonons or confined phonons.

[1] Gurevich V.L. and Yu. A. Firsov, *Sov.Phys.-JETP*, **13**, 137, 1961;

[2] E.M. Sheregii**,** et.al. *JETP Letters,***47,** 711, 1988;

[3] E. M. Sheregii, Yu. Ugrin, Sov.Phys.Solid State **32**, 27, 1990;

[4] J. Cebulski et.al. *J. Phys.: Cond. Matter*, **10**, pp. 8587,1998;

[5] J. Cebulski et.al *J. Alloys and Comp.*, **371**, 103, 2004;

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[7] G. Tomaka et.al. *Acta Phys. Pol. A*, **94**, 597, 1998;

[8] E.M. Sheregii et. al., *Low Temp. Phys.***30**, 1146, 2004;

[9] B.V. Robouch, A. Kisiel, E.M. Sheregii, *Phys. Rev. B*, **64,** 073204, 2001.

Coffee break

Wednesday morning, 17 September, 10:30
Main Hall

Parallel Session

SR as instrument for the phonon spectra research
Wednesday morning, 17 September, 11:00
Room 309
Chair: Prof. K. Kikoin

11:00 Invited oral

SR a brilliant sources for solid-state researches in the IR and far-IR energy domain

Augusto Marcelli

°Laboratori Nazionali Frascati INFN (INFN), Via E. Fermi 40, Frascati 00044, Italy

e-mail: marcelli@lnf.infn.it

IR spectroscopy probes rotations and vibrations of molecules, low-energy excitations of solids and many other phenomena in condensed matter physics, chemistry, biophysics and materials science. We discuss far and mid-IR spectroscopy and reflectivity measurements of metallic, semiconductor and insulator systems returning accurate information as a function of external parameters such as temperature or pressure. Reflectivity experiments were applied to investigate intrinsic point defects, a characteristic that affects properties of many solid solutions such as HgCdTe. Although limited in sensitivity far-IR reflectivity may be used for a quantitative determination of the vacancy concentration in a lattice thanks to the identification of additional vibrational modes. The same method can be used to identify in a semiconductor O or H impurities that affects crystal properties and limit applications.

Far-IR spectroscopy may be also used to investigate the pressure-driven insulator-to-metal transition, one of the most intriguing phenomena observed in colossal magnetoresistance (CMR) systems. We present high-pressure far-IR absorption measurements on LaCaMnO samples exploiting the unique characteristic of synchrotron radiation emission. The actual path followed by a system towards metallization is peculiar and volume compression affects the delicate balance among existing microscopic interactions. Far-IR spectra of manganites vs. pressure show a shielding of the phonon modes and a strong reduction of the gap, a clear behavior toward a metallic character at RT vs. pressure. Finally, because the superconducting energy gap is an important parameter, we will show that the best method to measure the gap is the measurement of the optical reflectance in the far-IR region below the transition. We will present reflectance curves addressing a typical metallic response in the new Fe-based layered superconductors that could be attributed to the gap formation in the density of state.

11:50 Oral

Far-infrared reflectivity as a probe of point defects in Zn- and Cd-doped HgTe

Józef Cebulski[1], Eugen M. Sheregii[1], Jacek Polit[1], Augusto Marcelli[2], M Piccinini[2], A Kisiel[3], Ina V. Kucherenko[4], Robert Triboulet[5]

1. *University of Rzeszow, Institute of Physics, Rejtana 16, Rzeszów 35-310, Poland* **2.** *°Laboratori Nazionali Frascati INFN (INFN), Via E. Fermi 40, Frascati 00044, Italy* **3.** *Jagiellonian University, Institute of Physics (IF UJ), Reymonta 4, Kraków 30-059, Poland* **4.** *Lebedev Physical Institute RAS, Leninskii pr.53, Moscow 117924, Russian Federation* **5.** *CNRS, Laboratoire de Physique des Solides et de Cristallogenese, 1 Place Aristide Briand, Meudon F 92195, France*

e-mail: cebulski@univ.rzeszow.pl

Intrinsic point defects often play a significant role in determining the properties of mercury-containing solid solutions such as HgCdTe or HgZnTe, which are fundamental materials for infrared (IR) devices [1]. Point defects are stochastic phenomena characterized by a random spatial distribution within the crystal, actually undetectable by methods sensitive only to long-range order such as x-ray diffraction [2].

We present a non-destructive method for quantitative determining the vacancy concentration in the lattice of Hg-based semiconductor alloys with tetrahedral structure. The method is based on the identification of additional vibrational modes (AVM) induced by lattice deformations in the far infrared (FIR) reflectivity spectrum. Although the method is restricted by sensitivity limitations, recent FIR experimental data carried out on HgZnTe and HgCdTe samples containing Hg-vacancies confirmed the presence of AVMs induced by Hg-vacancies in as-grown crystals.

References

[1] R. Dornhaus and G. Nimitz, *Sol.State Phys.*, **78**, 1-119 (1976).

[2] J. Cebulski, E.M. Sheregii, J. Polit, at oll, Appl. Phys. Lett. **92**, 121904 (2008).

cebulski@atena.univ.rzeszow.pl

12:10 Oral

Additional Phonon Modes related to intrinsic defects in CdHgTe

Jacek Polit[1], E Sheregii[1], A Kisiel[2], B V. Robouch[3], M Cestelli Guidi[4], J Cebulski[1], Andrzej Mycielski[5], M Piccinini[3]

1. *University of Rzeszow, Institute of Physics, Rejtana 16, Rzeszów 35-310, Poland* **2.** *Jagiellonian University, Institute of Physics (IF UJ), Reymonta 4, Kraków 30-059, Poland* **3.** *°Laboratori Nazionali Frascati INFN (INFN), Via E. Fermi 40, Frascati 00044, Italy* **4.** *Dipartimento di Fisica and Unita' INFM, Universita' di Roma "La Sapienza", Piazzale Aldo Moro 2, Roma 00185, Italy* **5.** *Polish Academy of Sciences, Institute of Physics, al. Lotników 32/46, Warszawa 02-668, Poland*

e-mail: polijack@univ.rzeszow.pl

Data of the optical reflectivity measurements obtained in far and middle infrared regions for 11 sample of $Cd_xHg_{1-x}Te$ (x=0.06-0.7) in temperature interval from 20 K to 293 K with using of synchrotron radiation (DAFNE- LIGHT in LNF, Italy) as source are presented. The curves of Im e (w) obtained by Kramers-Kroning transformation were analyzed by Lorentzian-approximation of dielectric function using model of deformed tetrahedra. Beside 8 canonical phonon modes observed earlier by Kozyrev et.al. [1], where the region below 120 cm^{-1} was excluded from consideration, the additional several lines were observed by us in this region. The same lines were presented in publications of another authors [2]. Our analysis is based on data for samples of different types (n- and p-type) and technology as well as on temperature dependences of the discussed line intensity in region from 70 cm-1 to 118 cm-1. This analyze shown that two kinds of lines are observed in this region: first type – generated by electronic structure; second one – generated by oscillations in defect-bearing tatrahedra. The last one are Additional Phonon Modes observed earlier in CdTe [3]. [1] Kozyrev et. al. *Phys. Rev. B*, **58,**3,1374(1998), ; [2] Li Biao, Appl.phys.lett, **73,**11,1538,(1998); [3] Polit J. Shereghii E.M., Cebulski J. et. Al., *J. Appl. Phys.***100,**013521, (2006).

Lunch break

Wednesday afternoon, 17 September, 12:30
Inner Courtyards

Parallel session

Manipulation of sound
Wednesday afternoon, 17 September, 14:00
Room 309
Chair: Prof. D. Zahn

14:00 Invited oral

Phononic Crystals and Manipulation of Sound

Yan Pennec, Bahram Djafari-Rouhani, Jérôme Vasseur

Institut d'Electronique, de Microélectronique et de Nanotechnologie (IEMN), cité scientifique, Lille 59655, France

e-mail: yan.pennec@univ-lille1.fr

Phononic crystals are composite materials made of periodic distributions of inclusions embedded in a matrix. Due to their periodic structure, these materials may exhibit, under certain conditions, absolute acoustic band gaps i.e. forbidden bands that are independent of the direction of propagation of the incident elastic wave. In the first part, we present some examples of two-dimensional bulk phononic crystals i.e. two dimensional arrays of inclusions assumed of infinite extent along the third spatial direction. We show that the existence and bandwidth of the gaps depend strongly on the nature of the constituent materials (solid or fluid), the contrast between the physical characteristics (density and elastic constants) of the inclusions and the matrix, the geometry of the array of inclusions, the inclusion shape and the filling factor. The second part is devoted to some possible applications of these composite materials. In particular, we show that defect modes (cavities, wave guides, stubs...) inserted inside the 2D periodic structure may lead to the possibility of manipulating the propagation of sound, very selective frequency filters and efficient devices for wavelength demultiplexing. We present also the possibility of devising sonic insulators for frequencies of the order of the *kHz* with relatively small thicknesses of the phononic crystal sample. Finally we report on the vibration modes of a 2D plate, i.e. a phononic crystal of finite thickness along the axis of the inclusions. We show the possibility of absolute band gaps in the band structure of the plate, either free or deposited on a substrate. We discuss the surface and guided modes which may occur in such a band gap. This should open new perspectives in the field of high-frequency radiofrequency devices.

14:45 Invited oral

Acoustic solitons in light emitting nanostructures

Alexey V. Scherbakov

A.F. Ioffe Physical-Technical Institute, Politekhnicheskaya 26, St-Petersburg 194021, Russian Federation

e-mail: scherbakov@mail.ioffe.ru

Acoustic soliton is the strain pulse with subpicosecond duration and amplitude up to 0.01. Such a giant strain produces significant changes in the energy spectrum of semiconductor nanostructure due to the modulation of its band gap. The energy shift of electron levels induced by acoustic soliton may reach the value of 100 meV. This ultrafast energy modulation of resonance states gives the opportunity to control frequency and intensity of light emitted from nanostructure. The resonance semiconductor nanostructures with an emitting layer placed into optical resonator are the most promising object for this purpose.

The present work is the review of our recent studies of the effect of acoustic soliton on electron spectra and light emission of semiconductor nanostructures [Phys. Rev. Lett **97**, 037401 (2006); Phys. Rev. Lett. **99**, 057402 (2007)]. The samples under study are structures with single quantum well (QW) and planar microcavity (MC). Strain pulse is generated by femtosecond laser heating of metal film evaporated on the back side of the studied sample. The pulse propagates through the sample and, if initial amplitude is high, transforms into the train of acoustic solitons due to the nonlinear elastic properties of the media. Reaching the semiconductor nanostructure acoustic soliton modifies the electron spectra, which are probed optically using time-resolved reflectivity or photoluminescence. In the structures with single QW the subpicosecond duration of a soliton is less than the coherence time of the optical transition between electron levels. The soliton-induced 10-meV energy shift of these levels leads to the chirping effect - frequency modulation of emitted light within the coherence time. The frequency and intensity modulation of photoluminescence on a picosecond time scale is realized in the structures with planar MC. The further fundamental and applied studies based on the energy modulation of resonance states by acoustic soliton are discussed.

Coffee break

Wednesday afternoon, 17 September, 15:30
Main Hall

Joint Poster Session 2

Wednesday afternoon, 17 September, 16:00
Main Hall

Thursday, 18 September

Phonons Spectra of Alloys

Local and Resonant vibrations
Thursday morning, 18 September, 9:00
Room 309
Chair: Prof. M. Valakh

9:00 Oral

Resonance Raman scattering and lattice dynamics of GaMnN crystals

Wojtek Gebicki[1], Pawel Dominik[2], Sławomir Podsiadło[2]

1. *Warsaw University of Technology, Faculty of Physics, Koszykowa 75, Warszawa 00-662, Poland* **2.** *Warsaw University of Technology, Faculty of Chemistry, Noakowskiego 3, Warszawa 00-664, Poland*

e-mail: wojtg@if.pw.edu.pl

We are presenting results of Raman scattering investigation of GaMnN crystals. The detailed study of polarization dependence Raman scattering enabled us to determine the symmetries of phonon bands characteristic for the system. It has been shown that the polarization dependence of the Raman spectra in the longtitudinal optical (LO) phonon spectral region is identical for all the peaks and suggests an impurity induced Fröhlich type resonance Raman scattering. This result is supported by measured dependence of the Raman spectra on excitation laser line. Phonon dispersion curves and density of phonon states have been calculated with use of a combination of VASP and Phonon computer codes. The phonon density of states has been compared with Raman scattering spectra. It has been shown that nitrogen vibrations are responsible for the new Raman bands observed at the LO phonon spectral region. The Mn vibrations are masked by the strong lattice bands. The role of nitrogen vacancy in lattice dynamics of the GaN:Mn system is discussed. Possible usage of the method for interpretation of the Raman spectra resulting from some other defects in GaN is suggested.

9:25 Oral

Point defect phonons in intermetallics: the case of $NiAl_3$ by atomic-scale simulation

Rémy Besson[1], David Tingaud[2]

1. *Laboratoire de Métallurgie Physique et Génie des Matériaux (LMPGM), Université de Lille 1, Villeneuve d'Ascq 59655, France* **2.** *Laboratoire Science des Procédés Céramiques et de Traitements de Surface - UMR 6638 CNRS - Université de Limoges, 123 avenue Albert Thomas, Limoges 87060, France*

e-mail: Remy.Besson@univ-lille1.fr

Although little is known about the influence of phonons on the point defect properties of ordered compounds, experimental measurements (positron annihilation) have pointed out the occurrence of unexpectedly strong effects, especially in iron aluminides. As a complementary approach, the present study, devoted to an atomic-scale simulation study of Al-rich Ni-Al intermetallic phases by means of embedded-atom potentials, aims at providing further insight into the role of this factor, presumably non negligible since it may drastically influence the diffusion of matter, and thus the microstructural evolution during the elaboration and ageing phases of the materials. The present work concerns $NiAl_3$ of cementite-type $D0_{11}$ structure, with a preliminary investigation of its low-temperature point defect structure, based on an independent-point defect approximation. The calculation of the T = 0 K grand canonical (GC) energies $E^0_{GC}(d)$ of the point defects shows the mixed antisite-vacancy character of this compound at low temperature. The defect-induced phonon properties are then tackled by means of a harmonic analysis around the T = 0 K relaxed configuration of each type of point defect: although point defects entail only minor changes in the overall shape of the phonon density of states with respect to that pertaining to the undefected reference crystal, they significantly modify the defect parameters, the relevant quantities becoming the (phonon-corrected) GC free energies $F_{GC}(d) = E^0_{GC}(d) + F^{vib}_{GC}(d)$, with $F^{vib}_{GC}= E^{vib}_{GC} -TS^{vib}_{GC}$. Our analysis demonstrates that, in the latter expression, none of the energy and entropy terms can be neglected in general. Moreover, the F^{vib}_{GC} term being a decreasing (resp. increasing) function of T for antisites (resp. vacancies), phonon-induced inversions of defect populations are expected at moderate temperatures.

9:45 Oral

Manifestation of single and coupled impurities in the vibration spectra of III-V and II-VI semiconductor alloys

Andrei V. Postnikov, Olivier Pagès, Jihane Souhabi, Ayoub Nassour, Joseph Hugel

Université Paul Verlaine, Laboratoire de Physique des Milieux Denses (LPMD), 1 Bd. Arago, Metz 57000, France

e-mail: jihane.souhabi@univ-metz.fr

We overview the study of vibration modes in the impurity limits of pseudobinary (substitutional) semiconductor alloys of the III-V or II-VI composition. On the side of experiments, such modes carry information about internal strains (the force constants being extremely sensitive to tiny variation/stretching of the bond lengths. On the side of ab initio calculations, the modes in question help to identify impurity-related peaks in experimental spectra (amidst a possibly confusing complex pattern), and relate the observed trends in their positions to the underlying structure models which can be thus tested. In the context of alloys study, the single impurity, as well as a couple of nearest (on the same, cation or anion, sublattice) impurities have a virtue of being clear-cut model systems, which allow nevertheless certain "extrapolation" towards further alloying effects.

A systematic study of single AND coupled impurities helps, moreover, to establish quantitative context for the so-called "percolation model" in the vibrational behaviour of mixed semiconductors. This model implies, throughout the whole concentration range, a manifestation of TWO separated vibration modes due to EACH type of cation-anion bond in a given pseudobinary alloy. The onset of such bimodal behaviour occurs already on coming from the single-impurity to impurity-pair regimes. We look into the microscopics of this transitions and discuss why in certain systems the corresponding splitting parameter is almost zero and in others quite large (up to tens of inverse cm).

The systems under study are (Zn,Be)Se, Zn(Se,Te), (Ga,In)As, (Ga,In)P etc., as well as some wurtzite systems. First-principles calculations of phonon spectra are done within the density functional theory, using either planewave/pseudopotential method with linear response (the Pwscf code), or finite-displacements approach with local-orbital method (Siesta).

10:10 Oral

Optical phonon dispersion for zinc-blende semiconductors

Wojciech Szuszkiewicz[1], Bernard Hennion[2]

1. *Polish Academy of Sciences, Institute of Physics, al. Lotników 32/46, Warszawa 02-668, Poland* **2.** *Laboratoire Leon Brillouin, CEA-CNRS, CE Saclay (LLB), Gif-sur-Yvette 91191, France*

e-mail: szusz@ifpan.edu.pl

The simplified model of the optical phonon dispersion has been analyzed in the case of binary semiconducting compound. As it is well known, the typical solution describing vibrations of one-dimensional atomic chain composed of two types of ions exhibits the maximal value of the optical phonon frequency corresponding to the wavenumber q = 0. This behavior of optical phonon modes is an excellent model of lattice vibrations for many important semiconductors, such as GaAs or ZnTe.

Our paper demonstrates that apart from a typical solution there exists also another one. Under particular conditions for selected parameters describing the constituent ions, the optical phonon dispersion may be completely flat or even can change the curvature (point q = 0 corresponds in this case to the frequency minimum). The “anomalous” behavior of the LO phonon mode have been observed by inelastic neutron scattering for a few real binary compounds. Between the oldest known examples of this kind is the lattice dynamics of CuCl, semiconducting compound crystallizing in the zinc-blende structure. More recent data concern mercury chalcogenides: HgSe and β-HgS, also crystallizing in this structure. The lattice dynamics of all compounds above mentioned has been reproduced previously by the rigid-ion model calculations, in the case of CuCl and HgSe an excellent description of the phonon dispersion has also been achieved by the *ab-initio* calculations. However, a simple physical model pointing out the basic factors responsible for the “anomalous” optical phonon behavior has not been previously discussed in these papers.

Coffee break

Thursday morning, 18 September, 10:30
Main Hall

Parallel Session

Interface Phonons and Phonon spectra of Alloys
Thursday morning, 18 September, 11:00
Room 309
Chair: Prof. A. Milekhin

11:00 Invited oral

Raman Monitoring of Organic/Inorganic Interface Formation

Dietrich RT Zahn

e-mail: zahn@physik.tu-chemnitz.de

Raman spectroscopy is a powerful technique to characterise organic and inorganic semiconductors, in particular when it is applied *in situ* during growth of semiconductor layers. In this paper recent results regarding the Raman monitoring of organic/inorganic interfaces are presented. This concerns both the formation of organic semiconductor layers on inorganic semiconductor substrates as well as the formation of metal interfaces with organic semiconductors. The organic semiconductors used are of the small molecule type, *i.e.* phthalocyanines and perylene derivatives, deposited onto silicon and GaAs, respectively, using organic molecular beam deposition under ultra-high vacuum conditions. Raman spectra are taken in a backscattering geometry using multi-channel detection. A prerequisite in order to be sensitive to ultra-thin coverages is the exploitation of resonance conditions. Then the Raman spectra reveal information about the any interaction of molecules with the substrate in the initial phase of deposition and further on about growth mode and molecular orientation. Considering metal deposition on organic semiconductor layers as substrates benefits from the surface enhanced Raman scattering effect and thus yields information about the intimate interface between metals and organic molecules relevant to contact formation in organic electronic devices. Using metals of varying reactivity, *e.g.* silver, indium, and magnesium, the effects of metal diffusion, growth mode, and chemical reactivity are revealed.

11:45 Invited oral

Theory of Lattice Vibrations of Solid Solutions and Examples of its Application

Vladimir S. Vinogradov

Lebedev Physical Institute RAS, Leninskii pr.53, Moscow 117924, Russian Federation

e-mail: vvs@sci.lebedev.ru

First a short historical rewiev of the theory development is given. The used methods, their advantages and limitations are outlined. The main obstacle in the way of the theory development was the difficulty of proper account for scattering of vibrational excitations by many-impurity complexes (clusters). In [1, 2] a solution of this problem was proposed. The main approach of these works is the two-staged averaging procedure. First the averaging and Fourier transforming of theory equations over positions of impurity clusters as a whole are performed. Then the averaging over the distances between impurities in the cluster is carried out. In order to avoid overcounting, each sum over cluster positions is multiplied by factor $1/n$, where n is the number of impurities in the cluster. The theory possesses all the needed physical properties and is capable of describing the complex structure of vibrational spectra of solid solutions. The calculated vibrational spectra of the random linear chain (using $n \sim 10$) are in perfect agreement with the results of the computer simulations by Dean for a linear chain of 8000 atoms [3]. Then the properties of the theory are illustrated using frequency dependences of spectra for different cases. The spectrum changes with a change of the impurity number in the cluster are shown. Physical nature, intensity and shape of different spectral peaks are discussed. The question related to a number of sites in the cluster, which is sufficient for describing the spectra of random lattices of different dimensions, and limits of applicability of the selfconsistent and non-selfconsistent approximations are also discussed. In conclusion the examples of experimental spectra explanation by the theory are presented.

[1] Vinogradov V S 2005 *Physics of the Solid State***47** 10 1937

[2] Vinogradov V S 2007 *Physics of the Solid State***49** 11 2163

[3] Dean P 1961 *Proc. Roy. Soc.* A**260** 1301 263

Lunch break

Thursday afternoon, 18 September, 12:30
Inner Courtyards

Friday, 19 September

E-MRS & EPDIC Joint Plenary Session

Friday morning, 19 September, 9:00
Small Hall (237)

Coffee break

Friday morning, 19 September, 10:30
Main Hall

Posters

Monday, 15 September

Joint Poster Session 1

The 1D Phonons, Lattice Dynamics, Electron-phonon coupling
Monday afternoon, 15 September, 16:00
Main Hall

16:00 Poster J01

Phonon spectroscopy of CdSe$_{1-x}$Te$_x$ nanocrystals grown in a borosilicate glass

Yuriy Azhniuk[1], Yuriy I. Hutych[1], Vasyl V. Lopushansky[1], Larysa A. Prots[1], Alexander V. Gomonnai[1], Dietrich RT Zahn[2]

1. *Institute of Electron Physics, Ukr. Nat. Acad. Sci., Universytetska Str., Uzhhorod 88017, Ukraine* **2.** *Technische Universitdt Chemnitz, Institut fur Physik, Chemnitz D-09107, Germany*

e-mail: azhn@ukrpost.net

Diffusion-limited growth in a glass matrix is a well elaborated technique to obtain ternary II-VI semiconductor nanocrystals where the confined exciton energy gap can be tuned by both compositional and size variation. Contrary to the CdS$_{1-x}$Se$_x$ system, the phonon spectra of which have been studied quite extensively, glass-embedded ternary CdSe$_{1-x}$Te$_x$ nanocrystals are much less investigated. CdSe$_{1-x}$Te$_x$ is known to be a solid solution system with a two-mode phonon spectrum transformation type, hence one can try to use phonon spectroscopy as an efficient and non-destructive tool to determine the nanocrystal composition.

Here we report on the studies of phonon spectra of CdSe$_{1-x}$Te$_x$ nanocrystals obtained in a borosilicate glass by diffusion-limited growth by heat treatment during 2–12 h at the temperatures ranging from 625 to 700^{o}C, resulting in the variation of the nanocrystal composition and size. Resonant Raman scattering studies were performed using a Dilor XY 800 triple monochromator with a CCD camera with excitation by a Kr$^+$ ion laser (647.1 and 676.4 nm). The measurements were carried out at room temperature.

First- and second- order Raman spectra of CdSe$_{1-x}$Te$_x$ nanocrystals were measured. The data obtained are compared with those for for the relevant bulk crystals obtained by Raman and infrared spectroscopy as well as with scarce data of other authors for CdSe$_{1-x}$Te$_x$ nanocrystals. The accuracy of determination of the nanocrystal composition from the phonon spectra is estimated.

A Raman feature near 215 cm-1, observed in the spectra of CdSe$_{1-x}$Te$_x$ nanocrystals, obtained at the heat treatment durations and temperatures below the optimal values for the nanocrystal formation, is attributed to vibrations of anion clusters being formed as an alternative to the diffusion-limited formation of II-VI nanocrystals.

16:00 Poster J02

Phonon spectra of quaternary II-VI semiconductor nanocrystals grown in glass matrices

Yuriy Azhniuk[1], Alexander G. Milekhin[2], Alexander V. Gomonnai[1], Yuriy I. Hutych[1], Vasyl V. Lopushansky[1], Dietrich RT Zahn[3]

1. *Institute of Electron Physics, Ukr. Nat. Acad. Sci., Universytetska Str., Uzhhorod 88017, Ukraine* **2.** *Institute of Semiconductor Physics SB RAS, Lavrentjeva 13, Novosibirsk 630090, Russian Federation* **3.** *Technische Universitdt Chemnitz, Institut fur Physik, Chemnitz D-09107, Germany*

e-mail: azhn@ukrpost.net

The II-VI semiconductor nanocrystals, obtained by various techniques, attract continuous interest due to confinement-related effects in their optical properties, leading to broad applications. Binary and ternary II-VI nanocrystals have been extensively studied by phonon spectroscopy with an emphasize on nanometer-size-related effects (phonon confinement, marked contribution of surface phonons due to the high surface-to-volume ratio, size dispersion of nanocrystals within the ensemble). For ternary II-VI nanocrystals, phonon spectroscopy has been proven to be a reliable and non-destructive tool for determinaton of nanocrystal composition for both one-mode and two-mode systems. As regards quaternary II-VI nanocrystals, their studies are extremely scarce.

Here we report on the studies of the quaternary Cd$_{1-y}$Zn$_y$S$_{1-x}$Se$_x$ and CdS$_{1-x-y}$Se$_x$Te$_y$ nanocrystals phonon spectra obtained in a borosilicate glass by diffusion-limited growth. The nanocrystal composition was varied by the concentration of their components in the initial mixture as well as by the variation of the heat treatment conditions (temperature and duration). Resonant Raman scattering studies were performed using a Dilor XY 800 triple monochromator with a CCD camera with excitation by Ar$^+$ and Kr$^+$ ion laser light being tuned from 476.5 to 647.1 nm. Measurements were performed at room temperature.

The Cd$_{1-y}$Zn$_y$S$_{1-x}$Se$_x$ nanocrystals, formed in the glass matrix, were observed to possess a basically two-mode type of the phonon spectrum transformation (for sulphur-rich nanocrystals) and a more complicated transformation type (for the nanocrystals with higher Se content). For CdS$_{1-x-y}$Se$_x$Te$_y$ nanocrystals a three-mode type of the phonon spectrum transformation was clearly revealed. The obtained results are compared with the calculations and experimental data for the bulk crystals of similar systems. The application possibilities of the phonon spectra to estimate the quaternary nanocrystal composition are discussed.

16:00 Poster J03

Resonant Raman spectroscopy of confined and surface phonons in CdSe-caped CdS nanoparticles

Volodymyr Dzhagan[1], Olexandra Rayevskaya[2], Alexander L. Stroyuk[2], Stepan Kuchmiy[2], Dietrich RT Zahn[3]

1. *Institute of Semiconductor Physics, National Academy of Sciences of Ukraine, Prospect Nauki,45, Kyiv 03028, Ukraine* **2.** *Institute of Physical chemistry of NAS of Ukraine (IFH), Nauky pr., 31, Kyiv 03028, Ukraine* **3.** *Chemnitz University of Technology, Semiconductor Physics, Chemnitz D-09107, Germany*

e-mail: dzhagan@isp.kiev.ua

A variety of mixed or composite II-VI semiconductor nanoparticles (NPs) have been developed and studied up to now in view of their novel physical properties and promising applications in biolabeling, catalysis, LED and photovoltaics technologies. Depending on the bands offset in the composite (core-shell) NPs, one can achieve either stronger confinement of the photogenerated charge carriers within the luminescing NPs, as in CdSe/CdS with consequent PL buildup, or escape of the charge carriers from the core to shell (well), as in CdS/CdSe, or quantum dot – quantum well NPs, such as CdS/CdSe/CdS. In the present report the photocatalytically-produced CdS/CdSe NPs are studied in dependence on the CdSe coverage and excitation wavelength of the Raman spectra. An “island-like” growth mode of CdSe on the CdS-core NP surface is derived from this study. This is in contrast to the generally observed smooth shells in common colloidal CdSe-core NPs, but resembles the case of epitaxially-grown nanoislands, self-assembled in the Stranski-Krastanow mode. The peculiarities of the Raman spectra of the CdS/CdSe/CdS quantum dot – quantum well NPs are also discussed.

16:00 Poster J04

Probing the structure of core-shell nanoparticles by resonant Raman scattering spectroscopy

Volodymyr Dzhagan[1], Mykhailo Valakh[1], Olexandra Rayevskaya[2], Alexander L. Stroyuk[2], Stepan Kuchmiy[2], Dietrich RT Zahn[3]

1. *Institute of Semiconductor Physics, National Academy of Sciences of Ukraine, Prospect Nauki,45, Kyiv 03028, Ukraine* **2.** *Institute of Physical chemistry of NAS of Ukraine (IFH), Nauky pr., 31, Kyiv 03028, Ukraine* **3.** *Chemnitz University of Technology, Semiconductor Physics, Chemnitz D-09107, Germany*

e-mail: dzhagan@isp.kiev.ua

Semiconductor nanoparticles of high structural and optical quality can be now produced in application-sufficient quantities. For a thorough understanding and precise manipulation of properties of composite (hetero-)nanoparticles, the knowledge about their interface structure is needed. A combination of resonant Raman scattering (RRS) with photoluminescence (PL) and optical absorption gives information on the surface and interface structure of heteronanoparticles, supplementary to X-ray, photoelectron spectroscopy and TEM. In the present report a complex effect of the confinement, strain, interdiffusion and distribution of the NP sizes within the ensemble onto the RRS spectra on optical phonons is investigated. In particular, the advantages and shortcomings of the size-selectivity of the resonant Raman scattering from the NP ensembles are discussed. A possibility to assess the interdiffusion extent and residual strain value at the interface of colloidal CdSe/MS (M=Zn, Cd, Pb, Ni, Mn) core-shell NPs from the resonant Raman spectra is demonstrated. CdSe NPs passivated with selenides - HgSe, Ag_2Se, CuSe, Bi_2Se_3 - have not revealed any shell-related phonon bands or shifts of the core phonon peak. The dependence of the surface phonon parameters on the passivating shell type and effective thickness is analyzed.

16:00 Poster J05

Raman scattering on semiconductor microtubes

Alexander G. Milekhin[1], Sergei Mutilin[1], Julia Yukecheva[1], Michael Putyato[1], Alexander Vorob'ev[1], Victor Prinz[1], Vladimir Kolchuzhin[2], Jan Mehner[2], Dietrich RT Zahn[2]

1. *Institute of Semiconductor Physics SB RAS, Lavrentjeva 13, Novosibirsk 630090, Russian Federation* **2.** *Technische Universitdt Chemnitz, Institut fur Physik, Chemnitz D-09107, Germany*

e-mail: milekhin@thermo.isp.nsc.ru

We focused on investigation of the strain in GaAs/InGaAs and InGaAs/InAs bilayer microtubes by means of micro-Raman spectroscopy and comparison of the experimental results with calculated data.

The GaAs/In0.15Ga0.85As and In0.85Ga0.15As/InAs bilayer-based structures were grown by molecular beam epitaxy on GaAs and GaSb substrates, respectively. The GaAs/InGaAs bilayer is formed by 20nm thick In0.15Ga0.85As layer and GaAs top layer of 80 nm. GaAs/InGaAs bilayer consists of InAs layer (15nm) and In0.85Ga0.15As top layer (12nm).

A diameter of InGaAs/InAs microtubes was estimated as 3 mkm while for GaAs/InGaAs tube it was varied from about 20 to 3 mkm due to decreasing upper GaAs layer thickness in the wet etching process.

The micro-Raman scattering experiments were performed using different laser lines at 300K. The scattered light was analysed in backscattering geometry using a Dilor XY triple monochromator. Using a micro-Raman setup the incident laser light was focused with a spot size of 1 mm on a sample surface.

Through analysis of the frequencies of InAs- and GaAs phonon modes observed in the Raman spectra of mictrotubes and as-grown bilayers and comparison with numerical calculations the residual strain in mictrotubes was estimated. The overheating effects in the tubes were excluded by measuring Stokes-anti-Stokes ratio of the Raman-active modes and controlling microtube temperature. A depth profile of residual strain is tested by measuring Raman scattering excited with different laser lines for which the laser light has different penetration depths.

The numerical analysis was carried out using a commercial FE code, the ANSYS Academic Research product. The bilayer structure is modelled with 3-D 8-Node Solid Shell element. Roller and fixed boundary conditions are applied along the axis of symmetry and at the end of the structure, respectively.

16:00 Poster J06

Phonon spectra of nanometric powders and composites of Cu_6PS_5Br superionic conductors

Ihor P. Studenyak[1], Mladen Kranjcec[2], Roman Buchuk[1], Volodymyr O. Stephanovich[1], Yaroslav I. Studenyak[1], Vasyl V. Panko

1. *Uzhgorod National University (UzhNU), Pidhirna str.46, Uzhgorod 88000, Ukraine* **2.** *University of Zagreb, Geotechnical Faculty, 7 Hallerova Aleja, Varazdin 42000, Croatia*

e-mail: studenyak@dr.com

Cu_6PS_5Br superionic conductors are characterized by high ionic conductivity and intrinsic structural disoder caused by the presence of vacancies in copper cation sublattice. Cu_6PS_5Br single crystals were grown by chemical transport reactions. Micro- and nanopowders with average grain size down to 15 nm were obtained by ball milling. The average grain size was estimated from the X-ray diffraction data. Cu_6PS_5Br nanopowder-based composites were obtained by embedding them in polymer films of polytrifluorethylene, polyvinyl chloride, and a copolymer of styrene and maleic anhydride. Raman spectra of the micro- and nanopowders as well as the Cu_6PS_5Br-based nanocomposites were measured at room temperature in a 90^o geometry using a double grating LOMO DFS-24 monochromator and a He-Ne laser (632.8 nm).

In comparison with the single crystals, in Cu_6PS_5Br micro- and nanopowders and in the composites on their base an essential increase of Rayleigh scattering is observed, masking the lower-frequency bands below 100 cm^{-1}. Therefore, in the Raman spectra two well separated bands are observed, the lower-frequency one being a superposition of the E and F_2 symmetry bands, the higher-frequency one corresponding to the A_1 symmetry mode. The crystallite size decrease results in a shift towards lower frequencies, broadening and decrease of intensity for both bands. The changes observed with the crystallite size decrease are explained by Frohlich surface modes revealed in the Raman spectra.

Contrary to the nanopowders spectra, in the Raman spectra of nanocomposites only the A_1 band is distinctly observed while the one due to the superimposement of the E and F_2 symmetry modes is extremely weak what is probably related to the insufficient concentration of the Cu_6PS_5Br nanocrystallites in the matrix. Besides, no changes in the Ramans spectra of the composites, dependent of the matrix type, are observed.

16:00 Poster J07

Influence of electron-phonon coupling on transport through the quantum dot in the Kondo regime

Renata G. Świrkowicz, M. Wilczyński

Warsaw University of Technology, Faculty of Physics, Koszykowa 75, Warszawa 00-662, Poland

e-mail: renatas@if.pw.edu.pl

Recent experimental data on electron transport through molecules and quantum dots have allowed to observe phonon satellites in the Kondo regime. Transport through a quantum dot attached to non-magnetic or ferromagnetic electrodes is studied theoretically within the non-equilibrium Green function formalism and effects of local vibrational modes are analyzed for different values of parameter *g* describing the coupling strength of electron-phonon systems. A presence of phonons strongly influences the spectral function and the differential conductance leading to an appearance of phonon satellites on both sides of the main Kondo anomaly. When the dot is attached to ferromagnetic electrodes with parallel magnetic moments the Kondo resonance is split due to the effective field generated by electrodes. The main components move away from the zero bias limit as polarization of electrodes increases. The Kondo satellites move accordingly and develop in a distance equal to the phonon energy from each Kondo component. The Kondo effect is strongly reduced due to polarization of electrodes and due to coupling to phonon bath. In systems in which spin voltage V_s is applied together with transport voltage V_e spin current I_s and charge current I_e can be carried out. The influence of electron-phonon coupling on the spin conductance $G_s=dI_s/dV_s$ and the charge conductance $G_e=dI_e/dV_s$ is discussed in detail. G_s reveals the dependence similar to that found for junction with ferromagnetic electrodes with two Kondo resonances accompanied by phonon satellites, but quite different behaviour is obtained for the charge conductance.

16:00 Poster J08

Characterization of the Individual Core/ Shell Silicon Nanowires

Marcin Marczak[1,2], Jarosław Judek[1,2], Anna Kozak[1], Wojciech Gębicki[1], Thierry Mélin[2], Djamila Hourlier[2], David Luxembourg[2]

1. *Warsaw University of Technology, Faculty of Physics, Koszykowa 75, Warszawa 00-662, Poland* **2.** *Institut d'Electronique de Micro-electronique et de Nanotechnologie, UMR CNRS 8520 (IEMN), BP 60069 - Cité scientifique-avenue Poincaré, Villeneuve d'Ascq 59652 Cedex, France*

e-mail: mm@if.pw.edu.pl

We report the results of a Raman scattering study of well-separated core/shell silicon nanowires grown by CVD (Chemical Vapor Deposition) and deposited on an Au surface. The diameters varies from around 100nm to 400nm. The analysis of Raman scattering shows a presence of both crystalline (520cm^{-1}) and amorphous (470cm^{-1}) phases of the silicon, forming quite independent fractions. From the growth conditions, nanowires are expected to form a core-shell cone, with the amorphous silicon phase (aSi) outside, and the crystalline silicon phase (cSi) inside. Raman spectra have been analyzed in three points along the examined nanowire length: base, middle and tip. Based on the Stokes/anti-Stokes (St/aSt) ratios, the position and full width at half maximum of the Raman peaks temperatures of the amorphous shell and the cSi core were determined [1]. Against our expectations, the crystalline silicon (cSi) temperature was found lower than the amorphous silicon temperature (aSi) [Fig. 1]. This suggests that the nanowire cSi core is in a good thermal contact with the metallic substrate, thus improving the heat evacuation of the SiNW, for which the thermal conductivity is known to be low [2].

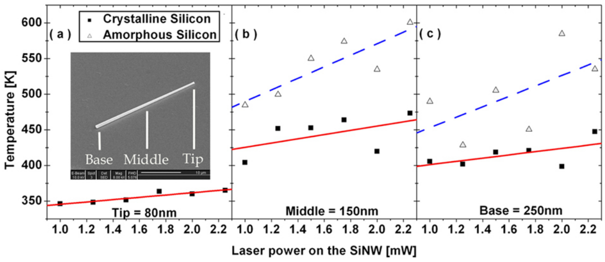

Fig. 1 Temperature of the silicon core and the amorphous shell obtained from St/aSt ratio for the 632nm laser line.

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[2] Piscanec *et al.* Phys. Rev. B, 68, (2003) 241312

16:00 Poster J09

Features of SH-waves propagation in the 1D magnetic phononic crystal

Tetyana V. Laptyeva[1,2], Sergey V. Tarasenko[1], Olga S. Tarasenko[1], Vladimir M. Yurchenko[1]

1. *National Academy of Sciences of Ukraine, A.Galkin Donetsk Institute for Physics & Technology (DonPTI NASU), Roza Luxemburg 72, Donetsk 83114, Ukraine* **2.** *Luhansk Taras Shevchenko National University (LNU), Oboronnaya str., 2, Luhansk 91011, Ukraine*

e-mail: lapteva@mail.fti.ac.donetsk.ua

The composite magnetic materials with a superstructure (magnetic photonic crystals) are actively investigated in view of the conditions of electromagnetic wave transmission [1, 2]. Some of these materials are the acoustically continuous media and then can be considered as magnetic phononic crystals (MPC). However, the acoustic dynamic peculiarities of such structures have been disregarded.

In this work the influence of magnetoelastic interaction on the normal SH modes spectrum of the semifinite 1D MPC with mechanically free surface has been analyzed using the transfer matrix method . In particular, the two-component magnetic superlattice similar to “easy axis ferromagnetic - nonmagnetic dielectric” structure and the MPC similar to “easy axis antiferromagnetic – ideal superconductor” structure were studied. For the represented data we assumed that elastic properties of magnetic and nonmagnetic components of the MPC are identical. Especially (it is necessary to specify that the undermentioned features are determined the magnetoelastic interaction influence):

(i) the existence conditions and dispersion relation for the three case of the surface acoustic SH-waves formation nearby the magnetic superlattice surface have been determined;

(ii) the criterion of a nonreflection transmission of shear bulk elastic wave through the semifinite acoustically continuous superlattice has been formulated;

(iii) the collective shear surface acoustic wave spectrum and the condition of nonreflection transmission can have a nonreciprocity relative to the inversion of the direction of SH-wave propagation along the MPC surface.

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[2] B. Bernard, Single-particle nanomagnetism, Solid State Sciences, 7 (2005) P. 668.

16:00 Poster J10

Lattice dynamics and Raman spectroscopy of ZnO:Mn crystals

Wojtek Gebicki[1], Andrzej Mycielski, Krzysztof Grasza[2]

1. *Warsaw University of Technology, Faculty of Physics, Koszykowa 75, Warszawa 00-662, Poland* **2.** *Polish Academy of Sciences, Institute of Physics, al. Lotników 32/46, Warszawa 02-668, Poland*

e-mail: wojtg@if.pw.edu.pl

Full density matrix functional calculations were performed to calculate structural properties and lattice dynamics of ZnO:Mn crystals. Wien2k and Phonon codes have been used. Both phonon dispersion curves and density of phonon states have been calculated. The phonon density of states has been calculated separately for Zn, Mn and O vibrations. The results of the calculations have been confronted with polarized Raman spectra. The symmetry of the Raman peaks assigned the Mn local vibrations has been identified and will be discussed. Fröhlich type resonant Raman scattering mechanism has been identified.

16:00 Poster J11

Phonon Dispersion Analysis as an Indispensable Tool for Correct Predictions of Solid State Polymorphism

Dominik Kurzydłowski[1], Tomasz Jaroń[1], Wojciech Grochala[1,2]

1. *Warsaw University, Faculty of Chemistry, Pasteura 1, Warszawa 02-093, Poland* **2.** *Warsaw University, Interdisciplinary Centre for Matematical and Computational Modeling (ICM UW), Pawinskiego 5,building D,floor 5, Warszawa 02-106, Poland*

e-mail: d.kurzydlowski@student.uw.edu.pl

Geometry optimization based on *ab initio* electronic structure calculations is a valuable tool for predicting structures of novel compounds in the solid state. But even the most precise optimization scheme can lead to a structure which is not a genuine minimum on the potential energy surface. That is the case for elusive bulk AuF for which three types of structures were proposed previously [1]. Our DFT (GGA/PBE) calculations of the phonon spectra revealed the presence of imaginary modes for all these polymorphs [2]. Distortion of the parent structures along the normal modes of imaginary phonons, and subsequent geometry reoptimization has led us to new polymorphs of AuF, free of imaginary lattice vibrations. Phonon - guided optimizations for a handful of possible polymorphs of XeAuF have yielded *inter alia* a quasi-molecular polymorph (derived from a well known InOBr structure) surpassing its predecessor in enthalpy by almost 0.4 eV [3]. These findings enabled us to propose viable high pressure ($p > 10\,000$ atm) synthetic routes for both compounds [2,3].

To further highlight the usefulness of phonon dispersion analysis we have conducted calculations of the lattice dynamics of solid compressed silane, SiH_4. The earlier theoretical studies have failed to correctly predict its crystal structure [4,5] (determined recently by x-ray diffraction [6]).

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[6] O. Degtyareva, M. Martínez Canales, A. Bergara, X. J. Chen, Y. Song, V. V. Struzhkin, H. Mao, R. J. Hemley Phys. Rev. B 76 (2007) 064123.

16:00 Poster J12

Application of Fourier Transform mid- and far-IR spectroscopy for studies of oxo– derivatives of Ag(II)

Przemyslaw Malinowski[1], Wojciech Grochala[1,2], Zoran Mazej[3]

1. *Warsaw University, Faculty of Chemistry, Pasteura 1, Warszawa 02-093, Poland* **2.** *Interdyscyplinarne Centrum Modelowania Matematycznego i Komputerowego (ICM), Żwirki i Wigury 93, Warszawa 02-089, Poland* **3.** *Jozef Stefan Institute, Jamova 39, Ljubljana, Slovenia*

e-mail: malin77@o2.pl

Three metathetical (ligand exchange) reactions have been performed: (i) $AgF_{2(s)} + CF_3SO_3H_{(l)}$, (ii) $AgF_2 + FSO_3H_{(l)}$, (iii) $Ag(SbF_6)_{2(\text{dissolved in HF})} + K_2SO_{4(\text{dissolved in HF})}$. The solid products have been subject to combined thermogravimetric / calorimetric / evolved gas analysis involving infrared spectroscopy of evolved gases using Bruker's Vertex 80V vacuum FT–IR spectrometer. All products decompose thermally in two distinct steps in the temperature range 80–400 ^{o}C yielding derivatives of Ag(I) and simultaneously evolving O_2 and/or SO_3, and peroxo dimers: $(SO_3F)_2$ or $(SO_3CF_3)_2$ (in equilibrium with their corresponding radicals: SO_3F, SO_3CF_3). Solid products of the metathetical reactions (i-iii) and solid products of their thermal decomposition have been studied with FT mid- and far-IR spectroscopy. Analyses performed indicate that reaction (i) leads to $Ag(SO_3CF_3)_2$, reaction (ii) to an unidentified oxo- derivative, possibly $Ag(SO_3F)_2$, while reaction (iii) to either $Ag^{II}SO_4$ or its electromeric peroxo form $Ag^{I}{}_2S_2O_8$. Complete thermal decomposition of (i) leads to $Ag^{I}(SO_3CF_3)$, that of (iii) to an unidentified product different from $Ag^{I}(SO_3F)$, while that of (iii) to $Ag^{I}{}_2SO_4$.

16:00 Poster J13

Model studies of transformation of dispersion of phonon spectra in defect structures of ABC_3 type

Ivan I. Nebola[1], Ivan M. Shkirta[2]

1. *Uzhhorod National University, Uzhhorod 88000, Ukraine* **2.** *Mukachevo Technological Institiute, Mukachevo 89600, Ukraine*

e-mail: nebola@univ.uzhgorod.ua

In the framework of superspatial symmetry concept we have elaboated a procedure for the calculation of dispersion of phonon spectrum, admitting continuous variation of force constant values and average values of mass characteristics at separate crystallographic sites. ABC_3 structure is considered as a $2a{\times}2a{\times}2a$

superlattice, for which a generalized dynamic matrix is constructed, involving an array of eight modulation vectors which determine the dynamic matrices of the protocrystal and mass defect matrices.

Based on the elaborated procedure, the transformation of dispersion of phonon spectra of $BaTiO_3$-type crystalline structures was studied, the formation of defects in all sites of this structure being simulated. The transformation was analyzed with both conservation and variation of space groups (O_h to D_{4h}). A detailed analysis of variation of the dispersion curves in the vicinity of the Γ point at small variation of the average is performed for defect structures of A (BaTiOOO$_d$) and B (BaTiOO$_d$O$_d$) type where *d* determines the position at which vacancies are located. Transitions between the defect-free structure and A or B type structures as well as the transition between these structures are analyzed. Dispersion curve families have been calculated. Complicated transformations of the phonon spectra degeneracies in some point of the Brillouin zone of the A and B type structures are shown to occur in the frequency range near 350 cm^{-1} at small variations of average mass characteristics, depending on these variation values.

16:00 Poster J14

Extended van Hove Singularity, Strong Electron-Phonon Interaction and Superconducting Gap in Doped Bi-2212 Single Crystals

Yaroslav G. Ponomarev, Mikhail Mikheev, Marina Sudakova, Sergeii Tchesnokov, Svetoslav Kuzmichev

M.V. Lomonosov Moscow State University, Vorobyevy gory, Moscow 119992, Russian Federation

e-mail: ponomarevy@mail.ru

According to A.A. Abrikosov a high T$_c$ in cuprates is caused by the presence of an extended van Hove singularity (EVHS) near the Fermi level. In Abrikosov's model, optical phonons with small wave vectors play a dominant role in pairing. In the present investigation the intrinsic Josephson effect in nanosteps (up to 30 nm) on the cryogenically cleaved surfaces of doped Bi-2212 single crystals has been studied. The obtained results support a previously observed scaling of a superconducting gap and a critical temperature. We have registered a sharp extra structure in the CVC's of perfect Bi-2212 nanosteps which could be caused by the presence of the EVHS close the Fermi level in slightly overdoped and slightly underdoped samples. An interaction between AC Josephson current and Raman-active phonon modes in the entire range of phonon frequencies (up to 20 THz) was observed in doped Bi-2212. It has been found that the structure related to generation of optical phonon modes can be observed in both underdoped and overdoped samples, with the doping level having only a negligible effect on the frequency of the main phonon modes. This means that the electron-phonon coupling in BSCCO does not change significantly over the entire region where superconductivity exists.

16:00 Poster J15

Discontinuity of the phonon mode frequency temperature dependence caused by a zero-gap state in HgCdTe alloys

Józef Cebulski[1], Augusto Marcelli[1,2], Eugen M. Sheregii[1], M Piccinini[2]

1. *University of Rzeszow, Institute of Physics, Rejtana 16, Rzeszów 35-310, Poland* **2.** *°Laboratori Nazionali Frascati INFN (INFN), Via E. Fermi 40, Frascati 00044, Italy*

e-mail: sheregii@univ.rzeszow.pl

Quasi-binary alloy HgCdTe (MCT) form a continuous series of solid solutions of
$Hg_{1-x}Cd_xTe$ over x = 0 to 1 with zinc-blend crystalline structure[1]. In these alloys a band inversion and, as a result, a zero-gap state $E_g \equiv G_6 - G_8 = 0$ is realised as a composition varies from HgTe to CdTe. The zero-gap state depends on temperature too because there are several dependences E_g (x,T) for that is realised $E_g = 0$. These type of peculiarity can be realised by changing of E_g using press or temperature. In this work are presented experimental results of optical reflectivity in far-infrared region (FIR) in wide interval of temperature (from 10 K to 290 K with step 10 K) for sample of $Hg_{1-x}Cd_xTe$ (x=0.115). For observation of effects described above a synchrotron radiation FIR source has a great advantage as compared with the classical sources, intensity of which drops abruptly in this spectral region. Obtained results evidently show that frequencies of optical phonon modes have discontinuity in their temperature dependence when the zero-gap state takes place.

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16:00 Poster J16

Raman scattering studies of disordering processes in $Cu_6P(S_{1-x}Se_x)_5Br_{1-y}I_y$ superionic conductors

Ihor P. Studenyak[1], Mladen Kranjcec[2], Volodymyr O. Stephanovich[1], Vasyl V. Panko[1]

1. *Uzhgorod National University (UzhNU), Pidhirna str.46, Uzhgorod 88000, Ukraine* **2.** *University of Zagreb, Geotechnical Faculty, 7 Hallerova Aleja, Varazdin 42000, Croatia*

e-mail: studenyak@dr.com

$Cu_6P(S_{1-x}Se_x)_5Br_{1-y}I_y$ mixed crystals, known as superionic conductors and ferroelastic materials, were obtained by chemical transport. Raman spectra were measured in a 90^o geometry using a LOMO DFS-24 double grating monochromator and a He-Ne (λ=632.8 nm) laser.

Here we report on the studies of the influence of temperature-related, structural (dynamic and static) and compositional disordering on the low-frequency range ($\omega<100$ cm^{-1}) of phonon spectra of $Cu_6P(S_{1-x}Se_x)_5Br_{1-y}I_y$ superionic conductors. In this frequency range the modes belonging to the diffusive-type vibrations of Cu atoms and Cu–Br(I) bond vibrations are observed.

The monotonous broadening of all phonon bands at the temperature increase from 77 K to the temperature of the transition to the superionic state is due to the temperature-related disordering caused by thermal vibrations of the lattice. Near the superionic phase transition, anomalies in the temperature dependences of the band frequencies are observed as well as their broadening by 10-20 cm^{-1}, explained by dynamic structural disordering of Cu sublattice at the transition to the superionic state.

Raman studies of $Cu_{6+\delta}PS_5Br$ crystals where δ is the deviation from stoichiometry, were performed. With the increase of δ, a high-frequency shift of the bands is observed, as well as an increase of intensity and halfwidth of the lower-frequency band, corresponding to Cu atom vibrations. Meanwhile, the intensity and halfwidth of the higher-frequency band, corresponding to Cu–Br bond vibrations, decrease.

For the phonon spectra of $Cu_6PS_5Br_{1-y}I_y$ mixed crystals the one-mode type of compositional transformation is shown, contrary to the two-mode type in $Cu_6P(S_{1-x}Se_x)_5I$ system. The most essential changes are revealed in the low-frequency range due to the cationic sublattice disordering and the motion of mobile Cu$^+$ ions in the superionic phase. The I→Br substitution results in a nonlinear decrease of the low-frequency band frequency and increase of its halfwidth.

16:00 Poster J17

Raman scattering and infrared spectroscopy of Si-doped GaN thin films

Mykola Vuichyk, Igor Yanchuk, Petro Gentsar, Oksana Lytvyn, Mykola Zayats

V.Lashkaryov Institute of Semiconductor Physics NAS Ukraine (ISP), Nauky prosp., Kyiv 03028, Ukraine

e-mail: vuychik@isp.kiev.ua

In the present work the Raman scattering spectra and infrared reflection spectra of GaN thin films with the thickness of 2-2.5 mm, grown by MOCVD method on sapphire substrates, oriented along the c axis, are investigated. The GaN thin films were doped with Si. AFM studies show the smooth surface of the GaN thin films. In the Raman spectra of the GaN thin films an E_2 phonon mode and an A_1(LO) phonon mode are revealed. In the infrared spectra an A_1(TO) mode and an A_1(LO) mode of wurtzite GaN are detected. The A_1(LO) mode is a function of the free electron density. From the known relationships, the density of free electrons was calculated from the A_1(LO) peak frequency. The presence of mechanical strain in the thin films and the substrate is shown. The experimental results of the studies of the Si-doped GaN thin films grown by MOCVD method, show the wurtzite hexagonal structure of the GaN thin films with the density of free electrons within $10^{18} – 10^{19}$ cm^{-3}.

16:00 Poster J18

Influence of hydrogen on hydrogenated cadmium telluride optical spectra

Malgorzata M. Pociask[1], Jacek Polit[1], E Sheregii[1], J Cebulski[1], A Kisiel[2], Andrzej Mycielski[3], Jerzy Morgiel[4], M Piccinini[5], Augusto Marcelli[5], B V. Robouch[5], M Cestelli Guidi[5,6], Victor Savchyn, I. I. Izhnin[7], Paweł Zajdel[8], A Nucara[6]

1. *University of Rzeszow, Institute of Physics, Rejtana 16, Rzeszów 35-310, Poland* **2.** *Jagiellonian University, Institute of Physics (IF UJ), Reymonta 4, Kraków 30-059, Poland* **3.** *Polish Academy of Sciences, Institute of Physics, al. Lotników 32/46, Warszawa 02-668, Poland* **4.** *Polish Academy of Sciences, Institute of Metallurgy and Materials Sciences (IMIM PAN), Reymonta 25, Kraków 30-059, Poland* **5.** *°Laboratori Nazionali Frascati INFN (INFN), Via E. Fermi 40, Frascati 00044, Italy* **6.** *Dipartimento di Fisica and Unita' INFM, Universita' di Roma "La Sapienza", Piazzale Aldo Moro 2, Roma 00185, Italy* **7.** *R&D Institute for Materials SRC "Carat", Lviv, Ukraine* **8.** *Jagiellonian University, Medical College, Department of Medicinal Chemistry, Medyczna 9, Kraków 30-688, Poland*

e-mail: pociask@univ.rzeszow.pl

The presence of oxygen impurity in semiconducting materials affects the electrical properties of crystals and significantly limits their application. To remove oxygen impurity, ultra-pure hydrogen is used while growing Te-containing crystals such as CdTe, CdZnTe, and ZnTe. The hydrogenation of CdTe crystals is a technological process that purifies the basic material from oxygen, mainly cadmium and tellurium oxide compounds incorporated in CdTe crystalline lattice. In the present work we analyses the deformations induced by hydrogen and oxygen atoms in CdTe crystals looking at their influence on the near fundamental band (NFB), middle infrared (MIR) and far infrared (FIR) reflectivity spectra as well as on cathodoluminescence (CL) spectra. Comparison of the hydrogenated CdTe phonon structure profiles confirms the presence of hydrogen atoms bounded inside the lattice. The possible localization of hydrogen and oxygen ions within the tetrahedron coordinated lattice is discussed in the framework of a model that shows a good agreement with recent NFB, MIR and FIR experiments carried out on hydrogenated CdTe crystals. Measured reflection spectra in the wavelength range 190-1400 nm (NFB) indicate the appearance in CdTe(H_M) and CdTe(H_L) of additional maxima at 966 nm related to the electron transitions from level about 0.2 eV above the valence band. The CL spectra confirmed existence of this electron level. We present a possible H_2 alignment similar to the single H model i.e., over the face (at about 0.38 Å). For this model the angle from the central atom to the H atoms is equal to 64° which is also close to the bonding angle of CdH_2. The propose model was verified by TEM images.

16:00 Poster J20

Confocal Raman microscopy of the strain AlGaN/GaN heterostructures on sapphire

Alexander E. Belyaev[1], Viktor V. Strelchuk[1], Alexander F. Kolomys[1], Svetlana A. Vitusevich[2], Hilde Hardtdegen[2]

1. *Institute of Semiconductor Physics NAS Ukraine, Kyiv, Ukraine*
2. *Institut für Bio und Nanosysteme and CNI Center of Nanoelectronic Systems for Information Tech., Forschungszentrum Jülich GmbH, Jülich D-52425, Germany*

e-mail: kolomys@isp.kiev.ua

Raman spectroscopy has proven to be an informative and nondestructive technique in characterization of nanostructures including local chemical and strain analysis. In this paper the confocal Raman microscopy have been used for the high-spatial-resolution characterization of phonon excitations in AlGaN/GaN heterostructures. These heterostructures were grown on Al_2O_3(0001) substrate with thickness 3 mm and 450 μm. The influence of the crystal inhomogeneous induced by strain, mosaic structure and dislocationson, on the phonon spectra of nitride layers, were studied. Stress values were obtained from the frequency shift of the E_2 (Al)GaN phonon. The measured micro-Raman results have shown the clear gradient distributions of strain along the heterostructure growth direction within both the wurtzite AlGaN/GaN layers and interface layers of the sapphire substrate. It is shown that considerable divergence in the deformation constant data in the literature, concerning of nitride heterostructures, are cased by the mosaic crystal structure peculiarities of nitride layers. Therefore, to characterize the local deformation states at nanoscale of the A^3N heterostructures, the combined micro-Raman microscopy together with high-resolution X-ray diffraction technique should be used. It enable us to calculate the exact value of the phonon deformation potential.

Mechanics of nanomaterials

Symposium K

Welcome

Nano-structured solids are an attractive group of modern engineering materials due to a range of properties in which they are superior to their coarse grained counterparts. In particular, this applies to their mechanical strength, fatigue resistance, faster hydrogen storage kinetics, and a number of other properties. In recent years, bulk nanomaterials suitable for structural applications have emerged due to the development of improved processing techniques, and there is a definite need to address their mechanical response by developing physically based *nanomechanics*.

Application of nanomaterials in new products hinges on a better understanding of the phenomena that control their mechanical properties. Simple extensions of the available models for mechanical properties of conventional materials do not hold for the nano-scale (cf. e.g. the breakdown of the Hall-Petch relationship). This calls for novel approaches in this area. One of them has been based on the concept of phase mixture modelling, while statistical methods have also been proposed as an alternative. Modelling at deeper length scales, including molecular dynamics and discrete dislocation, has been advancing fast, and the results provide a solid platform for developing constitutive models at a continuum level. A connection between the macroscopic quantities, such as stress and strain, and the properties at various length scales, including the nano scale, often needs to be established for an adequate constitutive description. A further important aspect is the non homogeneity of nanomaterials. Many materials that may be regarded as homogeneous at macro level exhibit heterogeneity at micro or nano level. Gradient plasticity approaches may be a way of addressing this issue.

Most real materials are so complex and irregularly heterogeneous that their description involves modelling in probabilistic terms. Methods of the theory of random fields, both continuous and discrete, are of special importance in this regard.

The aim of the Symposium is to provide a platform for exchanging information on the recent development in the field of mechanics of nanomaterials by bringing together diverse communities engaged in this nascent field.

Organisers

Radoslaw Iwankiewicz,

Hamburg University of Technology, Germany

Yuri Estrin,

Monash University, Australia

Programme

Monday, 15 September

Opening & Plenary Session

Czochralski Award Ceremony
Monday morning, 15 September, 10:00
Small Hall (237)

Lunch break

Monday afternoon, 15 September, 12:30
Inner Courtyards

Parallel Session

Monday afternoon, 15 September, 14:00
Room 215

14:00 Invited oral

Atomic-continuum equivalence at nanoscale

Ryszard Pyrz

Aalborg University (AAU), Pontoppidanstræde 101, Aalborg 9220, Denmark

e-mail: rp@ime.aau.dk

The most frequently used form for the stress at atomic level is based upon the Clausius virial theorem, which determines the stress field applied to the surface of a fixed volume containing interacting particles (atoms). It is essential to recognize that the stress at the location of an atom depends on the details of the interatomic interactions and the positions of interacting neighbours. Hence, the atomic stress is a non-local function of the state of the matter at all points in some vicinity of the reference atom, in contrast to the local stress field used in classical continuum theories.

It seems that the relationship between local displacements of atoms and the strain tensor is not as ambiguous as the concept of atomic stress. Strain measure is a relative quantity and one needs two configurations, the reference and the present, in order to define the local atomic strain which should provide detailed local information about kinematics of the atom in relation to its neighbours.

The atomic strain tensor is applied to investigate deformation of regular and disordered molecular systems. As classical continuum mechanics is inherently size-independent, inclusion of atomic strain gradients is used to analyse and predict the mechanical behaviour of nanomaterials in presence of size effects. It is shown that disordered systems exhibit significant nonaffine deformations. The characteristic length scale over which the nonaffine field is correlated serves as a lower limit beyond which classical continuum elasticity cannot be applied. The high non-affinity of disordered (amorphous) nanomaterials possibly stems from a group of strongly bonded atoms behaving as a unit and therefore high moment stresses may result. This effect can be captured by the atomic strain gradient tensor in a way similar to the strain gradient elasticity solution.

14:30 Oral

Molecular statics simulation of nanoindentation on nanocrystalline copper

Toby D. Young[1], Marcin Maździarz[1], Paweł Dłużewski[1], Piotr Traczykowski[1], Krzysztof J. Kurzydlowski[2], Tomasz Wejrzanowski[2,3]

1. *Polish Academy of Sciences, Institute of Fundamental Technological Research (IPPT PAN), Świętokrzyska 21, Warszawa 00-049, Poland* **2.** *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland* **3.** *Interdisciplinary Centre for Materials Modelling (ICMM), Woloska 141, Warszawa 02-507, Poland*

e-mail: tyoung@ippt.gov.pl

We present here a ‘multiscale’ model of nanoindentation of nanocrystalline copper operating on the micro-macro scale in the sense that the volume subjected to large forces (i.e. that directly under the nanoindenter) is represented by classical microscopic theory, whereas the more distant volume subjected to smaller residual forces is represented by a classical macroscopic theory [4]. In particular, by allowing the volume directly subjected to external forces to be governed by an interatomic potential the rearrangement of atomic bonds with the onset of plastic deformation may be observed. To complement this, the physical properties of the continuous region surrounding the atomic part are governed by elasticity theory in order to study the long-range effect of the nanoindentation process. The interaction between atoms is based on the empirical tight binding second moment approximation [1] suitable for systems involving dislocated sharing of free electrons, vis-à-vis copper. Since the behaviour of materials under compression and extension is known to be anharmonic, the surrounding continuum is governed by a nonlinear theory of elasticity. In our case the Hencky strain measure [2] is utilised (although alternative measures, namely Green and Biot, are also considered) [3]. Our multiscale model is therefore a quasistatic approach where contributions from kinetic energy terms have been ignored. This approximation is valid in the adiabatic limit where the process of indentation itself occurs within a short time.

Acknowledgements: This research was funded by the European Commission PARSEM project MRTN-CT-2004-005583.

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14:45 Oral

Molecular dynamics results showing continuum theory failure in describing the elastic behavior of nanoparticles embedded in Si-based systems

Pier Luca Palla, Stefano Giordano, Luciano Colombo

CNR-INFM SLACS and Dept of Physics, University of Cagliari, Cittadella Universitaria di Monserrato, Dept of Physics, University of Cagliari, Cagliari I-09042, Italy

e-mail: pierluca.palla@dsf.unica.it

In recent technological developments Si-based nanostructures have been widely investigated and utilized in many advanced applications, i.e. in optoelectronics, photonics and nanomechanics: typically, crystalline nanograins are dispersed into a silicon matrix in order to obtain desired physical properties such as the optical response, the quantum efficiency and the effective elastic moduli of different systems. The typical sizes of such nanostructures can range from the microscale to the nanoscale, generating several difficulties in the applications of the standard continuum approach to analyze the physical system response. From the mechanical point of view, the classical Eshelby theory describing the behavior of an inhomogeneity embedded in a matrix, does not take into consideration the actual size of the system at all, being this continuum approach a scale-free theory. Therefore, the atomistic structure of the medium is not considered and the results of the elasticity theory are meaningful only for geometrical structures ranging from the mesoscale to the macroscale. When the size of the embedded particles is comparable with the inter-atomic distance of the crystal lattice such results lose their validity and the atomistic simulation can be used to investigate the response at the nanoscale. In the present work we draw a comparison among the continuum theory and molecular dynamics results for Si-based composite systems formed by crystalline (or amorphous) inclusions embedded in a crystalline (or amorphous) bulk matrix. We performed a large campaign of simulations with decreasing radius (starting from a quite macroscopic one) of the cylindrical (or spherical) inhomogeneity. In particular, we observed a characteristic size of the embedded inhomogeneity, which represents the threshold of applicability of the Eshelby theory predictions. Moreover, we obtained the behavior of the elastic fields under such a scale threshold, for different properties of the involved phases.

15:00 Oral

Effect of hydrostatic pressure on defect diffusion in silicon: molecular dynamics simulations

Viktor I. Belko[1], Vasilii Gusakov[2], Nikolai N. Dorozhkin[1]

1. *Belarusian State University (BSU), F. Skaryna av. 4, Minsk 220050, Belarus* **2.** *The Joint Institute of Solid State and Semiconductor Physics of NASB, P.Brovki str., 19, Minsk 220072, Belarus*

e-mail: viktorbelko@yahoo.com

Because diffusion related phenomena become increasingly important as semiconductor device dimensions decrease, diffusion in Si has been heavily studied. The study of stress effects on diffusion is important, e.g., in the study of the stability for strained-layer epitaxial materials in semiconductor technology.

For studying the effect of hydrostatic pressure, we used molecular dynamic simulations with the modified Stillinger-Weber potential. The investigations of defect migration have been performed for a simulation cell, containing one <110> dumbbell interstitial or one di-interstitial with low formation energy.

The simulations for all interstitial configurations were performed at different temperatures and different hydrostatic pressures (zero, high and low). Fitting the data for the self-diffusion coefficient obtained in the simulations for mono-interstitial at zero pressure to the Arrhenius relation yields the values 0.012 cm^2/s and 0.82 eV for the pre-exponential factor and barrier energy, respectively. These values are in reasonable agreement with the values 0.019 and 0.98 from [1], where MD simulations with the same empirical potential have been performed. The values obtained at zero pressure for di-interstitial are $2.3\cdot10^{-4}$ (pre-exponential factor) and 0.54 eV (barrier energy).

The dependence of the resulting diffusion coefficients on pressure has been analyzed and discussed. We can conclude that the self-diffusion coefficients decrease at higher pressure and increase at low pressure for both mono- and di-interstitials. The results have been compared with literature values for the pressure effect on diffusion, and the resulting agreements and disagreements are discussed critically.

[1] Posselt M., Gao F., Zwicker D. Atomistic study of the migration of di- and tri-interstitials in silicon // Phys. Rev. B – 2005. – V. 71 – P. 245202 – 245217.

Coffee break

Monday afternoon, 15 September, 15:30
Main Hall

Joint Poster Session 1

Monday & Wednesday
Monday afternoon, 15 September, 16:00
Main Hall

Tuesday, 16 September

Parallel Session

Tuesday morning, 16 September, 9:00
Room 215

9:00 Invited oral

Homogenization of elastic-viscoplastic heterogeneous materials: Application to nanomaterials

Sebastien Mercier[1], Alain Molinari[1], Yuri Estrin[2]

1. *Laboratoire de Physique et de mécanique des matériaux, UMR CNRS 7554 (LPMM), Ile du Saulcy, Metz 57045, France* **2.** *CSIRO Division of Materials Science and Engineering, Private Bag 33, Clayton South MDC, Melbourne 3169, Australia*

e-mail: mercier@lpmm.univ-metz.fr

The purpose of this talk is to present new homogenization schemes for the prediction of the mechanical behavior of elastic-viscoplastic heterogeneous materials. In a first part, Mori-Tanaka and self-consistent approaches are developed based on an interaction law postulated by Molinari et al (Mech. Mater., 26, 43, 1997). Illustrations are given for two phase composite materials. In a second part of the present talk, we would like to emphasize how a simple homogenization technique can be useful for the prediction of the mechanical behavior of nanomaterials. Based on previous rigid viscoplastic models proposed by Kim et al. (Acta Mater, 48:493, 2000) and Kim and Estrin (Acta Mater, 53:765, 2005), the nanocrystalline material is described as a two phase composite material. Using the Taylor-Lin homogenisation scheme in order to account for elasticity, the yield stress of nanocrystalline materials can be evaluated. The transition from a Hall-Petch relation to an inverse Hall-Petch relation is defined and is related to a change in plastic deformation mode in the crystallite phase from a dislocation glide driven mechanism to a diffusion-controlled process.

9:30 Oral

Strain gradients and the strength of nanoporous gold

Brian Derby, Rui Dou

University of Manchester - School of Materials Science - Materials Science Centre, grosvenor street, Manchester M1 7HS, United Kingdom

e-mail: brian.derby@manchester.ac.uk

We propose a simple strain gradient plasticity model that predicts the very high strengths reported for ligaments in nanoporous gold. This is shown to predict that the yield strength of gold scales inversely with ligament diameter to the power -0.5 with yield stress levels consistent with literature values. The model assumes the predominant deformation mechanism to be the bending of ligaments within the structure of the nanoporous foam, as assumed by the model of Gibson and Ashby [1,2]. The validity of this assumption will be explored to further develop a model for the deformation of nanoporous metals that includes both the effect of a strain gradient and any intrinsic size effect.

1) L.J. Gibson and M.F.Ashby, Proc. Royal. Soc. Lon. **A382** (1982) 43.

2) L.J. Gibson and M.F.Ashby, Cellular Solids: Structure and Properties, second edition, Cambridge University Press, Cambridge, UK, 1997.

9:45 Oral

Study of dislocation nucleation activation from surface step by atomistic calculations

Pierre Hirel, Julien Godet, Sandrine Brochard, Laurent Pizzagalli

University of Poitiers Laboratoire Metallurgie Physique (LMP), Bld Marie et Pierre Curie Chasseneuil du poitou, Poitiers 86192, France

e-mail: pierre.hirel@etu.univ-poitiers.fr

Contrary to bulk materials, in which plasticity is often linked to the presence of Franck-Read sources, nanostructured materials are too small for such sources to operate. Plasticity is then mainly due to the nucleation of dislocations from surfaces and interfaces. In free surfaces, irregularities such as steps are expected to be favored sites for the formation of dislocations. Nucleation, happening at small spatial and temporal scales, is difficult to observe experimentally. An alternative is atomistic simulations, allowing to investigate the very first stages of plasticity.

We present here an analysis of the dislocation nucleation activation from a surface step in a crystal under stress, studied by atomistic calculations. Two model materials are considered: a face centered cubic metal (aluminum) and a diamond-like semiconductor (silicon), both of them being modeled with semi-empirical potentials.

Finite temperature simulations in aluminum lead to the formation of dislocation half-loops, and allow the determination of saddle-point configurations and the associated activation energies. In order to investigate a wide range of applied stress, different methods have been used: molecular dynamics simulations, and nudged elastic band calculations. The obtained results are then compared with those deduced from elasticity.

In the case of silicon, the determination of the activation parameters is more complicated because of the numerous different types of dislocation that can be obtained, depending essentially on the temperature. Nevertheless, the simulations bring important information on a possible change of nucleation mechanisms with temperature, namely nucleation of perfect dislocations in the shuffle set at low temperatures and partial dislocations in the glide set at high temperatures.

Coffee break

Tuesday morning, 16 September, 10:30
Main Hall

Parallel Session
Tuesday morning, 16 September, 11:00
Room 215

11:00 Invited oral

Motion of Connected Grain Boundaries and Stability of Nanocrystalline Systems

Lazar S. Shvindlerman[1,2], Günter Gottstein[1]

1. *Institute for Physical Metallurgy and Metal Physics RWTH Aachen University (IMM), Kopernikusstr. 14, Aachen 52074, Germany*
2. *Russian Academy of Sciences, Institute of Solid State Physics, Chernogolovka 142432, Russian Federation*

e-mail: shvind@imm.rwth-aachen.de

The presentation is dedicated to one of the major topics of modern materials science: evolution and stability of granular microstructures with special emphasis of fine grained and nanocrystalline materials. This problem is considered in the light of recent theoretical studies and computer simulations which provides evidence that the kinetics of connected grain boundaries might be essentially differnt from grain boundary kinetics. This effect is most prominent for fine grained and especially nanocrystalline materials. Major attention is paid to the contribution of grain boundary junctions (triple junctions and quadruple points) to grain microstructure stabilization. The results of recent experimental investigations of grain growth in nanocrystalline materials are discussed in the framework of developed approach.

The efect of faceting on the migration of high-angle boundaries is investigated. It is shown that the steady-state motion of a faceted boundary relates to a maximum dissipation rate of free energy.

11:30 Oral

Characterisation of silicon nitride thin films used as stressor liners on CMOS FETs

Gaetan Raymond, Pierre Morin, Arnaud Devos, Deborah Hess, Muriel Braccini, Fabien Volpi

STMicroelectronics, 850 rue Jean Monnet, Crolles CEDEX 38926, France

e-mail: gaetan.raymond@st.com

Performance enhancement due to process induced strained technology is mandatory in recent CMOS technology (90 nm and beyond) to meet the device specifications. In fact,the strain induced in a Si channel results in band structure distortion and mobility increase..Silicon Nitride (SiN) Contact Etch Stop Layers (CESL) are widely used for this purpose and bring for example an up to 70 % saturation current increase in PMOS transistors.

Standard physical and chemical characterisation is usually carried out, but mechanical measurements are not common on such high stressed thin films. The purpose of this paper is the measurement of Young's modulus and hardness by nanoindentation and picosecond acoustics.

In this paper, we demonstrate that contrary to what the nanoindentation theory expects, one can mechanically characterise our 200 nm thickness high stressed SiN thin film. Moreover, picosecond acoustics appears as the best method for mechanical characterisation of thinner films.

11:45 Oral

MgH_2-Mg interface: a first-principle molecular dynamics characterization

Massimo Celino, Simone Giusepponi

ENEA, via Anguillarese 301, Roma 00123, Italy

e-mail: celino@casaccia.enea.it

Nanostructured magnesium hydride MgH_2, prepared by a mechanical milling method, is considered an attractive hydrogen storage material. In particular, MgH_2 shows interesting properties such as high H_2 gravimetric storage capacity (7.6 wt%), low cost and high abundance. However, this material displays too high temperatures of decomposition, mainly owing to high thermodynamic stability and slow decomposition kinetics, so that several routes have been proposed in order to enhance the reaction and to reduce the decomposition temperature. These processes are based on the introduction of an high density of crystal defects or by ball-milling with intermetallic compounds with lower hydrogen desorption temperature than magnesium.

Since the desorption mechanism is strongly influenced by the chemical and mechanical properties at the interface between MgH_2 and Mg, a detailed study of this interface is needed. From an experimental point of view there is not a clear evidence of which interfaces are involved in the hydrogen diffusion and which is the atomic dynamics at the interfaces. However, extensive first-principle molecular dynamics simulations of the interface MgH_2-Mg give clear indications of both the equilibrium properties and the behaviour of the Mg and H atoms in terms of total energy calculations. The interface and the hydrogen desorption are studied as functions of the temperature. The atomic environment of the Mg atoms at the interface and hydrogen paths for desorption are characterized and studied. Furthermore some indications of the rearrangement of the magnesium atoms after desorption are provided to characterize the phase transition.

Lunch break
Tuesday afternoon, 16 September, 12:30
Inner Courtyards

Wednesday, 17 September

Parallel Session
Wednesday morning, 17 September, 9:00
Room 215

9:00 Invited oral

Nanotubes in global warming: From dynamic topology in superplasticity to hyperthermia in cancer treatment

Boris I. Yakobson

Rice University, 6100 Main St., Houston, TX 77005, United States

e-mail: biy@rice.edu

Two phenomena involving carbon nanotubes (NT) will be discussed. One occurs at very high temperature near 2000°C. Another takes place upon relatively minor yet biologically significant warming by just 10-50°C. Early considerations of dynamic topology of NT at high temperatures have predicted the possibility of plastic flow and quantized necking accompanied by the change of the electronic band gap. Past two years have brought spectacular experimental confirmations to those predictions, while also revealed new intriguing features of superplasticity. The glide of pentagon-heptagon defects and a particular type of their pseudo-climb, act concurrently to maintain the tube perfection, even in spite of great mass loss in sublimation [1-2]. Their dynamics disobey the Frank's rule, showing fundamental difference of dislocation theory in "non-Euclidean" 2D lattice of NT from the traditional 3D crystals.

Recently, our collaborators have discovered the ability of NT to heat up in a radiofrequency (RF) electromagnetic field, which can be used to locally induce hyperthermia to kill cancer cells and tumors [3]. One working hypothesis of RF-induced Joule heating emphasizes the role of large aspect ratio (length/diameter) and allows us to reconcile the high power deposition (<100,000 W/g of NT) with very low NT concentrations $(>10^{-5})$ in aqueous solution.

[1] F. Ding, et al., *Phys. Rev. Lett.***98***,* 075503 (2007); *Nano Lett.***7**, 681 (2007).

[2] J. Huang, et al., *Phys. Rev. Lett.***99**, 175503 (2007); *Phys. Rev. Lett.***100**, 035503 (2008).

[3] C. Gannon, P. Cherukuri, et al., *Cancer***110**, 2654 (2007)

9:30 Oral

On buckling of carbon nanotubes

Grzegorz Litak

Lublin University of Technology (LUT), Nadbystrzycka 38, Lublin 20-618, Poland

e-mail: g.litak@pollub.pl

We investigated single walled Carbon Nanotube under an axially directed compressive line loading applied at both of itsedges. The expected buckling behavior was studied by means of a molecular computation approach [1-2]. We formulated a globalpotential and searched for its minimum to obtain the equilibrium configuration. Beside the main parameter, viz. thevalue of the load, we were looking for a second parameter - the diameter of the tube. We were able to define the critical value of the diameter, forwhich the coincident case of local shell buckling was determined.

[1] D.W. Brenner, Empirical potential for hydrocarbons for use in simulating the chemical vapor deposition of diamond films, Phys. Rev.B 42, 9458–9471 (1990).

[2] A. Proykova and H. Iliev, Simulated Stress and Stretch of SWCNT, in Proceedings of SIMS 2004 Copenhagen, Denmark, September 23–24, 2004**, Editors: B. Elmegaard, J. Sporring, K. Erleben, K. Sorensen. Technical University of Denmark, Lyngby 2004.**

9:45 Oral

Characterization of Mechanical Properties of Nanowires by MEMS Actuator

Jung Mo Seo[1,2], Seung Woo Han[2], Hak Joo Lee[2], Hyun Woo Lee[1], Young Il Kim[3]

1. *School of Mechanical Engineering Pusan National University, Busan 607-735, Korea, South* **2.** *Korea Institute of Machinery and Materials (KIMM), Daejeon 305-600, Korea, South* **3.** *Technical Innovation Center, SUNGKYUNKWAN UNIVERSITY (TIC), Suwon 440-746, Korea, South*

e-mail: seo0918@kimm.re.kr

There is a growing interest in the use of nanostructures including nanotubes and nanowires, because they have demonstrated great potential in a variety of applications for NEMS (nanoelectromechanical systems). Understanding the mechanical behavior of nanowire is very important when it is adopted as the component of NEMS. This research has developed OCTT (on-chip tensile tester) which is designed to measure the mechanical properties of nanowires. OCTT consists of 3 parts: measurement part, actuator part, and supporting part. The OCTT is fabricated by MEMS process and makes from 6 inch SOI wafer with 350μm thickness. From the measurement beam, we can indirectly measure the specimen’s elongation by a scale bar on measurement part. In addition, the relation between specimen’s elongation and measurement beam’s deformation is calculated by traditional beam theory in the mechanics of solids. The driving principle of actuating part is that the electrostatic force between comb fingers is induced when the voltage difference occurs in comb drive fingers. In this research, OCTT contains 10,000 comb drive fingers. The specimen is the nanowire that is attached across the trench in specimen part of OCTT after OCTT was fabricated completely. The bonding condition and alignment of specimens are very important factor in acquiring accurate data of tensile test. The supporting part consists of the suspended beams with constant stiffness, and sustains the whole device. As a result, we obtain the mechanical properties of nanowire such as Young’s modulus, ultimate tensile strength, fracture strength, yield strength, and stress-strain curve.

10:00 Oral

The strength of gold nanowires

Rui Dou, Brian Derby

University of Manchester - School of Materials Science - Materials Science Centre, grosvenor street, Manchester M1 7HS, United Kingdom

e-mail: rui.dou@postgrad.manchester.ac.uk

Many experimental results in the literature show a distinct size effect for the measured yield strength at sub-micron length scales. Two possible mechanisms for this behaviour are strain gradient plasticity and dislocation starvation. Here, we report the yield strength of gold nanowire forests, with wire diameters in the range 30 – 80 nm, measured in uniaxial compression. The yield strength as a function of wire diameter continues to follow the trend reported for larger Au columns [1,2], with the yield stress of 30 nm diameter columns exceeding 1.4 GPa. No significant work hardening is observed at plastic strains up to 30% and because there are no strain gradients in this loading configuration, dislocation starvation is the only plausible hardening mechanism. TEM investigation of deformed nanowires found surface steps consistent with the nucleation of dislocations and their escape from the surface. Uniaxial compression results from nanoporous gold nanowires with 5 nm ligaments are also reported. In this case both strain gradient plasticity and dislocation starvation are thought to be possible strengthening mechanisms.

1) J.R. Greer and W.D. Nix, Phys. Rev. B **73** Art. No. 245410 (2006).

2) C.A. Volkert and E.T. Lilleoddon, Philos. Mag. Vol. **86**, Nos. 33-35, 5567-5579 (2005).

10:15 Oral

A novel three-tier reflective nanofibre structure for high performance thermal resistant but water vapor permeable insulations

Jintu Fan, Huijun Wu

The Hong Kong Polytechnic University (HK, PolyU), Hung Hom, Hong Kong, Hong Kong

e-mail: tchjwu@inet.polyu.edu.hk

A three-tier nanofibre assembly based on aluminum coated poly(vinyl alcohol) (PVA) nanofibres supported onto a spunbonded polypropylene (PP) web was fabricated via electrospinning and physical vapor deposition (PVD) for the first time. The scanning electron microscopy (SEM) and transmission electron microscopic (TEM) characterizations indicate that PVA nanofibers of approximately 430 nm in diameter and an aluminum coating of approximately 37 nm in thickness were successfully embedded on the supporting polypropylene web. Fourier transform infrared (FTIR) spectra and water vapor transmission rate (WVTR) were measured to determine the radiative heat and water vapor transfer through the materials with or without nanofibre or metal coating, respectively. Compared to the control uncoated PP web, the fabricated three-tier nanofibre assembly indicates a significant increase in thermal radiation extinction without noticeable weight increase or reduction in water vapor permeability. This represents a new and simple approach to produce light-weight hybrid layered assembly highly beneficial in reducing thermal radiation and heat loss in low density fibrous insulations without noticeable weight gain or reduction in water vapor impermeability for wide applications such as protective clothing, sleeping bags, building constructions and aircraft.

Coffee break

Wednesday morning, 17 September, 10:30
Main Hall

Parallel Session

Wednesday morning, 17 September, 11:00
Room 215

11:30 Oral

Tailoring mechanical properties by grain refinement and particle redistribution

Malgorzata Lewandowska, Kinga Wawer, Krzysztof J. Kurzydlowski

Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland

e-mail: malew@inmat.pw.edu.pl

Grain size refinement, in particular down to nanometer scale, causes a significant increase in mechanical strength. Among others, grain size refinement can be achieved via severe plastic deformation (such techniques as equal channel angular pressing, high pressure torsion, accumulative roll bonding and hydrostatic extrusion are commonly used in this context).

In this study, an attempt was made to combine grain refinement with controlled particle redistribution and their size reduction in order to improve thermal stability and strength/ductility balance of nanostructured aluminium alloys. The results show coupling of these processes during severe plastic deformation. The resulting microstructures consist of nanoscale grains and uniformly distributed second phase particles. Changes in strength/ductility balance, impact fracture, fatigue strength and thermal stability are measured and discussed.

11:45 Oral

Mechanical Properties of Lead Free Solder Material at High Temperature

Tae ok Kim[1,2], Seung-Woo Han[1], Hak-Joo Lee[1], Sang-Joo Lee[1], Hyun-Woo Lee[2]

1. *Korea Institute of Machinery and Materials (KIMM), Busan 305-343, Korea, South* **2.** *School of Mechanical Engineering Pusan National University, Busan 607-735, Korea, South*

e-mail: koeugeun@kimm.re.kr

For Flip Chip bonding, the solder bump is used commonly. In the solder bump structure, UBM (Under Bump Metallurgy), which is a multilayer of thin film interface metals, is one of the most important components to obtain reliable connections. Many studies have discussed the electromigration mechanism in lead free solder, however the mechanical properties in the high temperature range have still not been researched. When electrical current flows in the solder bump, it is heated and its temperature is raised quite significantly. In case of LED lamp that uses solder bump, the junction temperature as high as 125ºC. Thus the mechanical behavior of the solder bump material at high temperature will become increasingly important for reliability of Flip Chip bonding. We developed a micro-tensile testing system for evaluation of the mechanical properties of thin films at elevated temperatures. The testing system consists of a high temperature furnace, a motor actuator and a DIC (Digital Image Correlation) system which has 50 nm resolution and measures the strain of the specimen in real time. The testing system includes a 20N load cell whose resolution is 0.01N. Temperature range of the furnace is from room temperature to 350ºC. Programs for the testing system were written using LabVIEW 8.5 programming language and Vision Development Module 8.5. In this study, tensile tests were performed a various temperatures: room temperature, 80 ºC, 150 ºC and 210 ºC. The specimen material was electroplated thin film, which is a common solder bump material. Dog bone shaped specimens were fabricated by MEMS (Microelectromechanical System) process. As a result, stress-strain curves were obtained for each temperature and the mechanical properties such as Young's modulus, yield strength and tensile strength were determined.

Lunch break

Wednesday afternoon, 17 September, 12:30
Inner Courtyards

No session

Wednesday afternoon, 17 September, 14:00
Room 215

Coffee break

Wednesday afternoon, 17 September, 15:30
Main Hall

Joint Poster Session 2

Wednesday afternoon, 17 September, 16:00
Main Hall

Friday, 19 September

E-MRS & EPDIC Joint Plenary Session

Friday morning, 19 September, 9:00
Small Hall (237)

Coffee break

Friday morning, 19 September, 10:30
Main Hall

Posters

Monday, 15 September

Joint Poster Session 1

Monday & Wednesday
Monday afternoon, 15 September, 16:00
Main Hall

16:00 Poster K01

Modelling of plastic deformation of nano-polycrystalline materials

Romuald Dobosz, Tomasz Wejrzanowski, Krzysztof J. Kurzydlowski

Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland

e-mail: rdobosz@inmat.pw.edu.pl

Nano-polycrystalline materials are characterized by a significant volume fraction of atoms which need to be viewed as residing at the grain boundaries. The characteristics of these boundaries have a considerable influence on plastic deformation of nano-materials. In order to model this influence quantitatively, two-phase finite element model was developed in which the generalized Hill potential theory for modeling the anisotropic plasticity of grain boundaries was used. The results of numerical simulations show the influence of different parameters on plastic deformation of nano-polycrystalline materials. The simulations were also used to study the grain size effect and grain size homogeneity.

16:00 Poster K02

Peculiarities of structural changes and diffusion distribution of alloying elements in titanium alloys after mechanical-pulse treatment

Olha Kyryliv, Julia A. Budniak, Hryhoriy Nykyforchyn, Krzysztof J. Kurzydlowski

Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland

e-mail: okyryliv@yahoo.com

The influence of mechanical-pulse treatment (MPT) on diffusion (mass transfer) of alloying elements in surface layers of titanium alloys has been investigated. The studied materials were pure titanium VT1-0 (α-structure) and titanium alloy VT6 (α+β-structure). The MPT was carried out in special environments for carburizing and for nitriding. The results of investigations show that concentration of nitrogen and carbon in surface layers after MPT is higher in comparison to the virgin materials. The mechanism of diffusion of alloying elements from the technological environment to surface layers under conditions of high speed thermoplastic deformation is discussed. This fast diffusion leads to changes in structure and phase compositions of the treated surface layers and improvement of their physical and mechanical properties.

16:00 Poster K03

Influence of internal stresses on the properties of solids

Tatyana A. Ryumshyna, Peter Poliakov

Donetsk Physics & Technology Institute of the National Academy of Sciences of Ukraine (DonPhTI NASU), 72 R. Luxembourg St., Donetsk 83114, Ukraine

e-mail: r-tatyana@ukr.net

The experimental study of the resistance properties of many materials in the conditions of the simultaneous action of three thermodynamic factors (temperature, magnetic field, high pressure) [1,2] showed the importance of and the need for examining mechanical stresses in solid bodies. It was discovered that the observed linearity and the reversibility of the resistance properties of the materials correlate with the volume change over a wide range of temperatures, pressures and magnetic field. This leads us to assume that the properties being investigated are determined by the evolution of internal elastic stresses under the conditions of the external actions.

Internal "atomic" stresses appear as forces of elastic repulsion, arising due to deformation of electronic shells of atoms upon the association of separate atoms in a solid under the action of attractive chemical bonds. Including volume elastic forces in the balance of forces, which determine thee of the crystal lattice and the volume of the body, allows relating electrical, chemical and mechanical properties of a solid. According to estimation made on the basis of calculations for deformations of electron shells of free atoms on packing in a solid, and also on the basis of data for the volume change of solids at melting and results of [2], the internal stresses are large (about 100 GPa) and have periodic character consistent with the periodic table of the elements.

Internal stresses are new **collective** property of material, and can be examined, as a main parameter of solid. The distribution of atomic stresses in the solid is sensitive to their defect structure. The special structure of nanomaterials determines the specific field of internal stresses, and, correspondingly, the physical properties.

1. A.D.Bruce, R.A.Cowe. Structural Phase transformation. Taylor & Fransis, London (1981).
2. P.I.Polyakov, S.S.Kucherenko. JMM, 278, (2004), p. 138-155.

16:00 Poster K04

Deformation mechanisms in TiN/NbN multilayer thin films

Karolina A. Rzepiejewska-Malyska[1], Krzysztof Hejduk[2], Sandra Korte[3], William Clegg[3], Johann Michler[1]

1. *EMPA Materials Research and Technology (EMPA), Feuerwerkerstr. 39, Thun 3602, Switzerland* **2.** *Institute of Electron Technology (ITE), al. Lotników 32/46, Warszawa 02-668, Poland* **3.** *University of Cambridge, Pembroke Street, Cambridge, London CB2-3QZ, United Kingdom*

e-mail: karolina.rzepiejewska@empa.ch

The aim of the study was to compare polycrystalline and coherent, single crystal TiN/NbN multilayer thin films with respect to the deformation mechanisms during indentation. TiN/NbN films with different combinations of single layer thicknesses, 4/9 nm (80 periods) for single crystal and 25/25 nm (20 periods) for polycrystalline coatings were deposited in the sputtering process. Single layer reference coatings of TiN and NbN (1 µm thick) were synthesized for comparison in both cases. Hardness was determined by nanoindentation (TriboIndenter, Hysitron, Inc.) using a Berkovich indenter tip. In order to assess toughness, adhesion and deformation modes (pile-up, sink-in or crack propagation) of the coatings, a Hysitron PicoIndenter® integrated into a high resolution scanning electron microscope (SEM) was employed. We have observed a very different mechanical behavior of the reference coatings compared to the multilayer composition of same thickness. Also differences between polycrystalline and single crystal multilayers were observed. In order to get a complete understanding of the fundamental deformation phenomena occurring within the layers, transmission electron microscopy (TEM) observations on the cross-sections of the indented regions were carried out using a focus ion beam (FIB) technique. TEM images revealed that deformation mechanisms strongly depend on the microstructure of the coating. For polycrystalline multilayer films grain boundary sliding was identified as one of the acting mechanisms, while for coherent samples shear band formation and cracks perpendicular to the substrate were predominant. The difference in deformation mechanisms observed will be discussed and linked to the features observed on the load – displacement curves.

16:00 Poster K05

Characterization of the interface between nano crystalline diamond and Silicon substrate

Yoshiki Takagi[1], Takayuki Hirai[2], Toshiaki Suzuki[3]

1. *Teikyo University of Science and Technology, 2525, Uenohara, Yamanashi 409-0193, Japan* **2.** *University of Yamanashi, Takeda 4-437, Kofu 400-8510, Japan* **3.** *JEOL, Fujimicho 1-34-1, Tachikawa 190-0013, Japan*

e-mail: takagi@ntu.ac.jp

In this work, focused ion beam (FIB) technique was employed to characterize the interface between diamond and Silicon substrate. We used a hot filament chemical vapor deposition (HFCVD) reactor to synthesize the diamond and manufacture the cross-sectional parts.

Diamond synthesis from liquid carbon source has a relatively high growth rate and wide area of deposit among various carbon sources. HFCVD is a popular method for growing diamond particles or films. The HFCVD equipment used in the present work is simple and easy to operate.

First, we tried to synthesize a nano crystalline diamond (NCD) on Silicon substrate by HFCVD from liquid carbon source of ethanol. The structure, surface morphology, and grain size of the diamond were examined by field emission scanning electron microscopy (FE-SEM) and Raman spectroscopy. We confirmed our diamond particles as NCD with a typical Raman peak. We also observed diamond particles under 200nm in diameter with FE-SEM.

To analyze the interface between NCD and Silicon substrate with transmission electron microscope (TEM), a cross-sectional sample was prepared by FIB technique. Also, image analysis by STEM, element analysis, energy-dispersive X-ray spectroscopy (EDS) and electron energy-loss spectroscopy (EELS) were performed.

The intermediate thin layer between NCD and Silicon substrate a few nm in thickness was characterized and confirmed with EDS and EESL. Further important analysis will be presented at the meeting.

16:00 Poster K06

Hydrogen-free CVD nano diamond particle synthesis with graphite rod heating

Yoshiki Takagi[1], Takayuki Hirai[2], Hitoshi Kino[3], Osamu Shimizu[3], Yoshihisa Suda[3]

1. *Teikyo University of Science and Technology, 2525, Uenohara, Yamanashi 409-0193, Japan* **2.** *University of Yamanashi, Takeda 4-437, Kofu 400-8510, Japan* **3.** *MITSUBISHI PENCIL CO., LTD., Tateishi 1091, Fujioka 375-8501, Japan*

e-mail: takagi@ntu.ac.jp

A wide band gap semiconductor, diamond has recently emerged as an important and promising material for a wide field of optoelectronic and electronic applications. In traditional CVD (Chemical Vapour Deposition) diamond synthesis on substrate, such as on silicon single crystal, hydrogen radicals were thought to be inevitable. In this work, we synthesized diamond particles of wide band gap semiconductor on substrate without flammable hydrogen gas.

Through our work, safer and easier diamond synthesis was realized. We use graphite rods for heaters - Joule heating - and at the same time as carbon sources. With this method, we can synthesize diamond particles without hydrogen. We refer to our present technique as, "hydrogen-free diamond synthesis".

In argon (99.99%; 4N), high purity argon (6N), helium (4N5) or nitrogen (4N) atmosphere, without hydrogen gas, nano diamond particles were synthesized by the graphite rod heating method. One micrometer diameter particles in argon gas, 0.8 micrometer particles in high purity argon, 0.6 micrometer particles in helium, and 1 micrometer particles in nitrogen, were all confirmed as diamond by SEM micrographs and Raman spectroscopy.

We confirmed diamond particle morphological change with hydrogen content from high purity argon atmosphere up to pure hydrogen atmosphere. For gaseous species identification, OES (Optical Emission Spectroscopy) results will also be reported in this presentation.

16:00 Poster K07

Stochastic Approach To The Changes In The Mechanical Properties Of Nano-Crystalline Materials Induced By Grain Growth

Thomas B. Tengen[1], Tomasz Wejrzanowski[2,4], Radosław Iwankiewicz[3], Krzysztof J. Kurzydlowski[2,4]

1. *Department of Industrial Engineering and Operations Management, Vaal University of Technology (VUT), Vanderbijlpark 1900, South Africa* **2.** *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland* **3.** *Institue of Mechanics and Ocean Engineering, Hamburg University of Technology, Eissedorfer Strasse 42, Hamburg D-21073, Germany* **4.** *Interdisciplinary Centre for Materials Modelling (ICMM), Woloska 141, Warszawa 02-507, Poland*

e-mail: thomas@vut.ac.za

Polycrystalline nanomaterials can be manufactured through different processing routes. The consequence is that nanomaterials having the same mean grain size may have different grain size dispersion and, hence, different material properties.

The present paper studies the impact of detail microstructure evolution on the mechanical properties of nanocrystalline materials. The model for the evolution of the mechanical properties developed is tested on aluminium samples.
The results obtained from the present model reveal many salient features of the mechanical properties of the aluminium samples. Different mechanisms of grain growth impart different nature of response on the material mechanical properties. The conventional, homologous or anomalous temperature dependence of the yield stress has been revealed to be due to different nature of interactions of the microstructures during evolution.

16:00	Poster	K08

Transmission Electron Microscopy Studies of Nano Indented Zirconia Layers on Silicon Wafer Substrates

Lawrence C. Whitmore

University Service Centre for Transmission Electron Microscopy (USTEM), Wiedner Hauptstraße 8-10/138, Wien 1040, Austria

e-mail: whitmore@ustem.tuwien.ac.at

Indentation tests have been performed on silicon wafer substrates with surface layers of ZrO_2. The surface layers have been deposited with a newly developed atomic layer deposition (ALD) process using a Savannah 100 ALD reactor. Substrates with 50 nm nominal thickness layers have been tested using nano-indentation. Indentations were made using a Hysitron nano-indenter at 50 nm and100 nm depth. Subsequent indentations have been studied in cross-section using transmission electron microscopy with specimens prepared using the FIB lift-out technique and ion milling. The layer structure and the layer-substrate interface have been studied. Cross-sections show adhesion of the surface layers to the substrate even through the indentation profile. Underneath the indentations plastic deformation is observed to have occurred by dislocation generation, the formation of amorphous silicon a-Si, and by phase transformation from diamond silicon Si-I to the more dense Si-III phase. The contact surface is studied in detail to examine the contact-induced deformation in the ZrO_2 surface layer. Hardness and elastic modulus are determined from the indentation load-unload curves for the substrate and for the layer and these are compared with values in the literature.

New Scaffolds for Tissue Engineering: Materials and Processing Methods

Symposium L

Welcome

Tissue engineering (TE) is a multidisciplinary/interdisciplinary field, with potential for profoundly changing the medical practice, by regenerating diseased tissues and organs rather than repair. Substantial gains are expected to be obtained both from a medical and economic standpoint as a result of this emerging technology. The social and economical impact of such technology, regarding the patients' health care, are the major driving forces and justifications for the increasing research interests.
The proposed E-MRS Symposium "New Scaffolds for Tissue Engineering: Materials and Processing Methods" will address the latest evolutions and the most recent research challenges regarding the development and application of scaffolds or polymers and composites (including biodegradable ones) in the fields of tissue engineering, tissue regeneration and replacement applications.

The symposium on "New Scaffolds for Tissue Engineering: Materials and Processing Methods" will discuss new integrated advances on the field of Tissue Engineering of Soft and Hard Tissues. It will focus on the materials and techniques to develop adequate scaffolds for Tissue Engineering, as well as biodegradable and non-biodegradable materials and efficient processing methods.

This E-MRS Symposium aims to provide updated tools and innovative knowledge to contribute for the know-how of "hybrid" researchers, enforcing state of the art presentations within this area of Tissue Engineering. It is an objective conviction of the organizer and co-organizers to instruct participants through a tutorial and highly challenging symposium programme, addressing the latest TE scientific knowledge and R&D developments on Materials and Processing Methodologies.

Organisers

- **Dietmar W. Hutmacher**, *Queensland University of Technology, Australia*
- **Wojciech Święszkowski**, *Warsaw University of Technology, Poland*

Programme

Monday, 15 September

Opening & Plenary Session

Czochralski Award Ceremony
Monday morning, 15 September, 10:00
Small Hall (237)

Lunch break

Monday afternoon, 15 September, 12:30
Inner Courtyards

Session 1

Monday afternoon, 15 September, 14:00

14:00 Invited oral

Materiomics: dealing with complexity in Tissue Engineering

Clemens Van Blitterswijk, Dimitris Stamatialis, Hemant Unadkat, Bernke Papenburg, Jeroen Rouwkema, Roman Truckenmüller, Aart Van Apeldoorn, Matthias Wessling, Jan De Boer

University of Twente, Faculty Science and Technology, department of Tissue Regeneration, P.O. Box 217, Enschede 7500AE, Netherlands

e-mail: c.a.vanblitterswijk@tnw.utwente.nl

MATERIOMICS: DEALING WITH COMPLEXITY IN TISSUE ENGINEERING
C.A. van Blitterswijk, D. Stamatialis, H. Unandhar, B. Papenburg, J. Rouwkema, R. Truckenmuller, A. van Apeldoorn, M. Wessling, J. de Boer.

Departments of Tissue Regeneration and Membrane Technology, University of Twente, The Netherlands.
As the human body holds some 200 cell types that synthesize a multitude of both soluble and solid actives in addition to a variety of components that provide various means of mechanical support it will be clear that extremely complex interactions stand at the basis of the proper functioning of all tissues.
With the increase of complexity, certainly when this is associated with a, at best, only partial understanding of the underlying mechanisms, special strategies need to be applied to unravel or direct processes that result from such complex interactions. Rather than striving for a full understanding of the underlying mechanisms upon which to base ones actions, it might be more productive to rapidly screen a multitude of approaches and select the one with the most optimal result. Surprisingly, in tissue engineering this approach is still largely unexplored.
In this presentation, apart from a selective overview of the current state of high throughput in tissue enineering, we will discuss the production of large libraries of material geometries that will allow us to screen thousands to millions of substrates. We propose the name *MATERIOMICS* for the discipline of high throughput methods in biomaterials and tissue engineering science.

14:30 Invited oral

A tissue engineering approach to bone repair: coupling of bone formation and scaffold resorption in a Si-TCP/HA porous ceramic.

Ranieri Cancedda

University of Genova, Genova 16126, Italy

e-mail: ranieri.cancedda@unige.it

Among the different biomaterials considered as scaffolds for bone tissue engineering, calcium phosphate based ceramics have proven to be of great interest given their osteoconductivity and their ability to "integrate" with the bone tissue. We were the first to report the repair of large bone defects in humans by the use of autologous in vitro expanded bone marrow stromal cells (BMSC) associated to a 100% HA porous ceramic. A good integration of the implants with the pre-existing bone was maintained during the more than 7 year follow-up period and no major adverse conditions were observed. Nevertheless an important bias of this pilot study was represented by the low resorbability of the porous HA bioceramics. Therefore resorbable porous ceramic constructs, based on silicon-stabilized tricalcium phosphate, were implanted in critical-size defects of sheep tibias, either alone or after seeding with bone marrow stromal cells (BMSC). Only BMSC-loaded ceramics displayed a progressive scaffold resorption, coincident with new bone deposition. To investigate the coupled mechanisms of bone formation and scaffold resorption, X-ray computed microtomography with synchrotron radiation (mCT) was performed on BMSC-seeded ceramic cubes before and after implantation in immunodeficient mice for 2 or 6 months. With increasing implantation time, scaffold thickness significantly decreased while bone thickness increased. All scaffolds had a uniform density distribution before implantation. Areas of different densities were instead observed, in the *same scaffolds,* once seeded with cells and implanted in vivo. A mX-ray diffraction analysis revealed that at the bone/scaffold interface, the TCP component of the biomaterial decreased much faster than the HA component, highlighting coupling and cell-dependency of the resorption and matrix deposition mechanisms. Moreover, in scaffolds implanted without cells the TCP:HA ratio remained unchanged with respect to the pre-implantation analysis.

15:00 Oral

In-vitro bioactivity of bioresorbable porous polymeric scaffolds incorporating hydroxyapatite microspheres

L. H. Li[1,2], Inderchand Manjubala[1], Krishnaprasad Kommareddy[1], Christine Pilz[1], Changren Zhou[2], Peter Fratzl[1]

1. *Max Planck Institute of Colloids and Interfaces (MPIKGF), Research Campus Golm, Potsdam 14424, Germany* **2.** *Department of Materials Sciences and Engineering, Jinan University, Guangzhou 510630, China*

e-mail: i.manjubala@mpikg.mpg.de

Biomimetic composites consisting of organic polymer and inorganic mineral components, resembling bone in structure and composition, have been used successfully as scaffolds for bone tissue engineering. These scaffolds provide the necessary support for osteoblast cells to proliferate and maintain their differentiated function, spreading, growth and its architecture defines the ultimate shape of the newly formed bone. In the scaffolds produced by conventional techniques, the cell do not migrate more than 500 µm from surface due to lack of oxygen and nutrient supply in the interior as the pore channels are not interconnected. Solid freeform fabrication, popularly known as rapid prototyping (RP) technology brings solution for designing the scaffold with pre-defined and controlled external and internal architecture. Using indirect RP technique, a three component scaffold of wood-pile structure consisting of poly-L-lactic acid, chitosan and hydroxyapatite microspheres were produced having a macro-porosity more than 50% and also micropores in the polymer network. These scaffolds showed excellent biocompatibility and ability of 3D growth of the pre-osteoblastic cells. The MC3T3-E1 pre-osteoblastic cells cultured on these scaffolds formed a network on the hydroxyapatite microspheres and proliferated not only in the macropore channels but also in the direction of the micropores in the polymer network, as seen from the histological analysis and electron microscopy. The mechanical property of these scaffolds resembled that of a cellular structure and therefore can be used for non-load bearing applications.

15:15 Oral

High-throughput laser printing of cells and biomaterials for bone tissue engineering

Fabien Guillemot[1], Sylvain Catros[1], Agnès Souquet[1], Reine Bareille[1], Murielle Rémy[1], Patrick Chabassier[2], Jean-Christophe Fricain[1], Joëlle Amédée[1]

1. *Laboratoire de biomatériaux et réparation tissulaire, Université Victor Segalen Bordeaux 2, case postale 45, 146 rue Léo-Saignat, Bordeaux 33076, France* **2.** *NOVALASE, 6 impasse du Bois de la Grange, Canéjan 33610, France*

e-mail: fabien.guillemot@inserm.fr

Parallel to inkjet printing [1-3] and bioplotting, Biological Laser Printing (BioLP) using Laser-Induced Forward Transfer (LIFT) [4] emerges as an alternative method to assembly and micropattern biomaterials and cells. BioLP offers a wide range of advantages vs. inkjet techniques although this later benefits of a deep understanding and wide technological developments since its origin. BioLP specificities concern mainly the absence of clogging and the capacity of printing fluids with a wide range of viscosity. In addition, as an optics-based method, a laser printing device can also be set up for aiming and shotting as well as marking, cutting, exciting, photo-polymerizing or else foaming materials.

In this paper, we present results on high-throughput laser printing of different human cell lines (EAHy926 and MG63) and biomaterials (nano-sized HA synthesized by wet precipitation) giving an interest for 3D bone-like tissue building. First, a rapid prototyping workstation equipped with an infra-red pulsed laser (τ=30 ns,λ=1064nm, f=1-100kHz), galvanometric mirrors (scanning speed up to 500mm/s) and micrometric x-y-z translation stages has been set up. Droplets size (20 to 100 µm) has been controlled by monitoring laser fluence and focalisation conditions. Droplets of 70µm in diameter containing around 5-7 living cells per droplet has been obtained minimizing the dead volume of hydrogel around cells. In addition to cell transfer, we demonstrate the BioLP potential for creating well defined nano-sized HA patterns. Finally, in addition to these single- element printings, first multicolor laser printings of above-mentioned elements are presented.

1. RE Saunders et al. Biomaterials. 2008 Jan;29(2):193-203

2. EA Roth et al. Biomaterials. 2004 Aug;25(17):3707-15.

3. M. Nakamura et al. Tissue Eng. 2005 Nov-Dec;11(11-12):1658-66.

4. M. Colina et al. Biosens Bioelectron. 2005 Feb 15;20(8):1638-42.

Coffee break

Monday afternoon, 15 September, 15:30
Main Hall

Joint Poster Session 1

Monday & Wednesday
Monday afternoon, 15 September, 16:00
Main Hall

Tuesday, 16 September

Symposium H presentations

Tuesday morning, 16 September, 9:00
Room 213

Coffee break

Tuesday morning, 16 September, 10:30
Main Hall

Session 2

Tuesday morning, 16 September, 11:00
Room 213

11:00 Invited oral

Melt Electrospinning and its Potential for Tissue Engineering

Paul Dalton[1,2], Dirk Grafahrend[2], Kristina Klinkhammer[2], Doris Klee[2], Martin Moeller[2]

1. *University of Southampton, Southampton SO167PX, United Kingdom* **2.** *Deutsches Wollforschungsinstitut, Aachen D52076, Germany*

e-mail: dalton@soton.ac.uk

It is widely known that molten polymers may be electrospun; however there are comparatively few articles on melt electrospinning in the literature. Electrospinning from the melt may allow new approaches to certain aspects of electrospinning, particularly overcoming the technical restrictions governed by solvent accumulation and toxicity.

Both high and low melting point polymers can be melt electrospun, and electrospinning directly onto cells is feasible. In this research, biocompatible amphiphilic block copolymers of polyethylene glycol and poly(e-caprolactone) (PEG-*b*-PCL) are used, and their viscosity tailored through blending with other polymers. We also demonstrate that polypropylene fibers can be reduced from 35±8 mm in diameter, to 840±190 nm with a viscosity-reducing additive. Melt electrospun blends of PEG-*b*-PCL and PCL produced fibers with micron-scale diameters (2.0±0.3 mm); however this was lowered to 270±100 nm by using the gap method of alignment for collection, suggesting further extrusion of the fibers upon collection.

In preliminary investigations for tissue engineering applications, fibroblasts directly adhere to the electrospun fibres, wrapping around the fibres and attaching to multiple fibres. Since cells cultured *in vitro* can be used as collectors for melt electrospinning, the process promises to intimately combine the cell with the electrospinning collection process. In numerous ways, solvent accumulation has dictated the manner in which electrospinning has been performed. At the research level most electrospinning is perform in well-ventilated areas, and attaining industrial scale manufacture is associated with significant ventilation systems. Melt electrospinning is readily performed in a variety of spaces, ranging from confined and sealed vessels to cell culture hoods.

11:30 Invited oral

Dirty surface – cleaner cells? Some observations with a bio-assembled extracellular matrix

Michael Raghunath

National University of Singapore (NUS), Singapore, Singapore

e-mail: bierm@nus.edu.sg

Conventional culture is done on tissue culture polystyrene (TCPS) surfaces that have been treated to become hydrophilic and negatively charged. To improve cell growth and differentiation in vitro, TCPS surface modifications have been proposed including grafting surfaced with recombinant cell adhaesion peptides derived from extracellular matrix (ECM) proteins or using isolated ECM components to coat them. As the ECM represents an alloy of supramolecular assemblies carrying various biologically relevant ligands we hypothesised that such a complex ECM can only be laid down by professional matrix-making cells. Thus, it would be preferable to direct cellular activity rather than to control surface modifications. To this end, we directed EMC-deposition by human fibroblasts by adding negatively charged or neutral macromolecules to the culture medium thus creating a specific biophysical environment characterised by the excluded volume effect. This system allows for a complete conversion of procollagen to collagen by C-proteinase, drives the self-assembly of collagen and stimulates lysyl oxidase-mediated crosslinking of the matrix. As such, more collagen can be deposited in 48 hrs than in 4 weeks or longer, also the differntial usage of different charged macromolecular crowders allows the modulation of the depositional pattern. On this matrix, mesenchymal stem cells proliferated faster and retained their differentiation potential into osteogenic and adipogenic lineages compared to TCPS. Embryonic stem cells remained undifferentiated, formed tighter colonies and exhibited less runaway cells compared to Matrigel. In conclusion, a “dirtier” surface comprising of an ECM that has been bio-assembled under controlled conditions may provide preferable nanotopographic and chemical cues in comparison to artificial single component grafting.

12:00 Oral

Nanofiber sponge consisted of polymer-protein composite for vascular invasion bed

Hisatoshi Kobayashi, Chiaki Yoshikawa, Yoshiyuki Dobashi, Shinnya Hattori, Takako Honda, Yoshiro Yokoyama

National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba 305-0047, Japan

e-mail: kobayashi.hisatoshi@nims.go.jp

Introduction: Nano-scaffolds have provided good conditions for cell adhesion and are currently being applied to many different types of implantable medical device. The authors have produced and evaluated nanofibers made from biocompatible and biodegradable polymers for scaffold via electrospinning method. In general, when nanofiber nonwoven mats are used as scaffold, cells would not enter into a scaffold because of its high bulk density in the direction of the thickness. In this study, authors have contrived a convenient method to make spongiform nanofiber 3-dimensional fabric, which has spaces in moderation for scaffold. The property and tissue compatibility of nanofiber fabric made by this method was investigated. **Materials and Methods:** PGA (*Sigma-Aldrich, Inc.*, USA) was dissolved in 1,1,1,3,3,3 hexafluoro-2-propanol at concentration of 67 mg/ml. Collagen (Nippon Meat Packers, Inc., Japan) was dissolved HFIP at concentration of 100 mg/ml. The mixture at 5:5 solution was electrospunned at 3 ml/hr. The positive output lead of a high voltage supply, set to 30 kV, was attached to a 25 gauge needle on the syringe. Spinning stainless bath filled with t-butyl alcohol was used as a grounded target. A grounded target was placed 30 cm from the needle tip. After making nanofibers in the spinning stainless bath via electrospinning method, nanofiber fabric was vacuum-freeze dried using a t-BuOH freeze dryer in 1 day. Specimens were punched out from the nanofiber fabric. The fiber diameter and structure of nanofiber fabric were observed by scanning electron microscope (SEM, JSM-5600LV, JEOL Ltd., Japan). **Results and Discussion:** The nanofiber fabric consisted of fibers with diameters ranging from 140 nm to 1160 nm. Most of the fiber diameter are less than 1mm, and the average diameter is 760 nm (± 290 nm). The nanofiber fabric had a spongy structure with large spaces between the nanofibers. The tissue ingrowth in the spongiform nanofiber fabric was observed in vivo.

12:15 Oral

Combination of specifically designed cellular microenvironments and physical stimulation by pulsing hydrostatic pressure for osteogenic differentiation of human mesenchymal stem cells

Ricarda Hess[1], Timothy Douglas[1,2], Kenneth A. Myers[3], David A. Hart[3], Barbe Rentsch[1,4], Nigel G. Shrive[5], Hartmut Worch[1], Dieter Scharnweber[1]

1. *Dresden University of Technology, Mommsenstr. 4, Dresden D 01-062, Germany* **2.** *Christian-Albrechts-Universität Kiel, Kiel 24098, Germany* **3.** *McCaig Center for Joint Injury and Arthritis Research, Faculty of Medicine,University of Calgar, 3330 Hospital Dr. NW, Calgary, AB, Calgary T2N4N1, Canada* **4.** *Catgut GmbH, Markneukirchen 08254, Germany* **5.** *Department of Civil Engineering, University of Calgary, 2500 University Dr., Calgary, AB, Calgary T2N1N4, Canada*

e-mail: douglas@mkg.uni-kiel.de

Mesenchymal stem cells (MSC) from a number of sources have great potential for various tissue engineering (TE) approaches to repair connective tissues. To form the TE target tissue the differentiation pathways of the cells have to be stimulated. In vivo the cellular microenvironment and physical stimuli play an important role and thus the combination of biological and mechanical signals is likely to be critical. The goal of this work was to combine biochemical stimulation of cells with soluble factors or signals from substrates in defined microenvironments, plus mechanical stimulation via intermittent cyclic hydrostatic pressure (iHP) for osteogenic in vitro differentiation of human adult MSC. This hydrostatic pressure system allows for stimulation of all types and geometries of scaffold materials and cellular constructs. For these studies, a novel apparatus has been used that makes application of long term iHP to in vitro cell cultures [1]. Titanium discs and embroidered textile polycaprolactone substrates prepared were coated with collagen and/or chondroitin sulphate (CS), seeded with hMSC and subjected to iHP at various time points (1, 6, 13 days). Cell culture was performed either in DMEM (10 % FBS, 1 % P/S) or differentiation medium (50 µM ascorbic acid, 3.5 mM ß-glycerophosphate and 10 nM dexamethasone). It was shown that the extent of osteogenic differentiation as measured by ALP activity, mineral content, and expression of osteogenic markers is highly affected by the stimuli combinations applied. Thus, CS as a biochemical stimulus and iHP promoted stimulation with the effect of iHP being dependent on its timing within the time course of cell culture. Future work will study duration and details of HP application (duration, pressure level) on osteogenic differentiation together with more complex artificial extracellular matrices. [1] Myers K, Shrive NG, and Hart DA. J Biosci Bioeng 103:578-581 (2007)

Lunch break

Tuesday afternoon, 16 September, 12:30
Inner Courtyards

Session 3

Tuesday afternoon, 16 September, 14:00
Room 213

14:00 Invited oral

Response of Cell Types to Inkjet Printing

Brian Derby

University of Manchester - School of Materials Science - Materials Science Centre, grosvenor street, Manchester M1 7HS, United Kingdom

e-mail: brian.derby@manchester.ac.uk

Inkjet printing provides a versatile method for the simultaneous fabrication of tissue scaffold structures and parallel seeding. One of the potential benefits of this technology is the ability to fabricate structures with heterogeneous cell populations, with distinct cell types at specific locations within a printed structure. Our previous work has already demonstrated that human fibroblast cells can be successfully dispensed using commercial inkjet printing systems with cell death rates indistinguishable from that of control cultures [1]. However, in order for inkjet printing to be a viable technique for cell dispensing, we must be sure that it can be used with a range of cell types without damage. Here we present a survey of cell behaviour after inkjet printing of primary human fibroblasts and osteoblasts, fibroblast and oral keratinocyte cell lines and primary bovine chondrocytes. All cell types are shown to be printable and that conditions can be identified to minimise cell death after printing to levels that are indistinguishable from unprinted controls. Osteoblast and chondrocyte cells appear to show a response to printing that affects either their proliferation or metabolic rate after printing that is not seen with fibroblasts or keratinocytes. It is hypothesised that this may reflect the stress sensitivity of these cell types.

14:30 Invited oral

Dedicated nanometric surface topography and bone cell behaviour

Frank Walboomers[1], Edwin Lamers[1], Maciej Domanski[2], Regina Luttge[2], Louis Winnubst[2], Han Gardeniers[2], John A. Jansen[1]

1. *Radboud University Nijmegen Medical Centre (RUN-MC), po box 9101, Nijmegen 6500hb, Netherlands* **2.** *University of Twente, Faculty of Science and Technology, Low Temperature Division and MESA+ Research Institute, Postbus 217, Enschede 7500 AE, Netherlands*

e-mail: f.walboomers@dent.umcn.nl

The introduction of implants or tissue engineered scaffold materials into a living organism causes specific reactions of the biological environment. The bio-molecules and cells together with the intrinsic properties of the materials used, determine the biocompatibility and longevity of the biomaterial. Since the interaction of those bio-molecules and cells with the biomaterial surface is a vital element in evaluating the suitability of a biomaterial for its intended function, every attempt towards avoiding undesired and/or enhancing desired responses to implant or scaffold materials is of utmost importance. Recent developments in the field of nanotechnology offer powerful tools to modify the surface of biomaterials by introducing artificial topography on the material. The first objective of our studies was to deliver the relevant knowledge of the parameters that control the biological response at the nano-level. A screening chip was created using electron beam lithography, containing 50 nanotopographical fields different in design and size. Primary osteoblasts were seeded and the cell morphology was assessed as well as cell function through single cell based real-time PCR. It was found that nanometric topography, especially a groove and ridge design, were of great influence to cell reaction. On basis of the screening chip, parameters were chosen for the design of large area surfaces created by laser interference lithography. Osteoblast response was evaluated on basis of PCR; alignment of cells and mineral/matrix deposition; and interfacial analysis using TEM and dual-beam cryo SEM. We conclude that this type of nanotexturing later will be applicable to optimize performance of medical implant materials and scaffold surfaces.

15:00 Oral

Drop-on-demand inkjet printing of alginate gelation systems

Rachel E. Saunders[1], Andrew Starkie[1], Nicola Tirelli[2], Brian Derby[1]

1. *University of Manchester - School of Materials Science - Materials Science Centre, grosvenor street, Manchester M1 7HS, United Kingdom* **2.** *University of Manchester-School of Pharmacy and Pharmaceutical Sciences, Oxford Road, Manchester M13-9PT, United Kingdom*

e-mail: Saunders.rachel@gmail.com

A common approach to tissue repair is the use of a cell-seeded scaffold. Technology has advanced to provide complex scaffolds with controlled architecture and porosity although problems with incorporating cells into the scaffold structure still persist. Standard cell seeding techniques can result in poor cell seeding density, pore occlusion and are limited with regards to cell penetration, scaffold size and cell placement. Drop-on-demand inkjet printing is a fabrication technique which is capable of depositing materials layer-bylayer to form complex constructs. This technique has previously been proven to be a viable technique for use with mammalian cells yielding over 95% survival rates [1]. The simultaneous deposition of multiple cell types and scaffold matrix could yield a reality whereby human tissue could be fabricated with a precision not only applicable to scaffold architecture but also to the placement of multiple cell types.

This work presents the development of alginate solutions specifically for printing using a drop-on-demand piezoelectric inkjet system. Issues such as hydration of the alginate scaffolds throughout printing have been addressed and the printing parameters have been optimized for three dimensional fabrication.

1. Saunders, R.E., J.E. Gough, and B. Derby, Delivery of human fibroblast cells by piezoelectric drop-ondemand inkjet printing. Biomaterials, 2008. 29(2): p. 193-203.

15:15 Oral

Glutaraldehyde cross-linked gelatin/hydroxyapatite nanocomposite scaffold, engineered via compound techniques

Mahmoud Azami, Mohammad Rabiee, Fathollah Moztarzadeh

Amirkabir University of Technology (AUT), Hafez, Tehran 15914, Iran

e-mail: mazami@aut.ac.ir

In this study, a scaffold was designed for use in bone tissue repair and the effect of glutaraldehyde (GA) concentration as crosslinking agent was investigated. To mimic the mineral and organic component of natural bone, hydroxapatite (HA) and gelatin (GEL) were used as the main components of this composite. Nano-powders of HA were synthesized, and together with GEL, was used to engineer a three-dimensional nanocomposite with combination of three techniques of layer solvent casting, freeze-drying and lamination. The synthesized nanocrystalline hydroxyapatite and nanocomposite samples were characterized by the commonly used techniques. The results show that GEL/HA nanocomposite is porous with 3-dimension interconnected structure, pore sizes ranging from 300 to 500 μm, and about 85% porosity. In addition, increasing GA concentration provokes enhancement of compressive strength and reduction of toughness. It was concluded that optimum concentration for cross-linking GEL matrix for this purpose is 1%. Cultured osteoblast-like cells (SaOS-2) have shown an excellent level of cytocompatibility for nanocomposite scaffold. A specific cobmination of commonly used techniques was applied to engineer a scaffold with almost ideal properties intended for bone tissue engineering is introduced. In addition, scaffolds that are prepared via this compound process has the potential to be used in solid free form applications and so being formed in any dimention and geometry relevant to defect size and shape.

Coffee break

Tuesday afternoon, 16 September, 15:30
Main Hall

Session 4

Tuesday afternoon, 16 September, 16:00
Room 213

16:00 Invited oral

A bit of physics in our understanding of the cell and tissue interaction with scaffolds

Małgorzata Lewandowska-Szumieł

Medical University of Warsaw, Department of Biophysics and Human Physiology, Chałubińskiego 5, Warszawa 02-004, Poland

e-mail: mszumiel@ib.amwaw.edu.pl

The selected topics will be brought up in order to draw attention to the fact that the physical interaction between cell and scaffold is an important aspect of tissue engineering hybrid system consisting of a nonviable scaffold and living cells. Particularly, cell “feeling” of the support stiffness will be discussed on the basis of the recent scientific reports and the results from our group. Some attention will be paid to the new findings concerning mechanoreceptors of bone cells based on the patch-clamp methodology.

On the other hand, application of methods, which detect physical phenomena, to investigations of tissue organized inside the scaffold in vivo will be exemplified by a detection of bone formation in our tissue engineered product by means of the electron paramagnetic resonance (EPR).

16:30 Oral

Polymer-TiO$_2$ nanocomposites for soft tissue engineering

Miroslawa El Fray

Szczecin University of Technology, Polymer Instiute, Pulaskiego 10, Szczecin 70-322, Poland

e-mail: mirfray@ps.pl

Polymer-matrix nanocomposites are becoming emerging group of modern biomaterials with enhanced mechanical characteristics and biological performance. Nanocomposites containing ceramic nanofillers embedded in a termoplast or termoset polymer matrix are interesting group of materials where desired stiffness and biocompatibility can be achieved. However, many of these systems are rather stiff materials of limited elongation and thus application. Therefore, thermoplastic elastomers (TPE), as materials of high flexibility with wide range of possibilities to tailor their structure and properties represent interesting materials, especially for soft tissue applications. With the use of natural fatty acids, we produced an elastomeric polymer matrices, which were combined with nanometer-size ceramic particles (TiO$_2$) and showed various interesting mechanical properties [1,2]. *In vivo* tissue response to new elastomeric material containing nanocrystalline TiO$_2$ after 12 weeks implantation in rats was investigated. The superiority of fibroblasts, the little amount of histiocytes and lack of gigantiocytes reflects the development of nonprotracted–nonspecific inflammable reaction (a similar change comes in patients after grafting artificial silicone implants). Cell alterations were minimum with no evidences for contact necrosis being observed. Materials showed good biocompatibility, with no adverse biological effects. The lack of untoward effects of new nanostructured polymer/ceramic material on the adjacent tissues suggests good biocompatibility of material and indicated great potential for soft tissue engineering (current work is focused on application of these nanocomposites for myocardial tissue engineering).

References

[1] El Fray M., Nanostructured Elastomeric Biomaterials for Soft Tissue Reconstruction, Publishing House of the Warsaw University of Technology, Warszawa 2003, 1-144

[2] El Fray M., Boccaccini A.R.: Materials Letters 59:2300-2304, 2005.

16:45 Oral

Calcite-based material for tissue engineering ceramic scaffolds

Zbigniew Jaegermann[1], Sławomir Michałowski[1], Anna Chróścicka[2], Małgorzata Lewandowska-Szumieł[2]

1. *Institute of Glass, Ceramics, Refractory and Construction Materials (ISC), Postepu 9, Warszawa 02-676, Poland* **2.** *Medical University of Warsaw, Department of Biophysics and Human Physiology, Chałubińskiego 5, Warszawa 02-004, Poland*

e-mail: bioceramika@neostrada.pl

Tissue engineering applies biological, medical and technical science for the sake of regeneration, maintenance and improvement of tissue functions. Studies concerning new materials for cells culture scaffolds are a quickly developing domain of biomedical engineering.

The goal of the present research consisted in optimization of calcite materials chemical composition and possibility of quantitative analysis of porous scaffolds by micro-CT.

Several materials based on CaCO$_3$ were elaborated. Microporous samples were formed by uniaxial pressing. For macroporous ones the method of mapping the porous structure of polyurethane sponges was applied. Apparent density, total porosity and compressive strength of tested samples were determined. The porous structures were observed in stereoscopic, SEM and analysed by micro-CT method.

The microporous calcite materials were characterised by total porosity ranging from 0,7 to 27%, apparent density between 1,8 and 2,5 g/cm^3 and the compression strength ranging from 28 to 108MPa. These properties differed according to the chemical composition and sintering temperature.

The physical properties of macroporous calcite materials obtained by sponge method depended mainly on the technique of extrusion of the surplus slurry applied. The porosity of these materials ranged from 58 to 78%, apparent density from 0,55 to 1,07 g/cm^3 and compressive strength from 0,5 to 2,0MPa.

The biological study also shown higher viability of the cells cultured on the samples with a lower content of technical additives.

The analysis of results demonstrated that relative density and total porosity obtained by microtomographic method match the values measured by geometrical method. Micro-CT analysis enables to calculate supplementary information, such as: volume and surface of the material, width and number of struts, and other parameters describing architecture of porous material.

This work was supported by Ministry of Science and Higher Education (grant nr R13 01901).

17:00 Oral

Novel method for bone tissue scaffold fabrication. Influence of composition chitosan/beta-TCP matrixes on mechanical and biological properties.

Martyna A. Kucharska[1], Katarzyna Bocian[1], Beata Butruk[1], Tomasz Ciach[1], Wojciech Swieszkowski[2], Tomasz Brynk[2], Marcin K. Heljak[2], Małgorzata Szumieł-Lewandowska[3], Agnieszka Mikulska[3]

1. *Warsaw University of Technology, Faculty of Chemical Engineering, Warynskiego 1, Warsaw 00-645, Poland* **2.** *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland* **3.** *Medical University of Warsaw, Chałubińskiego 5, Warsaw 02-004, Poland*

e-mail: kucharska@ichip.pw.edu.pl

In this work authors present novel method of bone scaffolds fabrication. Matrixes are manufactured by chemical agglomeration of chitosan/β-TCP/collagen spheres and seem to be a promising bone tissue substitute. Fabrication process consists of the following steps: polymer based spheres extrusion, matrix formation by compression and spheres bonding with sodium tripolyphosphate (STPP) as cross-linking agent. Presented method allows to generate porous materials with controllable shape, pore size distribution and its interconnectivity. In this technique 3D scaffold porosity can be regulated by altering spheres diameter. Authors studied the influence of β-TCP, collagen and cross-linker concentrations on scaffold morphology, mechanical properties, enzymatic degradation rate (in presence of lysozyme), water absorption and osteoblast-like (MG-63) cells response. Influence of various chitosan molecular weights and length of STPP cross-linking on scaffold properties were also examined. Surface morphology and topography were evaluated by scanning electron microscope (SEM). Porosity and pores interconnectivity were observed via Micro-Computed Tomography (μCT) scanning. Mechanical tests showed that cross-linked chitosan performs compression characteristic (Young Modulus, maximum stress) similar to natural bone. Obtained matrices subjected to 10kN compression strength remain tough and not fractured. Cytotoxity evaluated by XTT assay shows that proposed composite materials don't exhibit any toxic properties against human cells. Osteoblast-like cells adhesion and morphology were analyzed both by SEM and optical microscope.

17:15 Oral

Bone tissue engineered product based on human bone derived cells and polyurethane scaffold

Piotr Woźniak[1], Monika Bil[2], Joanna Ryszkowska[2], Piotr Wychowański[3], Grażyna A. Hoser[4], Małgorzata Lewandowska-Szumieł[1], Krzysztof J. Kurzydlowski[2]

1. *Medical University of Warsaw, Department of Biophysics and Human Physiology, Chałubińskiego 5, Warszawa 02-004, Poland* **2.** *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland* **3.** *Medical University of Warsaw, Department of Dental Surgery, Nowogrodzka 59, Warsaw 00-006, Poland* **4.** *Medical Centre of Postgraduate Education, Department of Clinical Cytology, Marymoncka 99/103, Warsaw 01-813, Poland*

e-mail: pwozniak@ib.amwaw.edu.pl

Biodegradable polyurethanes are widely investigated as candidate material for scaffolds in bone tissue engineering (1-2). There are, however, only a few papers describing the formation of Tissue Engineered Product (TEP) based on polyurethane support and primary human osteoblasts. The aim of the present study was to fabricate TEP consisting of Human Bone Derived Cells (HBDCs) seeded on 3-D biodegradable polyurethane scaffolds and to evaluate its biocompatibility in vivo.

HBDCs were seeded (3,0x105 cells/sample) and cultured on specially developed polyurethane scaffolds in spinner flask type bioreactor for 14 days. The experiment was performed twice. Each time 6 samples were used for the evaluation of TEP in vitro and additional 22 scaffolds were used for the in vivo experiment. TEP samples and control samples (scaffolds without cells) were implanted subcutaneously into the SCID mice for the 4 and 13 weeks periods.

TEP examination in vitro was performed by means of: cell number (XTT assay), cell phenotype (RT-PCR) and cell distribution within the scaffold (fluorescence microscopy). Explants harvested from the animals were examined using histological (HE) and immunohistochemical (Collagen I and Osteopontin) methods.

It was found that dynamic cell seeding and cell culture conditions enable homogenous distribution, maintaining the proliferative potential and osteogenic phenotype of the HBDCs cultured on the selected three dimensional polyurethane scaffold – fabrication of TEP.

It was also found, that Human Bone Derived Cells implanted into the experimental animals as a component of TEP keep their ability to synthesize and secrete the specific components of the bone tissue Extracellular Matrix.

Acknowledgment: This work was supported by the Ministry of Science and Higher Education, grant R13 01901 and by the MUW (NZME/W2/08).

1 Guelcher, S.A. (2005) In An Introduction to Biomaterials (Eds, Guelcher, S.A. and Hollinger, J.O.) pp. 576.

2 Bil et all. J Mater. Sci. in press.

Wednesday, 17 September

Session 5

Wednesday morning, 17 September, 9:00
Room 213

9:00 Invited oral

Development of Porous Scaffolds for Tissue Engineering by Template and Hybridization Methods

Guoping Chen, Naoki Kawazoe, Tetsuya Tateishi

National Institute for Materials Science, Ibaraki 305-0047, Japan

e-mail: Guoping.CHEN@nims.go.jp

Many porous scaffolds have been prepared for tissue engineering from naturally derived polymers such as collagen, and synthetic polymers such as poly (glycolic acid) (PGA), poly (L-lactic acid) (PLLA), poly(lactic-co-glycolic acid) (PLGA). However, development of functional porous scaffolds with controlled pore structures and high mechanical properties remains a great challenge.

To control the porous structure of porous scaffolds, we developed a template method by using biodegradable polymer template and ice particulate template. Collagen mesh scaffolds were prepared by using a PLGA knitted mesh as a template. At first a hybrid mesh of PLGA knitted and collagen was prepared by forming web-like collagen microsponges in the openings of a PLGA knitted mesh. And then the PLGA knitted mesh was selectively removed. Collagen sponge with an open surface structure was prepared by using embossing ice particulates as a template. Ice particulates were formed on a plate and collagen aqueous solution was poured onto them. The collagen sponge was prepared after freeze-drying. These collagen scaffolds were used for cell culture of human dermal fibroblasts. The open surface and interconnected porous structures facilitated cell seeding and cell distribution.

To improve the mechanical properties of porous scaffolds, we developed a hybridization method to prepare hybrid scaffolds of synthetic and naturally derived polymers. PLLA-collagen and PLGA-collagen hybrid porous scaffolds were prepared by forming collagen sponge in a PLLA sponge cylinder mold or a PLGA mesh cylinder mold. The PLLA sponge and PLGA mesh cylinder molds provided the hybrid scaffolds with high mechanical strength. The collagen sponge caged in the PLLA sponge or PLGA mesh cylinder mold facilitated cell seeding and cell distribution. Cartilage-like tissue was regenerated when mesenchymal stem cells or chondrocytes were cultured in the hybrid scaffolds.

9:30 Invited oral

Non invasive microscopy of bioscafflolds and their interface with calcified and soft tissue in 3D with a novel multiscale x-ray tomography system (CT)

Siew H. Lau[1], Margam Chandrasekaran[2], Victor Fan[3], Mohd Nazul[3], Tiffany Fong[1], Tom Case[1], Susan Candell[1]

1. *Xradia Inc, 5052 Commercial Circle, Concord 94520, United States* **2.** *Bio-scaffold International Pte. Ltd, Singapore 117525, Singapore* **3.** *Faculty of Dentistry, National University of Singapore, Singapore 119074, Singapore*

e-mail: shlau@xradia.com

Evaluating bioscaffolds and its interface with tissue and cells are unsatisfactory with conventional histology, imaging modalities and conventional x-ray micro tomography system (microCT). Histology can take up to a few weeks and are prone to artifacts. Electron optics imaging requires extensive sample preparation, while AFMs are confined to surface characterization of a very small sample area. Conventional microCT lacks the contrast to image soft tissue and cartilage and does not have the resolution to detect fine microstructures. In the current work we have used a novel multiscale CT system to develop a rapid technique for non invasive 3D characterization of a variety of biomaterials, tissue engineering scaffolds and their interaction with soft and calcified tissue, often without much sample preparation or contrast agents, and with spatial resolution from a few microns to sub 50 nm. A clinical application involving evaluation of porosity of a PLGA bioscaffold during fabrication and its subsequent implant and bone quality studies in a patient will be discussed. Other examples include imaging 3D distribution of hepatocyte cells on tissue engineered PCL-collagen scaffold; cartilage imaging in murine bones without contrast agents. Finally, the power of non invasive multiscale tomography characterization of complex biological systems from meso to nanoscale resolution will also be illustrated . Comparison of CT results with conventional histology, SEM and MRI will be shown. The novel Multiscale CT comprises a MicroCT and nanoCT module and uses proprietory optics. Unlike conventional microCTs which rely on point projection technique, hence resolution is limited by source spot size and its sample-source distance, the resolution of the novel CT is not dependant on these parameters. With significantly higher contrast than conventional CTs, it is possible to image most biomaterials and soft tissue without contrast agents.

10:00 Oral

Investigation of the Biocompatibility of Carbon Nanotube-Based Matrices by Study the Adhesion Behavior of Osteoblast-like Cells

Izabela Firkowska, Eva Godehardt, Michael Giersig

center of advanced european studies and research (caesar), Ludwig-Erhard-Allee 2, Bonn 53175, Germany

e-mail: firkowska@caesar.de

It is well known that cell adhesion to the surface of the substrate is the first phase of cell-substrate interaction, and the quality of this adhesion plays an important role in the modulation of cell functions such as morphology, proliferation, protein production and differentiation. As shown by several studies, the surface chemistry and the topography of the substrates are responsible for the variation in cytoskeleton organization and proliferation. Since the cytoskeleton is believed to be responsible for the mechanical properties of cell, the alteration in its architecture upon adhesion to diverse substrates may lead to changes in the mechanical stiffness of the cell. This fact assumes that a high value of Young's modulus is directly correlated with a good cell adhesion.

In this work, we have used atomic force microscopy (AFM) to investigate the biocompatibility of carbon nanotube-based constructs by studying the adhesion behavior of osteoblast-like cells. Exploiting the ability of AFM to image cells under physiological conditions we were able to determine the cytomechanical properties of living osteoblasts cultured on substrates with randomly-distributed CNTs, cavity-like assembled nanotubes, and smooth glass surface.

Experimental data show that the elastic modulus of the osteoblast cells is modulated by the substrate to which they adhere. We have found that the osteoblasts plated on non-nanostructured substrate (glass) have the lowest cell stiffness (3.71 ± 1.48 kPa), whereas cells adhered to the cavity-like topography expressed an increased average cellular elasticity ($E = 5.43 \pm 2.05$ kPa). Moreover, we observed that irregular topography has a weaker influence on osteoblast adhesion, which results in a decreased elastic modulus in the case of cells cultured on randomly distributed carbon nanotubes.

10:15 Oral

Investigation Of The Processing and Materials Related Factors On The BCP Scaffolds Containing Naphthalene As A Pore Forming Agent For Bone Tissue Engineering Applications

Ranna Tolouei, Aliasghar Behnamghader, Roghieh Nemati

Ceramics department from Materials and Energy Research Center, Tehran 15914, Iran

e-mail: ranna.tolouei@gmail.com

the object of this study was to produce absorbable biomaterials containing tricalcium phosphate (TCP) and hydroxyapatite (HA). Naphtalene was used as a pore forming agent. The conventional pressing and sintering were utilized to produced the disc shape samples. The sintering temprature and the applied pressure were selected as the variable factors. The phase composition and chemical structure analysis were performed using XRD and FTIR. The size and distribution of the porosities as well as the connection of porosities with each other were studied by SEM. The sintered sampleds consisted of the HA and TCP phase. No impurities, remaining from the additives were detected in the sintered samples. The optimum sintering temprature and applied pressure parameters were 1200^{o}C and 220 MPa, respectively. The pores of 50-300 micrometers size illustrating the rough enough internal surfaces, were obtained for potential use in hard tissue engineering.

Coffee break

Wednesday morning, 17 September, 10:30
Main Hall

Session 6

Wednesday morning, 17 September, 11:00
Room 213

11:00 Invited oral

Biosynthetic hydrogels for cell and drug delivery: Challenges in fabricating functional 3D constructs

Laura A. Poole-Warren

University of New South Wales (UNSW), Sydney 2052, Australia

e-mail: L.Poolewarren@unsw.edu.au

11:30 Oral

Selective laser sintering of hydroxyapatite/poly-ε-caprolactone scaffolds

Szilvia Eosoly[1], Dermot Brabazon[1], Stefan Lohfeld[2], Lisa Looney[1]

1. *School of Mechanical and Manufacturing Engineering, Dublin City University, Dublin Dublin9, Ireland* **2.** *National University of Ireland, Galway (NUIG), University Road, Galway none, Ireland*

e-mail: szilvia.eosoly2@mail.dcu.ie

Selective Laser Sintering (SLS) has the potential to fabricate complex geometries with intricate and controllable internal architecture. Numerous polymeric biomaterials can be processed by SLS given that they are available in the form of powder. However to process calcium phosphate bioceramics a thermoplastic polymer functioning as a binder material is required. In this study hydroxyapatite and poly-ε-caprolactone were used with a weight ratio of 30/70. These materials are suitable for hard tissue engineering purposes. SLS process parameters were examined in the following ranges: outline laser power (3-7 W), laser fill power (8-12W), scan spacing (0.1-0.2 mm) and building direction (X, Y, Z). The effect of feature size (0.5-0.7 mm) was also included in the design. All factors except manufacturing direction were examined at five levels using a Box-Wilson Central Composite Design (CCD) frequently used for process optimization. Mathematical model for estimating the mechanical properties, surface roughness and accuracy was developed and used for the optimization where the measured responses were the objective functions. As laser power and scan spacing determine the delivered energy density, the design also enabled the examination of its effect on the response functions in the range of 0.008 -0.02 J/mm^2. In general higher energy density resulted in better mechanical properties due to lower porosity in the designed solid regions, increased dimensions and decreased surface roughness due to lower polymer viscosity during processing. The accuracy of fabricated parts was poor as deviation from nominal dimensions could reach 50%. Compressive moduli for geometries with relative density of 0.25 were in the range 1 - 5 MPa and compressive collapse strengths were in range 0.2-1 MPa. These values do not qualify the fabricated scaffolds for load bearing application however mechanical properties can be improved by post processing.

11:45 Oral

REDV peptide patterning onto PET using Laser Induced Forward Transfer

Fabien Guillemot, Christel Chanseau, Stéphanie Lesage, Marion Dulpuch, Murielle Rémy, Laurence Bordenave, Marie-Christine Durrieu

Laboratoire de biomatériaux et réparation tissulaire, Université Victor Segalen Bordeaux 2, case postale 45, 146 rue Léo-Saignat, Bordeaux 33076, France

e-mail: fabien.guillemot@inserm.fr

Tissue engineering aims to create functionally active tissue by mixing biomaterials with cells and cell components.Since tissues *in vivo* are often composed of several types of cell layers, cell/cell interactions are important in the maintenance of a normal physiology in organ systems.To fabricate functional tissue architectures, it is necessary to precisely allocate specific cells to a desired location.Micropatterning of cells is a possible approach for this purpose.One suitable method is to functionalize the surface of the materials with “pro-adhesive” ligands, likely improving subsequent cell adhesion.Our work has concentrated on promoting human endothelial cells(ECs) isolated from human saphenous veins(HSVECs) to adhere to polyethylene terephthalate (PET) substrates.We have grafted REDV peptides onto the surface of a PET template in well-controlled patterns.

For this study,we have used a simple and rapid cell-patterning procedure.Direct-writing techniques,capable of depositing tiny amounts of biological material onto different substrates,are emerging as promising tools for the preparation of miniaturized biosensors due to their versatility,accuracy, low cost and speed.The Laser Induced Forward Transfer (LIFT) technique offers an interesting approach providing a good spatial resolution: tiny amount of material to be deposited was removed from a thin film (inks differing biomolecularly were used) and transferred onto a receptor substrate parallel with the film by the action of a laser pulse.

The main objective is to demonstrate the successful transfer and grafting of REDV peptide spots regardless the solvent used onto pre-functionalized PET by a LIFT technique.The distributions and densities of the peptides were evaluated by high resolution µ-imager using radiolabeled biomolecules.Neither direct nor indirect cytotoxicity to PET-REDV was found to exist regardless the transfer solution used.Finally, surfaces seeded with HSVECs were investigated for cell attachment.

12:00 Oral

Engineered composite materials for improved cellular response: CeO_2 loaded PLGA films

Corrado Mandoli, Francesca Pagliari, Stefania Pagliari, Giancarlo Forte, Paolo Di Nardo, Enrico Traversa

Universita di Roma 'Tor Vergata', Roma 00133, Italy

e-mail: corrado.mandoli@uniroma2.it

Nanotechnologies offer a rational approach to the development of scaffolds for tissue engineering. The polymeric biomaterial can be manipulated at any level and can be designed with specific geometries in the range from 1 to 100nm.

Synergistic effects deriving from the interaction with inorganic components may lead to a new class of hybrid systems whose mechanical and chemical properties can be entirely tailored to maximize bio-affinity. Using ceramic oxides particles as dispersed phase may result in improving the polymer-based composite structure both in terms of mechanical and biomimetical properties. It is known that free radical formation during cellular growth limits cells proliferation. Such problem may be overcome by using ceramic oxides as dopants such as cerium oxide (CeO_2), to act as radical scavengers.

Our study relies on synthesis and characterization of CeO_2 loaded PLGA scaffolds for stem cells culturing *in vitro*. Cells capability to adhere and proliferate on newly designed scaffolds has been analyzed with molecular and electronic microscopy analysis, vitality and toxicologic assays. Results show the tuning effect exerted by ceramic load in terms of concentration and grain size on cell systems through the modification of scaffold’s mechanical and topographical properties, respectively. Scaffold's stiffness and roughness conditions able to improve cellular adhesion and proliferation respect to unloaded PLGA supports have been identified. CeO_2 scavenging property towards cell system has been investigated by comparison with TiO_2 and SiO_2 loaded PLGA scaffolds, at given stiffness and roughness. Results suggest that CeO_2 exerts some kind of stimuli towards cell culture able to promote larger adhesion and proliferation maybe related to CeO_2 anti-oxidative properties.

Moreover, cells have shown spontaneous tendency to coordinate along oriented arrays once seeded onto μ-scale pre-patterned PLGA scaffolds of suitable geometry, regardless the material employed.

12:15 Oral

Physical and chemical techniques to improve surface proprieties of polyesters films

Magdalena Aflori, Mioara Drobota, Mihaela A. Olaru, Iuliana Stoica

Petru Poni Institute of Macromolecular Chemistry of the Romanian Academy, Aleea Grigore Ghica Voda 41A, Iasi, Romania

e-mail: maflori@icmpp.ro

Although the use of medical devices is widespread, there is an increasing demand for new biomaterials used as implants or for preparing bioartificial organs. Several surface modification techniques have been developed to improve wetting and adhesion of polymer surfaces by introducing a variety of polar groups, with little attention to functional group specificity. When surface modification was a precursor to attaching a bioactive compound, these techniques must be tailored to introduce a specific functional group. The ideal surface modification techniques are those that introduce as close to a monolayer as possible of a desired functional group without causing irregular etching or producing significant hazardous waste.

The aim of this work is to improve the superficial hydrophilic properties of poly(ethyleneterephthalate) (PET) films. To achieve this object, amide and amine groups were produced by chemical and plasma-precursor treatments with triethylenetetramine. In order to obtain information about the chemical and morphological modifications of polymers, modern and high performant techniques were used: FTIR- ATR, XRD, contact angle, AFM. Treatment time dependency of amine concentration is depicted; more amines were incorporated after exposure to a longer time at the same temperature. For surface activation, plasma-precursor treatment was more efficient than simple chemical treatment. For all the treatments surface modifications are at nanometer scale. Because of the high number of identical hillocks, a relatively homogeneous surface occurred at several treatment times.Optimal treatment parameters were found by fluorescence optical microscopy measurements after collagen deposition.

Nitrogen containing PET films can be considered as potential biomaterial substrates for the attachment of proteins and other biologically active molecules because they allow direct attachment of bioactive molecules.

Lunch break
Wednesday afternoon, 17 September, 12:30
Inner Courtyards

Symposium H presentations
Wednesday afternoon, 17 September, 14:00
Room 213

Coffee break
Wednesday afternoon, 17 September, 15:30
Main Hall

Joint Poster Session 2
Wednesday afternoon, 17 September, 16:00
Main Hall

Thursday, 18 September

Coffee break
Thursday morning, 18 September, 10:30
Main Hall

Session 7
Thursday morning, 18 September, 11:00

11:00 Invited oral

Injectable scaffolds that harden in vivo

Kevin M. Shakesheff

University of Nottingham, Nottingham, United Kingdom

e-mail: kevin.shakesheff@nottingham.ac.uk

This talk will describe a process called liquid sintering in which an injectable paste can convert into a mechanically strong and highly porous material at body temperature. Liquid sintering does not involve any chemical crosslinking or solvent removal. There is no exothermic reaction to achieve the hardening. Therefore, the material can act as a deliver system for temperature and/or solvent sensitive molecules and cells. The work presented here describagain an injectable scaffold for orthopaedic applications that hardens to the compressive strength of cancellous bone in vivo. We demonstrate the delivery of BMP-2, VEGF and mesenchymal stem cells to accelerate bone regeneration.

11:30 Invited oral

Interaction between 3D scaffolds and blood vessels – Implications for generation of axially vascularised bioartificial tissues

Ulrich Kneser, Justus P. Beier, Andreas Arkudas, Elias Polykandriotis, Oliver Bleiziffer, Subha Rath, Dietmar W. Hutmacher, Raymund E. Horch

University Erlangen, Erlangen 91054, Germany

e-mail: ulrich.kneser@uk-erlangen.de

Vascularization is one of the major challenges in tissue engineering. Sufficient engraftment of large volume bioartificial tissues requires not only rapid ingrowth of blood vessels but also a well balanced interaction between vascularization and formation of fibrovascular tissue. Transfer of initially vascularized, functional bioartificial constructs may be facilitated by certain microsurgical approaches based on one dominant vascular axis. Arteriovenous loops or arteriovenous bundles could be applied for transformation of 3D scaffolds into axially vascularized functional tissue units. Our group developed a microsurgical AV loop model based on the saphenous artery and vein that allows generation of large amounts of vascularized tissue in small and large animals. Vascularization kinetics and differentiation of the vascular system could efficiently be modulated by immobilized angioinductive growth factors (VEGF and bFGF). The effect of these factors is dose-dependent and the drug release system has been combined with several porous 3D scaffolds for bone tissue engineering applications. Visualization of the vascular network and determination of vascularization kinetics require sophisticated imaging tools such as high resolution MRI or CT scans either for intravital or post mortem studies. Transplantation of specific adult or fetal cells (e.g. osteoblasts, myoblasts or fetal liver cells) allows generation of functional *neo*-tissues for applications in regenerative medicine. Application of tissue-inductive factors (BMPs) is being assessed as an alternative approach at the moment. Innovative biomimetic scaffolds with graded porosity, appropriate orientation of the internal structures, functionalized surfaces for optimal cell attachment and binding sites for angioinductive or tissue-specific growth factors will eventually allow growing large volumes of axially vascularized autologous bioartificial tissues suitable for transfer to distant defect sites.

12:00 Oral

Processing strategies in sol-gel derived scaffolds with dual pore structure for bone tissue regeneration

Ana Gama, Rui M. Almeida

Instituto Superior Técnico, Lisboa 1049-001, Portugal

e-mail: rui.almeida@ist.utl.pt

Development of optimal scaffolds for bone tissue regeneration is still a challenge. The present work deals with the preparation and characterization of SiO_2-CaO and SiO_2-CaO-P_2O_5 sol-gel derived monoliths, with potential application as glass scaffolds for bone regeneration. The aim was to achieve a hierarchical dual pore structure including pores of both ~100's of micrometers and a few to 10's of nanometers in size, leading to a coral-like morphology with interconnected macropores, based on polymerization-induced (spinodal-type) phase separation made to occur in parallel with the sol-gel transition, by adding a water soluble polymer to the sol-gel solution. The SiO_2 content was varied between 60 – 77 mol% and different processing strategies have been tested, namely by varying the Si alkoxide (TEOS or TMOS), the CaO precursor (Ca nitrate or acetate), the type and concentration of polymer (PEO or PEG) and the temperature/time schedule during sol processing and gel drying and heat treatment.

The morphological and textural characterization of the scaffold materials, performed by field emission SEM, nitrogen adsorption and mercury intrusion porosimetry, confirmed the presence of a dual pore structure including interconnected macropores (~ 10 - 200 μm) plus the inherent nanopore (~ 5 - 40 nm) structure tailored by solvent exchange procedures. Scaffold bioactivity has been demonstrated by the precipitation of hydroxyapatite after immersion in simulated body fluid, by means of SEM and infrared (IR) spectroscopy. The effect of the non-bridging/bridging oxygen ratio of the gel derived glass was also investigated and it was verified by IR and Raman spectroscopies, combined with EDX analysis, that the net amount of Ca^{2+} incorporated into the glass network tended to be lower than the nominal batch concentration and it depended on the CaO precursor and the processing conditions. The influence of these factors on the scaffold bioactivity is discussed in detail.

12:15 Oral

Metallic and ceramic porous bone scaffolds by gel casting and 3D fiber deposition

Steven Mullens, Wim Bouwen, Ivo Thijs, Pieter Nuyts, Jan Luyten

Flemish Institute for Technological Research (VITO), Boeretang 200, Mol 2400, Belgium

e-mail: steven.mullens@vito.be

Bone tissue engineering is an emerging interdisciplinary field in science, combining expertise in medicine, material science and biomechanics. It aims at a patient specific reconstruction of large bone defects by applying a porous scaffold that acts as a (temporary) skeleton for biologically active substances. The requirements posed on the possible candidate for bone scaffold are numerous, ranging from material aspects to the porous architecture itself. Pore size distributions and interconnectivity should be sufficient for cell seeding and cell migration, vascularization and mass transport from and to the cells.

This study focus on 2 manufacturing routes which are applied on calcium phosphates and titanium (alloys). Gel casting is a direct foaming technique starting from a metallic or ceramic suspension. The biomimetic architecture consists in pore size distribution from 100 μm to 800 μm. The porous structure is characterized with electron microscopy, image analysis and Hg intrusion porosimetry. Bioresobable ceramic foams are manufactured with well controllable composition of (biphasic) calcium phosphates. Preliminary in vitro testing yield different dissolution rates for the varying compositions. When aiming at load bearing applications, titanium foams can be produced, with a tunable mechanical strength and high ductility values.

Rapid prototyping technologies include a large number of technologies, among which 3D fiber deposition (3DFD). Starting from a highly viscous paste, a computer controlled 3D movement of the paste reservoir allows the continuous deposition of thin fibers of a ceramic or metallic paste. The porous architecture is governed by the fiber thickness and fiber spacings and is characterized by narrow distributions. Due to the high mechanical properties and the influence on cell behaviour, the introduction of microporosity in the fibers is achievable.

Session 8

Thursday afternoon, 18 September, 14:00

14:00 Invited oral

Imaging and probing cellular interactions with collagen type I down to molecular scale

Anna Taubenberger, Clemens M. Franz, Jens Friedrichs, David Cisneros, Daniel J. Mueller

Biotechnology Center, University of Technology Dresden (TUD), Am Tatzberg 47-49, Dresden 01307, Germany

e-mail: anna.taubenberger@biotec.tu-dresden.de

The extracellular matrix in tissues such as bone, tendon and cornea contains ordered, parallel arrays of collagen type I fibrils. Cells embedded in these matrices frequently co-align with the collagen fibrils, suggesting that ordered fibrils provide structural or signalling cues for cell polarization. To study mechanisms of matrix-induced cell alignment, we developed nanoscopically defined two-dimensional matrices assembled of highly aligned collagen type I fibrils. The matrices were characterized by atomic force microscopy (AFM) to study the influence of buffer conditions on the collagen type I assembly. The growth of collagen fibrils into these matrices was followed by high-resolution time-lapse AFM. Individual fibrils exhibited an axial D-periodicity of ≈ 67 nm such as typically observed for *in vivo* assembled collagen fibrils from tendon. When seeded onto the collagen matrices, cells started to reorganize the collagen I matrices. This cellular remodelling of individual fibrils could be visualized by time-lapse AFM. Next we studied specifically the role of integrin alpha2beta1 in mediating adhesion to the collagen matrices by single-cell force spectroscopy. In the early steps (5-30sec) the integrin alpha2beta1 -mediated cell adhesion was dominated by the binding of individual integrins. At prolonged adhesion time (60-600sec), the cellular adhesion process significantly increased suggesting that integrins switched from individual to a co-operative binding behavior.

14:30 Oral

Nanostructuring of PEG-Fibrinogen Polymeric Scaffolds

Havazelet Bianco Peled[1], Ilya Frisman[1], Dror Seliktar[2]

1. *Technion Israel Institute of Technology Dept. of Chemical Engineering, Technion City, Haifa 32000, Israel* **2.** *Technion Israel Institute of Technology Dept. of Biomedical Engineering, Technion City, Haifa 32000, Israel*

e-mail: bianco@tx.technion.ac.il

Poly (ethylene glycole)-Fibrinogen (PF) hybrid scaffold are prepared by the cross-linking of PEGylated fibrinogen precursors molecules. The fibrinogen provides to this hydrogel an inherent enzymatic degradability and cell-specific interactions, while the poly (ethylene glycole) (PEG) provides mechanical strength and a means to control the cross-linking density of the scaffold. It was previously shown that variations in the molecular weight of the PEG, the protein concentration, or the addition of PEG cross-linker, can be used to alter the biochemistry and physical properties of the scaffold. Following recent studies that demonstrated the effect of scaffold nanostructuring on cell behavior, we hypothesize that nanostructuring of PF scaffold could provide an additional means to control both their physical properties and their interaction with cells. In the current study we have developed a methodology for the nanostructuring of PF hydrogels. Our experimental approach utilizes the self-assembly tendency of the biocompatible amphiphilic block-copolymers poly(ethylene oxide)/poly(propylene oxide) (Pluronic ®), and is based on embedding micelles within the gel. Small angle x-ray scattering (SAXS) and cryo- transmission electron microscopy (cryo-TEM) experiments have verified existence of structural features of nanometric size within the scaffold. Cell seeding assays have demonstrated faster cell growth within the nanostructured scaffolds. Furthermore, the cell morphology was affected from the nanostructuring. This research is expected to lead a better understanding of the influence of structural modification on the cell activity to improved properties of PF scaffolds.

14:45 Oral

Preparation and rheological properties of calcium phosphate-based paste used for treatment of vesicoureteral reflux

Masoud Hafezi-Ardakani[1], Saeed Hesaraki[2], Fathollah Moztarzadeh[1]

1. *Amirkabir University of Technology (AUT), Hafez, Tehran 15914, Iran* **2.** *Ceramics department from Materials and Energy Research Center, Tehran 15914, Iran*

e-mail: mhafezi@aut.ac.ir

Vesicoureteral reflux (VUR) is the abnormal backflow of urine from the bladder into the ureter and up to the kidney. The endoscopic injection of bulking agents for correction of VUR is an outpatient procedure used to correct reflux in children. Calcium phosphate (CaP) pastes have been in clinical use. Most of these materials have been claimed to be injectable. However, most surgeons complain that CaP pastes poorly injectable .In the present study, we evaluated a new CaP paste as a potential injectable bulking agent for the injection therapies.

The calcium phosphate paste used in this study was prepared by mixing hydroxyapatite (HA), polyethylene glycol 400 (PEG 400), glycerol and ringer solution. HA was synthesized and other materials was commercially obtained. The synthesized HA with two kinds of particle size prepared as solid phase. Two liquid compositions were obtained and used as liquid phase of the paste. The paste was obtained by mixing the powder (P) to the two liquids (L) at P/L ratio 1.

The results of the rheological test showed that the paste containing of PEG 400 was less sensitive to the rate of shear and had much more viscosity. Also injectability results containing of PEG 400 showed that a filterpressing phenomenon was happened but the paste containing of glycerol had a good injectability and require less force for injection. Also, it was found that the injectability of a new CaP paste can be improved by using of glycerol. It has the potential to be delivered through needles and applicators for practices that involve minimally invasive methods.

15:00 Oral

3D Laser Synthesis of Porous Tissue Scaffolds as repository for stem cells

Igor V. Shishkovsky[1], Yuri G. Morozov[2], Larisa T. Volova[3]

1. *P.N. Lebedev Physics Institute of RAS, Samara branch, Novo-Sadovaja st. 221, Samara 443011, Russian Federation* **2.** *Institute of Structural Macrokinetics and Materials Science, Russian Academy of Sciences, Chernogolovka 142432, Russian Federation* **3.** *Samara State Medical University, Samara 443096, Russian Federation*

e-mail: shiv@fian.smr.ru

General approach to the synthesis of porous functional meso-devices – bio compatible tissue-cellular scaffolds the based nitinol (NiTi phase with Shape Memory Effect property) or titanium by the SLS method and directed management (a priory, i.e. on stage of CAD) their physical-mechanical and physical-chemical characteristics is described.

Layer by layer It was synthesized as porous volume parts, which could be recommended for tissue-cellular scaffolds (matrixes), as solid 3D parts - from those biocompatible implant materials. Comparative histological and morphological analysis of medical applications for porous nitinol and titanium 3D parts is presented with connect to SEM-EDX structure and chemical element verification.

It was shown, that sintered porous titanium and nitinol is comfortable environment for stem cells. It allow to propose such tissue-cellular scaffolds as repository (matrix) for stem cell keeping and may be as basis for growth (recovery) demanded organs. It was remarked, that fabrication of nano substructure during SLS with self-organization by fractal type could be promoting the biomechanical integration of implant to a living tissue.

15:15 Oral

Soft chemical methods integration in developing new scaffolds for tissue engineering

Roxana M. Piticescu[1], Tinca Buruiana[2], Nicoleta Plesu[3], Eugeniu Vasile[4], Bogdan Firtat[5], Cristina F. Rusti[1]

1. *National Institute for Nonferrous and Rare Metals (IMNR), 102 Biruintei Blvd., Pantelimon 077145, Romania* **2.** *Petru Poni Institute of Macromolecular Chemistry of the Romanian Academy, Aleea Grigore Ghica Voda 41A, Iasi, Romania* **3.** *Institute of Chemistry Timisoara of Romanian Academy, Bdul Mihai Viteazul 24, Timisoara 300223, Romania* **4.** *METAV-CD SA, CA Rosetti Nr 31 Sect. 2, Bucharest 70000, Romania* **5.** *National Institute for Research and development in Microtechnologies (IMT-Buchares), P.O.Box 38-160, Bucharest 023573, Romania*

e-mail: roxana@imnr.ro

The aim of the work is to develop new scaffolds for tissue engineering. This supposes to integrate soft chemical methods (hydrothermal and electrochemical methods) for preparing multifunctional biomaterials based on hydroxyl-apatite and functionalized polyurethanes. The innovative part is represented by the following aspects:

- synthesis, in situ under hydrothermal synthesis at low temperatures and high pressures, of new nanostructured hybrid materials with a strong chemical/physical bonding between the components;

- applying the cyclic voltametry to monitor the electrical response of the nanostructured hybrid thin films deposited by spin-coating on gold-plated silicon wafers used as substrate. Electrochemical measurements were used to monitor cell adhesion, and experiments were designed to determine how various changes in substrates influence the cell adhesion and proliferation. To accomplish these studies, cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) were performed. As the cell number increases, the covered surface of electrode with cells will increase and the electrode impedance will change. Depending on the structural and compositional factors of the nanostructured hybrid thin films, the electrical response could be useful in monitoring by electrical simulation of the cell response. The processes at the substrate/hybrid interface have been studied by SEM and HRTEM methods. Biocompatibility studies by in-vitro tests of different immobilized biomolecules are under working.

Acknowledgements: The researches are financially supported by National Authority for Scientific Research in the frame of project 71-004/2007.

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Coffee break

Thursday afternoon, 18 September, 15:30
Main Hall

Posters

Monday, 15 September

Joint Poster Session 1

Monday & Wednesday
Monday afternoon, 15 September, 16:00
Main Hall

16:00 Poster L01

Optimization of polyurethane structure as the potential materials for bone tissue engineering applications

Monika Bil[1], Joanna Ryszkowska[1], Piotr Woźniak[2], Małgorzata Lewandowska-Szumieł[2], Krzysztof J. Kurzydlowski[1]

1. *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland* **2.** *Medical University of Warsaw, Department of Biophysics and Human Physiology, Chałubińskiego 5, Warszawa 02-004, Poland*

e-mail: mbil@meil.pw.edu.pl

Polyurethanes are microphase separated polymers, containing hard and soft segments. The hard, rigid segments are produced by a reaction between diisocyanate and chain extender while polyether, polyester or polycarbonate diol comprises the soft segments. Hard domains act as reinforcing filler in the soft matrix. The hard segment content influences the degree of the phase separation, which further affects the physical and mechanical properties and biocompatibility. By varying the composition of the polyurethanes their properties can be tuned to use in many areas of tissue engineering, either for reconstruction of soft tissue or for cartilage and bone regeneration.

The objective of this study was to develop polyurethane scaffolds with optimal hard segment content for human osteoblast culture. The aliphatic poly (ester-urethanes) were synthesized from poly(ε-caprolactone) diol with different molecular mass, cycloaliphatic diisocyanate 4, 4’-methylenebis(cyclohexyl isocyanate) and ethylene glycol as a chain extender. The structure-property relationships and behavior of Human Bone Derived Cells (HBDCs) in direct contact with the solid segmented polyurethanes containing from 22 to 70% (w/w) of the hard segments were investigated. Tensile strength and hardness of the polyurethanes were in the range of 1.6 - 48 MPA and 22- 61 Sh D, respectively. Increasing content of the hard segments results in an increasing surface hydrophilicity determined by contact angle measurements. Crystalline phase of polyurethane was characterized by differential scanning calorimetry and chemical structure by infrared spectroscopy. The best biocompatibility of HBDCs cultured in vitro demonstrates polyurethane containing 50% (w/w) of hard segments. This type of polyurethane was selected for porous scaffold fabrication.

Acknowledgements

This work was supported by the Ministry of Science and Higher Education, grant R13 01901.

16:00 Poster L02

Exploring the potentiality of MAPLE technique for biopolymer coatings

Valeria Califano[1], Francesco Bloisi[1,2], Luciano Vicari[1,2], Aldo R. Boccaccini[2]

1. *INFM - Coherentia, Via Cinthia, Napoli 80125, Italy* **2.** *Imperial College London, Department of Materials, London, United Kingdom*

e-mail: valeriacalifano@hotmail.com

Matrix Assisted Pulsed Laser Evaporation (MAPLE) technique is a thin film deposition technique developed to minimize the photochemical damage that results from direct interaction of the laser light with fragile organic molecules (polymers and biomolecules). In fact, in MAPLE the target is composed by a dilute (1-5%) frozen solution of a volatile and light absorbing solvent, which contains the molecules of interest as solute. When the laser pulse impacts the target, most of its energy is absorbed by the solvent, which vaporizes explosively entraining the polymer molecules in the plume. This provides a softer desorption of intact polymer molecules. The volatile solvent is pumped away by a vacuum pump, resulting in a non-contact deposition technique.

For the deposition of biopolymer thin films, the MAPLE technique is a suitable alternative to solution-based processing techniques due to the following facts: (1) MAPLE is a non-contact deposition technique, thus eliminating a major source of contamination, i.e., the solvent and its impurities, and it can be integrated with other sterile processes; (2) The accurate thickness control is beneficial to tailor the in-vivo degradation rate of bioresorbable polymers, being the time of degradation proportional to the thickness of the film; (3) MAPLE allows multiple-layer depositions without the risk of re-dissolving the first deposited layer. This characteristic offers interesting perspectives for multilayer deposition of composite coatings.

This study concerns the exploration of the possibility of biopolymer coatings by MAPLE and of the possible advantages on the properties of the obtained composite materials that this technique can have. In particular, among the applications we also explored the possibility of coating three-dimensional porous scaffolds using (D,L-lactide) (PDLLA) as coating material and 45S5 Bioglass® as scaffold material.

16:00 Poster L03

Immobilization of bioactive moieties on polycaprolactone scaffold surface: RGD sequence bioconjugation after aminolysis

Filippo Causa[1], Edmondo Battista[1], Raffaella Della Moglie[3], Paolo A. Netti[2,3]

1. *Dipartimento di Medicina Sperimentale e Clinica (UMG), Viale Europa, Catanzaro 88100, Italy* **2.** *Department of Materials & Production Engineering, University of Naples "Federico II" (DIMP-CRIB), Piazzale Tecchio, 80, Napoli 80125, Italy* **3.** *Interdisciplinary Centre on Biomaterials (CRIB), Napoli 80125, Italy*

e-mail: causa@unicz.it

PCL is a semicrystalline thermoplastic polyester widely used in biomedical field. This popular biomaterials for tissue engineering scaffold often has suboptimal properties when analyzed for cell attachment and growth, thus, it should be desirable to improve its performance by immobilization of bioactive moieties on its surface.

Moreover, short amino acid sequence such as arginine-glycine-aspartic acid (RGD) has been widely used as recognition motif to mediate cell attachment.

The aim of this work is to set-up a procedure to covalently immobilize RGD-based peptide sequences onto functionalized PCL surface. The procedure consists of three steps: aminolysis of polymeric scaffold, grafting of a tether and peptide immobilization.

The aminolysis of PCL substrates with 1,6-hexanediamine has been investigated and the yield of the reaction evaluated. In particular, the amount of amino group introduced, measured by Ninhidryn assay reached a maximum NH_2 density of ~$1*10^{-7}$mol/cm^2 (30 minutes, 37°C)(fig 1).

Contact angles decrease with increasing time of treatment, ranging from 76° (pure) to 67° (90 min at 37°C). The rates of NH_2 grafting at different temperatures (from 24 to 37°C) ranged from 0.92 to $3.2*10^{-8}$ mol/cm^{2}min, and, an activation energy of 59 kJ/mol have been evaluated.

Moreover, ATR-FTIR spectroscopy characterization evidenced the presence of amine group (3337cm^{-1} NH stretch, 1639cm^{-1} and 1556cm^{-1} -CONHR- absorption) (fig 2). Afterwards, indeed, glutaraldeide solutions were used to graft GRGDY-Rho sequences on scaffold surface after reaction in mild aqueous conditions by reductive amination.

CLSM observations were also preformed on cross-sections of 3D PCL scaffolds demonstrating the capability to control in space and amount the peptide immobilization also in the case of 3D PCL substrate to be used as scaffold for tissue engineering.

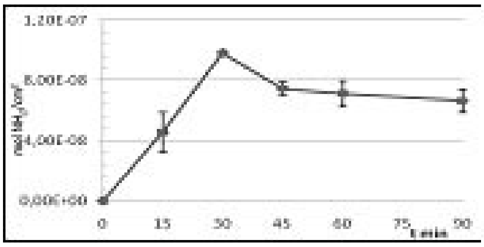

Fig 1

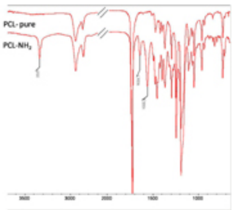

Fig 2

16:00 Poster L04

Synthesis of thermo-responsive hyaluronic acid based hydrogel and its application in cartilage tissue engineering using mesenchymal stem cells

Jyh-Ping Chen, Chia-Hsin Lu

Chang Gung University, Taoyuan 3330, Taiwan

e-mail: jpchen@mail.cgu.edu.tw

An injectable polymer hydrogel with hyaluronic acid as the backbone and end-grafted poly(*N*-isopropylacrylamide) as the thermo-sensitive moiety was synthesized. The thermo-responsive hyaluronic acid-*g*-poly(*N*-isopropylacrylamide) (HPN) copolymer was used a scaffold for cultivation of bone marrow mesenchymal stem cells (MSCs), which could be induced into articular chondrocytes in vitro for the treatment of cartilage defect. The copolymers exhibited temperature-sensitive reversibly soluble-insoluble characteristics with the lower critical solution temperature (LCST) being around 30°C, which depends on polymer compositions during grafting reactions. Results from scanning electron microscopy (SEM) confirmed a porous, interconnected, 3-D structure of this polymer at the physiological temperature. Other temperature-dependent physical properties of the copolymer hydrogel, such as rheological properties, water content and volume change, phase transition kinetics, and reusability were also characterized in detail. For MSCs culture, 3-D cultures with HPN copolymer hydrogels were compared with 2-D cultures on TCPS for cell functionality. In addition, gelatin and transforming growth factor-β1 (TGF-β1) was incorporated into HPN by conjugating the protein to the copolymer through the carboxylic groups of HA with 1-(3-dimethylamino-propyl)-3-ethyl-carbodiimide hydrochloride (EDC) as a crosslinking agent. MSCs were seeded in HPN scaffolds with and without TGF-β1 and cultured under conditions of different periods of chondrogenic differentiation induction. Results including cell proliferation, cell viability, light microscopy and SEM observations, and glycosaminoglycans (GAG) and collagen synthesis were studied. From the experimental results obtained, we concluded that MSCs can be successfully induced into articular chondrocytes in HPN and the hydrogel shows a promising potential to be a suitable 3-D scaffold for tissue engineering of cartilage.

16:00 Poster L05

Preliminary examinations of mechanical properties of DLC and novel DLC-polymer hybrid coatings for resurfacing hip prostheses

Emilia Choinska[1], Maciej M. Spychalski[1], Wojciech Swieszkowski[1], Ingrid Milosev[2], Veli M. Tiainen[3], Krzysztof J. Kurzydlowski[1]

1. *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland* **2.** *Jozef Stefan Institute, Department of Physical and Organic Chemistry (JSI), Jamova 39, Ljubljana 1000, Slovenia* **3.** *The Invalid Foundation, ORTON Research Institute, Tenholantie 10, Helsinki 00280, Finland*

e-mail: choinska.emilia@gmail.com

Resurfacing hip implants are promising type of hip implants, since they allows maximum preservation of the patient's own bone. This speeds up the healing process and facilitates eventual later revision surgery. But there are some problems with metallic wear debris, which induce metallosis. They can also lead to aseptic loosening of the implant.

The diamond-like carbon (DLC) and novel DLC-polymer hybrid (DLC-p-h) nanocomposite coatings, deposited with filtered pulsed arc discharge method (FPAD), have the potential to improve greatly the tribological properties of these implants by decreasing the friction and wear.

The aim of the present study was preliminary examinations of the DLC and DLC-p-h anti-wear coatings deposited on AISI316L stainless steel. The different composition of cathodes and parameters of FPAD process were used to fabricate the 3 types of coatings: DLC, DLC-PDMS-h and DLC-PTFE-h. These deposited coatings were investigated in terms of surface characterization, chemical composition, mechanical and electrochemical properties, using optical profilometer, SEM, FIB, nanoindenter Hysitron, XPS, Raman spectroscopy and electrochemical methods.

The results show that coatings deposited with FPAD method are homogenous and good quality. The two types of novel coatings has similar mechanical properties (E_r = 5-13GPa, H=0,2-0,7GPa), which are different (much lower) than for DLC (E_r = 200-230GPa, H=21,6-22,3GPa). Further examination will be focus on the tribological properties of novel hybrid coatings.

The deposited coatings offer a good corrosion protection under physiological conditions, as investigated by electrochemical potentiodynamic measurement in Hank's simulated physiological solution at 37ºC. The corrosion resistance deduced from polarization resistance measurements increases in the following order: DLC<DLC-PTFE-h and DLC-PDMS-h.

16:00 Poster L06

Bioactive hydroxyapatite coatings on polyurethane implants

Gabriela Ciobanu[1], Gabriela Carja[1], Simona Ratoi[1], Octavian Ciobanu[2], Ion Sandu[3]

1. *Technical University from Iasi (UTI), Bd.D.Mangeron 63, Iasi 700050, Romania* **2.** *"Grigore T. Popa" Medicine and Pharmacy University, 16 University, Iasi Ro 6600, Romania* **3.** *Iasi, Al.I.Cuza University (Iasi, UAIC), 11 Carol I Blvd., Iasi 700506, Romania*

e-mail: gciobanu03@yahoo.co.uk

Polyurethane is a biocompatible material that is used for biomedical applications, especially in the fields of tissue engineering, tissue regeneration and replacement applications. Hydroxyapatite is widely used as a bioactive ceramics since it forms a chemical bonding to bone. Applications include coatings of orthopedic and dental implants and scaffolds for bone growth. This work presents an alternative coating method based on biomimetic techniques which are designed to form a crystalline hydroxyapatite layer very similar to the process corresponding to the formation of natural bone. The hydroxyapatite deposits are investigated by means of scanning electron microscopy (SEM) and energy dispersive X-ray analysis (EDX). In vitro hydroxyapatite formation studies show that the morphology and structure of hydroxyapatite layers alter in different condition of preparation.

Acknowledgments: This research was supported by the Grant al Academiei Romane no. 59/2008 and the PNCDI II - NATOEPA no. 71-020/2007.

16:00 Poster L07

Alginate/lactose-modified chitosan hydrogels: a bioactive biomaterial for chondrocyte encapsulation

Ivan Donati

Università di Trieste, Trieste, Italy

e-mail: idonati@units.it

Cartilage degeneration represents a serious health problem, causing progressive debilitation and marked decrease of quality of life. Cartilage damages occur as a consequence of congenital abnormalities, diseases and traumas, and are related to the limited intrinsic healing potential of this tissue. Because of the lack of blood supply and subsequent insufficient inflammatory response, lesions to cartilage result in an incomplete repairing attempt by local chondrocytes leading to mechanically inadequate resident fibrocartilage formation. During the past decade tissue engineering procedures have been widely studied for the treatment of articular cartilage damages, exploiting the basic knowledge gained in the fields of cell and molecular biology and the advances of biomaterial research.

A new bioactive scaffold has been prepared from a binary polysaccharide mixture (AC-mixture) composed of a polyanion (alginate) and a polycation (a lactose-modified chitosan, chitlac) and its potential use for articular chondrocytes encapsulation and cartilage reconstructive surgery applications has been studied. The hydrogel combines the ability of alginate to provide for a supporting structure with the capability of the second component (chitlac) to directly interact with porcine articular chondrocytes. Physico-chemical characterisation of the scaffold was accomplished by gel kinetics and compression measurements and demonstrated that AC-mixture hydrogels exhibit improved mechanical properties when compared with sole alginate hydrogels. Furthermore, biochemical and biological studies showed that these 3D-scaffolds are able to maintain chondrocyte phenotype and particularly to significantly stimulate and promote chondrocyte growth and proliferation. In conclusion, the present study can be considered as a first step towards an engineered biologically active scaffold for chondrocyte *in vitro* cultivation, expansion and cell delivery.

16:00 Poster L08

Polymer-Ceramic Composite Scaffolds for Osteochondral Tissue Engineering

Timothy Douglas[1], Betül Temel[1], Bodo Kurz[1], Sureshan Sivananthan[2], Jörg Wiltfang[1], Patrick H. Warnke[1,3]

1. *Christian-Albrechts-Universität Kiel, Kiel 24098, Germany* **2.** *Epsom and St Helier University Hospital, University of London, London SM51AA, United Kingdom* **3.** *Faculty of Health Sciences and Medicine, Bond University, Gold Coast Queensland, Australia*

e-mail: douglas@mkg.uni-kiel.de

Polymer-Ceramic Composite Scaffolds for Osteochondral Tissue Engineering

One popular approach in osteochondral tissue engineering for the treatment of osteochondral defects is the use of polymer-ceramic composite scaffolds. The purpose of this study was to evaluate the in vitro biocompatibility for osteoblasts of a new composite scaffold type, Osteochondral Plugs (Biocomposites Ltd., U.K.). These consisted of Poly-L-lactid Acid (PLLA) fibres, Polycaprolactone (PCL) and Tricalcium Phosphate (TCP) sprayed with Hydroxyapatite (HAP). Average pore size was approximately 200-250 µm. Two versions of Plugs were compared. Version 1 contained $CaSO_4$, whereas Version 2 was $CaSO_4$-free. Plugs were seeded with human osteoblasts. Cell morphology was assessed using scanning election microscopy (SEM). Cell vitality was evaluated using fluorescence microscopy after staining with fluorescin diacetate (FDA) and propidium iodide (PI). Standard tests for biocompatibility (WST, LDH, MTT) were performed. SEM investigation showed that osteoblasts adhered to the surface of both versions of Osteochondral Plugs and demonstrated good spreading. Fluorescence microscopy and standard tests for biocompatibility (WST, LDH, MTT) showed superior biocompatibility of Version 2 to Version 1. It can be concluded that the incorporation of $CaSO_4$ into Plugs is disadvantageous for biocompatibility in vitro. Further tests are needed to assess biocompatibility in vivo.

16:00 Poster L09

Rapid Prototyping: Porous Titanium Alloy Scaffolds produced by Selective Laser Melting (SLM) for bone tissue engineering

Timothy Douglas[1], Patrick Wollny[1], Betül Temel[1], Stephan T. Becker[1], Ingo N. Springer[1], Sureshan Sivananthan[2], Jörg Wiltfang[1], Patrick H. Warnke[1,3]

1. *Christian-Albrechts-Universität Kiel, Kiel 24098, Germany* **2.** *Epsom and St Helier University Hospital, University of London, London SM51AA, United Kingdom* **3.** *Faculty of Health Sciences and Medicine, Bond University, Gold Coast Queensland, Australia*

e-mail: douglas@mkg.uni-kiel.de

Selective Laser Melting (SLM), a method used in the nuclear, space and racing industries, allows the creation of customized titanium alloy scaffolds with highly defined external shape and internal structure (pore size) using rapid prototyping as supporting external structures within which bone tissue can grow. Human osteoblasts were cultured on SLM-produced 3D titanium alloy (Ti6Al4V) mesh scaffolds to demonstrate biocompatibility using Scanning Electron Microscopy (SEM) and fluorescence microscopy after cell vitality staining. The occlusion of pores of different widths (0.45 - 1.2 mm) by osteoblasts was evaluated. SEM investigations showed osteoblasts with well-spread morphology and multiple contact points. Cell vitality staining confirmed osteoblast vitality. 1 week after seeding, only 0.45 mm pores showed any occlusion by osteoblasts (21%). At 3 weeks the occlusion of 0.45 mm, 0.5 mm, 0.55 mm, 0.6 mm and 0.7 mm pores was 79%, 67%, 67%, 44% and 10%, respectively. At 6 weeks the occlusion of 0.45 mm and 0.5 mm pores had risen to 100%, but no increase was observed for 0.55 mm, 0.6 mm and 0.7 mm pores. No pore occlusion was observed on pores of width 0.9 – 1.2 mm. In summary, the scaffolds are biocompatible and pore size influences pore overgrowth.

16:00 Poster L10

Ceramic scaffolds produced by rapid prototyping: characterisation and biocompatibility investigations

Timothy Douglas[1], Betül Temel[1], Hermann Seitz[2], Sureshan Sivananthan[3], Jörg Wiltfang[1], Patrick H. Warnke[1,4]

1. *Christian-Albrechts-Universität Kiel, Kiel 24098, Germany* **2.** *University of Rostock, August-Bebelstr. 55, Rostock 18055, Germany* **3.** *Epsom and St Helier University Hospital, University of London, London SM51AA, United Kingdom* **4.** *Faculty of Health Sciences and Medicine, Bond University, Gold Coast Queensland, Australia*

e-mail: douglas@mkg.uni-kiel.de

Ideally, scaffolds used as bone replacement materials should fit the defect site exactly and have tailored porosity and pore size. Commonly used ceramic materials in general are not easily to form to individual patient needs. Using rapid prototyping methods, three-dimensional ceramic scaffolds of hydroxyapatite (HAP) and tricalcium phosphate (TCP) have been produced with defined external shape and internal structure by sintering ceramic powder. These scaffolds also demonstrate microporosity due to gaps in the sintered particles. The goal of this study was to evaluate the in vitro biocompatibility of these new HAP and TCP scaffolds compared to the material BioOss®, which is widely used in oral and maxillofacial surgery. To this end, human osteoblasts were cultured in eluate from the aforementioned scaffolds and also seeded onto scaffolds directly.

Using commonly used biochemical tests (LDH, MTT, WST) and cell vitality assessment by fluorescence microscopy after staining with fluorescin diacetate (FDA) and propidium iodide (PI), it was found that the new ceramic HAP scaffolds produced by rapid prototyping have superior biocompatibility for osteoblasts than the material BioOss®. However, new ceramic TCP scaffolds produced by rapid prototyping appear to be less biocompatibile than BioOss®. Scanning electron microscopy (SEM) revealed colonisation and spreading of osteoblasts on HAP and TCP scaffolds. It can be concluded that HAP scaffolds in particular are biocompatible for use as bone substitute materials.

16:00 Poster L11

Fabricationg polyurethane/calcium carbonate composite scaffold for bone tissue engineering

Ida O. Dulińska-Molak, Joanna Ryszkowska, Monika Bil, Anna Wolska, Krzysztof J. Kurzydlowski

Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland

e-mail: idad@meil.pw.edu.pl

The main function of a tissue engineering scaffolds is to act as a substrate for depozition of cells, and their subsequent growth and proliferation.

The basic requirements for the scaffold material are biocompatibility, degradability, mechanical integrity and osteoconductivity. Novel biodegradable scaffolds made of poly (e-caprolactone) urethane (PCL_PUR) porous matrix and calcium carbonate ($CaCO_3$) were developed and studied for bone tissue engineering.

The scaffolds were prepared by *in situ* polymerization. Porous structure of the scaffolds was obtained by combining leaching and coagulation techniques, using NaCl with the grain size 250-500 um as a porogen. An influence of solution concentration on scaffolds structure and properties was evaluated.

The structure and properties of scaffolds were studied by scanning electron microscopy and thermal analyse. The scaffolds were incubated in a buffered simulated body fluid at 37°C for certain periods of time to allow for apatite formation and potential improvement of osteoconductivity.

Calcium phosphates formation of the apatite layer on three dimensional scaffolds was investigated by X-ray diffraction (XRD), X-ray Photoemission Spectroscopy (XPS), Scanning Electron Microscope (SEM) equipped with Energy-Dispersive Spectrometer (EDS) and Fourier transformed infrared spectroscopy-attenuated total reflectance (FTIR-ATR). The thermal and mechanical properties of composites were investigated using Thermal Gravimetric Analysis (TGA), Differential Scanning Calorimeter (DSC) and Dynamic Mechanical Analysis (DMA).

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The authors thank Dr Zbigniew Jaegermann from Institute of Glass and Ceramics forsupplying us calcium carbonate. This scientific work was funded from the finances for education in the years 2006-2008 as research project no. R1301901

16:00 Poster L12

Nanomechanical measurements of thin dextran layers

Wojciech R. Fabianowski[1], Beata Polak[1], Ude Hangen[3], Tomasz Kobiela[1], Radosław M. Olkowski[2], Małgorzata Lewandowska-Szumieł[2]

1. *Warsaw University of Technology, Faculty of Chemistry, Noakowskiego 3, Warszawa 00-664, Poland* **2.** *Medical University of Warsaw, Department of Biophysics and Human Physiology, Chałubińskiego 5, Warszawa 02-004, Poland* **3.** *Hysitron, Munich 85737, Germany*

e-mail: wofab@ch.pw.edu.pl

Surface modifications play a crucial role in tissue engineering for bone regeneration. There are many important factors for biomaterials that have to be fulfilled in order to ensure a proper growth and proliferation of bone cells.

In this study the influence of surface mechanical properties on osteoblasts in culture was investigated. Thin dextran films with 8 different thickness were deposited from water solution on silicon wafers. After radiation sterilization Human Bone Derived Cells (HBDC) were seeded under standard conditions. Mechanical properties, i.e. reduced elastic modulus - Er and hardness - H of prepared modifications, were investigated using Hysitron Triboindenter. Reduced elastic modulus was measured both on dry samples as well as on samples dipped in solution of culture medium – DMEM. Mapping of reduced elastic modulus on selected hybrid surfaces was performed. Cell viability (XTT) was performed after 1 week of culture.

After Er and H measurements in DMEM we observed swelling effect for 8 layers of dextran. Dextran films consisting of 8 layers were the most elastic and soft. Cell viability was found to be changed depending on the thickness of the dextran deposits.

It is concluded that the elasticity and the topography of the surface influence cell behaviour in direct contact.

16:00 Poster L13

The influence of graphene layer on the cholesterol lodgement: molecular dynamics simulation

Krzysztof M. Górny, Przemysław Raczyński, Zygmunt Gburski

University of Silesia, Institute of Physics, Uniwersytecka 4, Katowice 40-007, Poland

e-mail: kgorny@us.edu.pl

The dynamics of cholesterol molecules forming an ultrathin layer (lodgment) around an extracellular domain protein has been studied *via* molecular dynamics (MD) simulations. We have also investigated the impact of the graphene layer on the nanosystems studied. The graphene wall influences the motion of cholesterol molecules forming the thin layer developed over the surface of a protein.

16:00 Poster L14

Implants with carbon coatings

Jacek D. Grabarczyk[1], Ireneusz Kotela[2]

1. *Technical University of Lodz, Institute of Materials Science and Engineering, 1/15 Stefanowskiego, Łódź 90-924, Poland* **2.** *Wojewódzki Szpital Zespolony, Lwowska 178a, Tarnów 33-100, Poland*

e-mail: jacek.grabarczyk@p.lodz.pl

Contact allergy on metals is a cause of complications in application of metal implants in human body. In clinical practice are known the patients with the Irritation Reaction (IR) and typical Contact Allergy on nickel, chromium and cobalt which are used as a components of biomaterials in implantology. The very important problem is a hypersensitivity to titanium which was recognized as a safe biomaterial for human body as far.

The idea of this research is the manufacturing the thin carbon layer on the metal implant surface and changing the biocompatibility of its.

Carbon as a biocompatible biomaterial is a diffusion barrier between material of implant and human body. Metal ions from the implant cannot penetrate form metal to tissue.

Hermetic carbon coating completely prevents agaimst developing of contact allergy after implantation.

Authors of article present the research which have been done on patients with a allergy to nickel, chromium and cobalt. The patch tests have been done on patients. These results indicate that the application of carbon coating on the surface of metal implants eliminate allergic reaction.

In this article will be present the patients with contact allergy on metals after implantation of prostheses covered by carbon coating and results of treatment.

The examinations show that metal implants with carbon coating decrease the risk of the contact allergy on metals. Biocompatible and chemical resist carbon coating additionally increases corrosion resistance of implant and thus this stable isolation layer between organism and metal is very good for short- and long-term implants.

16:00	Poster	L15

Optimization of the polymeric scaffolds for bone tissue engineering fabricated by rapid prototyping method

Marcin K. Heljak[1], Wojciech Swieszkowski[1], Christopher Lam[2], Dietmar W. Hutmacher[3], Krzysztof J. Kurzydlowski[1]

1. *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland*
2. *National University of Singapore (NUS), Singapore, Singapore*
3. *Queensland University of Technology (QUT), Queensland 4001, Australia*

e-mail: marcin.heljak@gmail.com

The favourable scaffold for bone tissue engineering should be characterized, among others, by high mechanical strength and 3D open porosity, which guarantee biocompatibility and suitable environment for tissue regeneration. Numerical modeling could be used as a tool for preclinical evaluation and optimization of the scaffold. In fact, optimization of such complex structures like bone scaffolds is a great challenge for investigators. In the paper optimization of material application for particular fiber of scaffold fabricated by FDM was described. The objective of optimization is the best possible mechanical strength – degradation rate ratio. The used method of optimization was standard Genethic Algorithm, which is efficient method of discrete optimization, especially when solved problem is characterized by a great number of variables. In case of optimization of bone scaffold, number of variables is equal to number of fibers. Each of fibers could be made by different material (number of used materials is 5). The ultimate goal of study was to created optimal scaffold model for simulations of new bone formation.The numerical models of the scaffolds were generated using MSC/Patran. The generated mesh was optimized by SED criterium and finally consisted of about 270,000 finite elements. Results showed that, application of different material for particular fiber is very efficient method of controling the scaffold behaviour during healing process.

16:00	Poster	L16

Biodegradable and bioabsorbable polymeric - ceramic composites for medical applications

Tomasz Jaroszewicz[1], Barbara D. Ostrowska[1], Wojciech Swieszkowski[1], Miroslawa El Fray[2], Krzysztof J. Kurzydlowski[1]

1. *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland*
2. *Szczecin University of Technology, Polymer Instiute, Pulaskiego 10, Szczecin 70-322, Poland*

e-mail: t_jaroszewicz@o2.pl

Bioabsorbable and biodegradable materials are expected to maintain their mechanical properties for an amount of time and then eventually degrade and be resorbed or excreted. Biodegradable polymers, especially those belonging to the family of polyglicolic acid (PGA) and polylactic acid (PLA) together with poly e-caprolactone, play an increasingly important role in medical applications. Due to their properties, they find their place in orthopaedics and tissue engineering. They can be used to manufacture a wide range of bone implants, porous scaffolds and cell carriers for tissue engineering.

Initial durability of polymer made device or the time, when it is suitable, are to small to ensure patient’s full reconvalescence or proper cells density on the scaffold. Therefore, using polymer-ceramic composites as a timber, besides only polymer or co-polymer made, seem to be more favourable. Ceramics improves implant’s/scaffold’s mechanical properties and vitality which eliminates the risk of to early disintegration.

The aim of the study was to develop a strong biodegradable implant material which could be used for medical application. Different polymer-ceramic composites were fabricated using combined mixing and extrusion process. PLA, PGA and PCL were selected as a matrix materials. HAp and TCP (10-30%) have been used to reinforce the polymeric matrixes.

Extensive mechanical tests were performed to investigate the mechanical properties of the composite. µCT and nCT as well as SEM, were used to study the ceramic particles distribution in the polymeric matrix. Mechanical tests results show the increase of stiffness, improved tensile and breaking strengths and very low sterilization influence on mechanical properties. The particles were distributed homogeneously in the polymer. The conclusion is that the developed composites may be used as implant materials.

16:00 Poster L17

Comparative study of hydroxyapatite and hydroxyapatite mixed with bioglass coatings for metallic implants, deposited by PLD method.

Waldemar Mróz[1], Sylwia Burdyńska[1], Marcin Jedyński[1], Artur Prokopiuk[1], Anna Ślósarczyk[2], Maria Łączka[2], Katarzyna Cholewa-Kowalska[2], Elżbieta Menaszek[4], Anna Ścisłowska-Czarnecka[5], Agata Niedzielska[3]

1. *Military University of Technology, Institute of Optoelectronics (IOE), Kaliskiego 2, Warszawa 00-908, Poland* **2.** *AGH University of Science and Technology, Faculty of Materials Science and Ceramics (AGH UST), Mickiewicza 30, Kraków 30-059, Poland* **3.** *Technical University of Lodz, Institute of Materials Science and Engineering, 1/15 Stefanowskiego, Łódź 90-924, Poland* **4.** *Jagiellonian University, Collegium Medicum, Department of Pharmaceutical Microbiology, Medyczna 9, Kraków 30-688, Poland* **5.** *Academy of Physical Education, Faculty of Anatomy (AWF), Al. Jana Pawła II 78, Kraków 31-571, Poland*

e-mail: jedynski@ippt.gov.pl

Hydroxyapatite and Bioglasses are important bioactive materials as they exhibit direct bonding with human bone. Therefore they are used as a coatings for metallic implants. The aim of the study was to compare two types of layers: hydroxyapatite (HA) and hydroxyapatite mixed with bioglass (BG) (HA+BG, 50% of BG) during initial stage of their interaction with cell medium. The layers were deposited by pulsed laser deposition technique on 316L stainless steel with nanocrystalline diamond as a buffer film. The *in vitro* study was performed in order to determine the effect of the two layers on the cells response. Human osteoblast-like cells (MG-63) were cultured on examined surfaces and on polystyrene commercial 48-well cell culture plates (TCPS) used as a control. After 3 and 7 days the behaviour of the cells grown on different surfaces was compared through determination of cell adhesion (CV colorimetric assay). Cell morphology and properties of biomaterials surfaces were analysed by atomic force microscopy (AFM).

The results of CV tests performed after 3 days of culture proved the much better ability of HA/BG layers to stimulate cell adhesion in its initial stage compared to HA and TCPS. After 7 days' culture the results of CV tests didn't differ significantly for HA and HA+BG but were still much better than in the case of TCPS.

16:00 Poster L18

Electrospun polymeric fibers for cartilage regeneration

Ewa Kijeńska, Wojciech Swieszkowski, Krzysztof J. Kurzydlowski

Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland

e-mail: ewakijenska@gmail.com

The aim of tissue engineering is to allow the regeneration of natural tissues and to create biological substitutes for injured organs. The formation of new cartilage tissue is one of the most significant problems that tissue engineering encounts. Bioactive microporous scaffolds covered with nano- or subimcrofibers seem to be a promising solution for these problems. One of the best methods to prepare such fibers is electrospinning. Electrospinning is a fiber formation technique that uses electrostatic forces to create continuous fibers.

The aim of this study was to investigate the influence of electrospinning process parameters on fibers diameter and to obtain electrospun PDLA fibers suitable for cartilage scaffolds. Parameters of electrospinning process like applied voltage, polymer concentration, solution conductivity, needle diameter and working distance (distance between needle and collector) were studied to fabricate fine fibers. The choosing of optimum parameters (voltage U=10kV, needle inner diameter Ø = 0.41mm, working distance 180mm and conductivity K=0.035 uS/cm) allowed for obtaining fibers with diameter from tens nanometers to submicrons. This kind of fibers combined with microporous scaffolds should support formation of new cartilage tissue.

16:00 Poster L19

Kinetic study of hydroxyapatite formatioin from $Ca(OH)_2$ and H_3PO_4

Dong Wook Kim[1], In-Sun Cho[1], Hae Lin Jang[1], Hyun Suk Jung[2], Kug Sun Hong[1]

1. *Seoul National University, Department of Materials Science and Engineering (MSE, SNU), San 56-1, Sillim-dong, Gwanak-gu, Seoul 151-744, Korea, South* **2.** *Kookmin University, School of Advanced Materials Engineering, Seoul 136-702, Korea, South*

e-mail: dong0414@snu.ac.kr

The process of hydroxyapatite (HAp) formation was investigated via an in-situ analysis by freeze drying the sampled products during the reaction. It is confirmed that HAp is formed from $Ca(OH)_2$ and H_3PO_4 via dicalcium phosphate dihydrate (DCPD) phase as an only precursor, which has been monitored by XRD, FT-IR, ^{1}H and ^{31}P MAS NMR and pH measurements. Additionally, we demonstrated the kinetics of HAp formation with an experimental proof that is the FESEM images of powders at various time intervals. It was directly observed how the change of plane and cross-section in powders were developed. The process of HAp formation was made up of the formation of DCPD and the transformation of DCPD to HAp. This transformation was developed by initially (1) heterogeneous nucleation-controlled and then (2) gradual transformation in volume of DCPD. However, the transformation was retarded by the slow diffusion process and the slow dissolution of residual $Ca(OH)_2$. Further works are needed to enhance the crystallization process with a fairly simple process.

16:00 Poster L20

Structure evaluation of Porcine Cornea Decellularized by Ultra High Hydrostatical Pressurization

Hisatoshi Kobayashi[1], Tsuyoshi Kimura[2], Seiichi Funamoto[2], Yoshihide Hashimoto[2], Syuji Sasaki[2], Manabu Mochizuki[2], Shinnya Hattori[1], Takako Honda[1], Toshiya Fujisato[3], Akio Kishida[2]

1. *National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba 305-0047, Japan* **2.** *Institute of Biomaterials and Bioengineering, Tokyo Medical and Dental University, Tokyo 101-0062, Japan* **3.** *Osaka Institute of Technology, Osaka 535-8585, Japan*

e-mail: kobayashi.hisatoshi@nims.go.jp

Introduction: The success rate of a corneal transplantation is high compared to other forms of tissue transplantation, but many complications still occur. Also, an absolute shortage of donor corneas has been an important problem in many countries. Artificial corneas have been studied as alternatives in order to overcome these problems. Acellular cornea scafforld seems to natural cornea same structure without host cells and antigen molecules. Therefore, acellular cornea scaffold was expected to infiltrate the donor cells into the scaffold and regenerate the tissues. We made acellular cornea scaffold using ultra-high pressure (UHP) method without detergents. Our objective of this study is to investigate the structual difference of acellular corneas between UHP method and current methods. **Materials and Methods:Decellularization of corneas:** The corneas were pressurized at 4,000 or 10,000 atm at 10 or 30˚C for 10 min using a high-pressure machine, washed by continuous shaking in an EGM-2 medium containing DNase I (0.2 mg/ml), antibiotics and 3.5 % w/v dextran at 37˚C under 5% CO2, 95% air for 72 hours. **Ultrastructure of decellularization corneas:** After decellularization, each cornea was fixed with glutaraldehyde and osmium tetraoxide. After fixation, tissues were enbedded with epoxy resin. 80nm thickness sections were obtained. Cutting sections were observed using transmission electron microscopy. **Results and Discussion:** Ultrastructual properties of decellularized corneas made by UHP method were resembled with natural cornea. Collagen bundles were observed by TEM. In addition, there were no host cells in the UHP decellurized corea. On the other hand, microstructual properties of SDS decellularized corneas were far from natural cornea. No collagen bundles were in it. The results indicated that UHP decellurized cornea might be had a potential ability for the scaffold to regenerate cornea tissue. The results of 6 month implantation will be presented.

16:00 Poster L21

Bioresorbable and bioactive PGLA/bioglass composites – mechanical properties and in vitro studies

Justyna Kokoszka[1], Maria Łączka[1], Elżbieta Pamuła[1], Katarzyna Cholewa-Kowalska[1], Anna M. Osyczka[2]

1. *AGH University of Science and Technology, Faculty of Materials Science and Ceramics (AGH UST), Mickiewicza 30, Kraków 30-059, Poland* **2.** *Jagiellonian University, Faculty of Biology and Earth Science, Institute of Zoology (UJ), Kraków 31-007, Poland*

e-mail: j.kokoszka@poczta.fm

The polymer base composites are considered as one of the most promising groups of materials in medicine. The combination of polymers with bioactive component like bioglass, takes advantage of the osteoconducting properties – bioactivity and of their strengthening effect on polymer matrices.

The aim of this study was preparation and investigation of new polymer/bioglass composites of enhanced bioactivity. The composites were manufactured in form of foils by volume dissolving of PGLA and Bioglass. As a component of composites were used sol-gel derived bioglasses: S2 – high silica bioglass, and A2 – high lime glass. In this work PGLA composites containing 12% vol., 21% vol. and 33% vol. bioglass additions were manufactured. The obtained PGLA/Bioglass composites were characterized under mechanical properties, wettability and hydrolytic degradation. Hydrolytic degradation was realized in distilled water at 37^{o}C for 3 months. The degradation process was monitored by pH and conductivity measurements of incubation medium. In order to estimate bioactivity of composites the surface changes of composites were investigated as a function of soaking time in simulated body fluid (SBF) after 5 and 10 days using SEM/EDAX analysis. Simultaneously, the interaction of composites with human stem cells was tested under *in vitro* conditions.

The results of the degradation studies in SBF indicate the possibility to modulate the degradation rate of the composite. The rapid formation of HA on composite foils after incubation in SBF indicates the high bioactivity of the material. Future work will focus on preparing the bioglass/polymer scaffolds for tissue engineering and tissue repair.

16:00 Poster L22

Selective Laser Melting for medical models processing from Ti alloys

Edward Chlebus, Bogdan Dybała, Tomasz Kurzynowski

Politechnika Wrocławska (PWR), Wybrzeże Wyspiańskiego, Wrocław 50-370, Poland

e-mail: tomasz.kurzynowski@pwr.wroc.pl

Rapid Manufacturing Technologies as methods of free-form fabrication have found a widening area of applications in the medical field. Nowadays medical models, scaffolds, implants and prostheses may be highly individual and customised. Biomodels should have a porous outer layer to increase bone osseointegration and a compact core to provide a required mechanical strength. It is possibile to produce a highly complex geometrical internal structure to reduce weight keeping mechanical properties of the medical part. It is expected that besides small batch or one-off production for the industry, additive metal RM technologies may be applied to provide customised biomodels for individual patients, and – what is most promising – end-use medical products.

16:00 Poster L23

Poly(lactic acid) with a sugar moiety at a terminal group as a transdermal permeation enhancer

Chia-Chang Liu, Ken Yuan Chang, Yng Jiin Wang

National Yang Ming University, Taipei 112-21, Taiwan

e-mail: lcceric90@yahoo.com.tw

The objective of this study was to synthesize and characterize a series of novel diblock copolymer containing sugar moiety at a terminal group as a transdermal penetration enhancer.Sugar-based micelles are advantageous because they are highly biodegradable and non-toxic.Those amphiphilic diblock copolymers may be regarded as a building block for the micellar drug carriers and cosmetic delivery systems. Normally transdermal permeation enhancers are of relatively low molecular weight, probability that they permeate through the skin and cause unfavorable side effects. Polymeric transdermal enhancers may exhibit a high enhancing activity and non-toxic due to the bulkiness of enhancer and the physiological inertness. The enhancing activity of poly(lactic acid) end-capped lactose (PLL), poly(lactic acid)-b-hyaluronan (PLH) on the permeation through the nude mice dorsum skin were evaluated by in vitroexperiments using a franz cell and lidocaine chloride as a model drug. As a result, PLL exhibited a higher enhancing effect on the permeation the drug through the skin, which may suggested that a suitable balance of polarity and hydrophobicity of the penetration enhancers would be necessary to appear the high enhancing effect.

16:00 Poster L24

Chitosan-Multiwall Carbon Nanotubes For Applications in Tissue Engineering

Imelda O. Armendariz[1], Perla E. Garcia-Casillas[1], Alberto M. Villafañe[2], Carlos A. Martínez[1]

1. *Universidad Autonoma de Ciudad Juarez, Ave. del Charro 450 Norte, Juarez 32360, Mexico* **2.** *Centro de Investigaciones en Materiales Avanzados, SEP-Conacyt (CIMAV), Miguel de Cervantes No. 120, complejo industrial Chihuahua, Chiuahua 31109, Mexico*

e-mail: camartin@uacj.mx

In the search for ideal materials for tissue engineering where the properties of scaffolds are dictated concurrently by different factors such as degradation rate, mechanical properties, site of implant, kinetics of cell growth, etc. it's common to blend or make composite of two or more materials in order to modulate its properties. In this work the preparation of Chitosan-MWCNT Scaffold by thermal induced phase separation technique (TIPS) is presented. The effects of the different parameters as solvent type, polymer concentration, and quenching temperature for the production of the scaffolds were studied. Biodegradable materials with 3D interconnected porous with pore size between 100-300 µm were obtained. The incorporation of the MWCNT improved the mechanical properties of the scaffolds. The bioactivity of the materials was tested in vitro using a simulated body fluid (SBF). The Scaffolds were soaked in this solution for different period of time showing the formation of biological apatite alike that shows its potential in tissue engineering.

16:00 Poster L25

Investigation of cells interactions with textile scaffolds for bone tissue enginnering

Maryla Moczulska[1,2], Malak Bitar[2], Wojciech Swieszkowski[1], Arie Bruinink[2], Krzysztof J. Kurzydlowski[1]

1. *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland* **2.** *EMPA, Materials Science and Technology, Laboratory for Advanced Fibers, Lerchenfeldstrasse 5, St.Gallen 9014, Switzerland*

e-mail: maryla.moczulska@gmail.com

Textile scaffolds for bone tissue regeneration should take into consideration the effect of its composition and structure on cell function. The scaffolds architecture should initially permit and promote cell colonization, and drive the population towards osteoblastic differentiationn.

The aim of the present study was to develop a textile scaffold as a tissue engineering support in vivo natural tissue regeneration. Monofilament polyethylene terephthalate and polyamide woven fabrics were evaluated in this study by correlating fibre diameter and mesh size to cell proliferation and migration.

In the first series of experiment reaggregates of primary adult trabecular bone derived human osteoblast (HBC), and of human skin fibroblast (NHDF), were used to assess the capacity of the cells population in covering the textile scaffolds as a function of fibre diameter and mesh gap size. In the next part cells were seeded on the mesh scaffolds, and proliferation was assessed using BrdU.

The results obtained in this study strongly suggested that fibre diameter and mesh size influenced cell outgrowth out of reaggregate. Fibres of 42/105 permitted significantly greater extent of reaggregate spreading in comparison to a fibre diameter of 77 µm.However, the cell population response to the physical character of the scaffolds appeared to be cell type dependant.

Future studies will focus on cellmigration and osteoblast differentiation with the overall aim of optimisng mesh chemical composition and most important, physical geometry for enhanced bone cell recruitment.

16:00 Poster L26

Culture of osteoblasts on nanostructured titanium – preliminary observation

Halina Garbacz[1], Małgorzata Lewandowska-Szumieł[2], Edyta Wróbel, Barbara D. Ostrowska[1], Krzysztof J. Kurzydlowski[1]

1. *Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland* **2.** *Medical University of Warsaw, Department of Biophysics and Human Physiology, Chałubińskiego 5, Warszawa 02-004, Poland*

e-mail: bostrowska@gmail.com

Commercial titanium of technical purity (c.p.) is an excellent implant material because of its high corrosion resistance and outstanding biocompatibility. It is known as not causing allergic reactions, preferred when infection is a risk. However, the applications of titanium are limited by relatively poor wear resistance and tensile strength. This stimulated interest in improving the mechanical properties of c.p. titanium, among others by hydrostatic extrusion which is a method of grain refinement by severe plastic deformation. Hydrostatic extrusion (HE) allows to obtain nanograins in bulk samples, which achieve strength similar to that of titanium alloys. This opens the new possibility for application of c.p. titanium in the biomedical devices. The present study reports the results obtained in the investigations of osteoblast culture on nanocrystalline titanium. The material examined in the study was c.p. extruded titanium with the mean grain size of 60 nm. HE titanium was examined by scanning and transmission microscopy (SEM/STEM Hitachi S 5500) and using a computer image analysis. The mechanical properties of the titanium were characterized using a HYSITRON Triboindenter. Titanium with a grain size of 20 µm and Ti6Al4V alloy were used as the reference materials. Human bone derived cells were observed in direct contact with investigated materials in vitro. Cell morphology and proliferation on nano-titanium was found to be comparable to those for micro-titanium and for Ti6Al4V alloy. This indicates, that nanocrystalline titanium obtained by hydrostatic extrusion may be taken into account as a material for bone reconstruction.

Acknowledgements

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16:00 Poster L27

The influence of fullerenol on the dynamics of nitric oxide molecule in water solvent - computer simulation

Adam Piątek, Zygmunt Gburski

University of Silesia, Institute of Physics, Uniwersytecka 4, Katowice 40-007, Poland

e-mail: afriday@interia.eu

The potential nitric oxide-scavenging activity of polyhydroxylated derivative of fullerene, fullerenol $C_{60}(OH)_{24}$, has been tested using the computer simulation (MD) method. The impact of water soluble fullerenol on the dynamics of NO molecule has been observed by calculating several quantities: radial distribution function, linear and angular velocity correlation functions, diffusion coefficient, mean square displacement, etc. at physiological temperature.

16:00 Poster L28

Novel coating materials based on sol-gel process. Preliminary investigations.

Anna Pytel, Maria Zielecka, Elżbieta Bujnowska

Industrial Chemistry Research Institute (ICRI), Rydygiera 8, Warszawa 01-793, Poland

e-mail: anna.pytel@ichp.pl

The sol-gel technology is regarded as the fastest growing domain of contemporary chemistry. This process can be used to prepare organic and inorganic materials, as well as organically and inorganically modified materials, which are being studied for diverse range of applications.

Characteristic sol-gel process implicate metal alkoxide precursors $M(OR)_Z$ when R is an alkyl group (e.g. R = Me, Et); it can be represented by the following overall chemical equation:

$$Si(OR)_4 + (4-x)H_20 \rightarrow SiO_x(OH)_{4-2x} + 4ROH$$

Reaction takes place through hydrolysis and condensation of monomeric alkoxysilanes.

Sol-gel process depends on several factors: pH, presence of admixture, mixing rate or water to precursor ratio etc, which determinate various chemical and physical features of received materials. For example pH and drying conditions affect structure and porosity of materials based on sol-gel process.

One of the most important applications of sol-gel technology is the production of coatings. It is possible to apply coatings based on sol-gel process with almost all types of chemical compositions, which can be adaptated not only as automotive clearcoats, hard coats for plastics or anit-graffiti coatings, but also as new materials for bioengineering.

The results of preliminary investigations of coating materials for sophisticated applications will be presented focusing on the effect of sol-gel process factors on characteristic of surface layer of coating materials based on the following methods: Scanning Electron Microscope, Fourier transform infrared spectroscopy, Photon Corelation Spectroscopy.

16:00 Poster L29

Features of growing of bone tissue in the porous titan received from a powder of different morphology

Vadim Savich, Oleg Smorygo

Research institute of powder metallurgy, Platonova 41, Minsk 220071, Belarus

e-mail: VSavich@yandex.ru

Work is devoted to research of influence of morphology of a surface porous implants on their adhesion to bone tissue.

Material of researches - porous samples in diameter 8 and height 12-14 mm from spherical and spongy powders of technically pure titan. The average of pore sizes 120-160 microns, porosity 0,42-0,56. Samples were implanted in bone tissue by a laboratory animal and in terms 1, 3 and 6 months left together with near bone fragments. Durability of coupling implants with a bone was investigated, and also preparations for histologic researches prepared. The effect of influence of a condition of a surface of particles of the titan on process of growing - ingrowth bone tissue is established. In case of ideally smooth spherical particles bone tissue simply fill pore space, being kept in it mainly due to an interlacing and jamming in the goffered pores. Only in case of spongy particles with a rough and microporous surface bone tissue form close intimate

16:00 Poster L30

Tissue formation in cellular ceramic scaffolds for motile orbit stump

Vadim Savich, Oleg Smorygo, Victoria Krasilnikova, Axana Dudich, Yury Kovalenko

Research institute of powder metallurgy, Platonova 41, Minsk 220071, Belarus

e-mail: VSavich@yandex.ru

Formation of a motile supporting orbit stump is of special importance for the social rehabilitation of patients who lost the eyeball. Implant material ensuring formation of the stump must meet the following requirements: low weight, high strength-to-density ratio, stability in biological environment, rapid tissue ingrowth and uniting with extraocular muscles. Foam-structure ceramic scaffolds are excellent candidates for this purpose.

In this work the scaffolds were manufactured from alumina-zirconia ceramics via the polyurethane foam replication technology. In some cases a nanocrystalline hydroxiapatite was synthesized and deposited over the scaffold structural elements. The fibro-vascular ingrowth process was studied depending on the scaffold pore size and the availability of the nanocrystallyne hydroxiapatite coating. Materials with optimum parameters were used to manufacture the orbit implants. Results of in-vivo and clinical studies are summarized.

16:00 Poster L31

Synthesis of Mg-doped biphasic calcium phosphate via sol-gel method

Iis Sopyan, Toibah Abdurrahim

International Islamic University Malaysia (IIUM), PO Box 10, Kuala Lumpur 50728, Malaysia

e-mail: sopyan@iiu.edu.my

Magnesium-doped biphasic calcium phosphate (Mg-BCP) was synthesized through sol-gel method using calcium nitrate tetrahydrate and diammonium hydrogen phosphate as the precursors. Magnesium nitrate hexahydrate was used as the source of the dopant; magnesium concentration was varied between 0.5 to 15 mo%. The monomers were heated in an ammonium solution until a white gel formed. The obtained gel was then dried and subsequently subjected to 500 - 900 ºC calcination. Morphological evaluation by SEM measurement shows that the particles of Mg-BCP are tightly agglomerated, globular in shape with primary particulates of 50-200 nm diameters. Successful incorporation of Mg into BCP lattice structure was confirmed by higher crystallinity of Mg-BCP and by shifting of tricalcium phosphate (TCP) peaks in XRD patterns to higher 2q angles as the increased Mg content. No hydroxyapatite (HA) peak shifted in the XRD patterns. Doping magnesium into BCP particles caused fusion of particles leading to more progressive densification of particles as shown by higher concentration magnesium doping. This result is in good agreement with the FESEM analysis showing larger Mg-BCP particles as the increased dopant concentration. XRD and FTIR measurement showed that the increment of crystallinity is directly proportional to the amount of the dopant showing a sintering additive properties by the addition of magnesium. Both analyses also revealed that TCP appeared only after calcination of 700 ºC and above. Preliminary test on powder performance was done by making aqueous slurry of the powder. Soaking cellulosic sponge into the stable slurry followed by drying and burning at 1250ºC gave porous bodies with high consistency macro- and micropores. With macropores of 100-500 microns diameter, the samples are applicable for human spongy bone substitutes. Surprisingly, doping 10 mol% of magnesium has increased the compressive strength by over 10 times compared to pure BCP (0.4 MPa) to 5 MPa.

16:00 Poster L32

The effect of kind of manufacturing on the certein physico-mechanical properties of the bioglass composite

Barbara Staniewicz-Brudnik[1], Lucyna R. Jaworska, Krystyna Wodnicka[2]

1. *Institute of Metal Cutting, Wrocławska 37A, Kraków 30-011, Poland* **2.** *AGH University of Science and Technology, Faculty of Materials Science and Ceramics (AGH UST), Mickiewicza 30, Kraków 30-059, Poland*

e-mail: bbrudnik@ios.krakow.pl

The basic problem while designing composite materials for medical application is:proper selection of reinforcement (strengthening phase) ,matrix and their kind of manufacturing.Biomaterials of submicrocrytalline sintered corundum ceramics (reinforcement) covered with bioactive glass(CaO-SiO2-P2O5 system-as a matrix) can be used as one of possibilities in invasive medicine. The influence of kind of manufacturing (sintering,sintering with densification) on the bioglass composite properties is examined.

The following technique are used:

-for densification bioglass composite describing: zeta potential;

-for morphology and bioglass composite structure describing:SEM,EDX,XRD;

-for certein physico-mechanical properties describing: microhardness test,strengthening test,wetting test,adhesion force after SBF immersion.

16:00 Poster L33

Fabrication Porous Ceramic Body by Negative Polymer Replica as a Bone Tissue Engineering Scaffold

Ranna Tolouei[2], Aliasghar Behnamghader[1], Sayed Khatiboleslam Sadrnezhaad[3], Morteza Daliri Joupari

1. *Ceramics department from Materials and Energy Research Center, Tehran 15914, Iran* **2.** *Islamic Azad university, Science and research branch, Tehran 1445-14655, Iran* **3.** *Materials and Energy Research Center, Tehran 15914, Iran*

e-mail: ranna.tolouei@gmail.com

The porous calcium phosphate scaffolds with defined pore-channel interconnectivity were successfully prepared via negative replica method. The internal channel architecture was achieved using a water-insoluble polyurethane sponge. This material is thermally decomposable into gaseous residues. The PU sponge was first filled with aqueous slurry of biphasic calcium phosphate material containing pore forming agent. After drying at room temperature, a heat treatment was employed to remove all organic material. The bodies were finally sintered at the temperature of 1200°C. The phase composition and chemical structure of bodies were determined by X-ray diffraction (XRD) and FT-IR methods. Scanning electron microscopy (SEM) was used to study the pore size and distribution and pore-pore and pore-channel interconnectivity. The scaffold bodies were principally composed of HA and β-TCP with some traces of α-TCP. No residue of polymer replica or pore agent was identified. The scaffolds contained an interconnected pore-pore and pore-channel structure with a pore size less than 500 µm. The company of desired phase composition and pore-channel structure increases the hope for the production of more effective biodegradable scaffolds for hard tissue engineering.

16:00 Poster L34

The porous ceramic grafting material

Tatyana M. Ulyanova[1], L.V. Titova[1], V.L. Evtukhov[2]

1. *Institute of General and Inorganic Chemistry of NAS of Belarus (IGIC), Surganov str., 9, Minsk 220072, Belarus* **2.** *Belarusian State Medical University, Minsk 1111, Belarus*

e-mail: ulya@igic.bas-net.by

The preparation of a biocompatible, slowly resolved material and its replacement by the living bone tissue due to natural regeneration of the cells of bone substance is a significant task. The present work is devoted to preparing a porous grafting ceramic material and to performing medical-biological experiments on it. Samples of porous implants were fabricated from natural raw material containing mineral and organic components. Heat treatment was made within a special step-by-step regime involving isothermal annealing. Moulding and mechanical processing were conducted at certain stages. For the influence of the heat treatment temperature on the structure and properties of porous ceramics to be studied, the implant samples were annealed in air over the temperature range 300-1400^{0}C, their crystal and porous structures as well as the physicochemical and mechanical properties were examined by X-ray and SEM methods. The obtained results have revealed that the implant consisted of calcium and phosphate as well as magnesium phosphate and calcium carbonate admixtures. It was characterized by two levels of pores: macropores 300-400 mm in size in the material volume as well as by micro- and transient pores up to 100 nm located over the material surface of the dividing walls. The experiments have supported that in 7-30 – days at the implant - cortical or spongy bone boundary the muscle and bone tissue gradually germinates into the implant holes. The formation of protein substance in the samples of the calcium-phosphate implants being in contact with the bone for 21 days developed so intensely that it was impossible to separate the implant from the bone, not disturbing its completeness. The developed grafting material is compatible and promotes the bone regeneration process.

16:00 Poster L35

Porous alumina via protein foaming-consolidation method

Iis Sopyan, Ahmad Fadli

International Islamic University Malaysia (IIUM), PO Box 10, Kuala Lumpur 50728, Malaysia

e-mail: sopyan@iiu.edu.my

We have succeeded in developing a novel method for preparation of porous alumina using egg yolk both as consolidating and foaming agents. This strategy allows the control of porosity not only by the varied concentration of yolk but also by managing the foaming process. Slurries of alumina powders and yolk was prepared by stirring the mixture with an alumina-to-yolk ratio of 1.0 for 3 h and the resulting slip was poured into cylindrical shaped molds. The slurries show a slight shear thinning behavior for a lower range of shear rates, and it changed to shear thickening at higher shear rates. Their viscosities are in the range of 0.6 - 1.1 Pa.s at 1000 s^{-1} shear rate, thus indicating that the slurries are pourable under shear. Subsequently, they were subjected to drying at 110, 150, and 180 °C with the varied time of 8, 12, and 60 min for foaming and/or consolidation. Foaming process condition determined mean pore size and pore distribution. The dried green bodies of the samples were then burned to remove the pore creating agent at 600 ºC for 1 h accordingly, followed by sintering at 1550°C for 2 h. Pore size distribution measurement showed that macropores of the sintered alumina porous bodies increased with the increased time and temperature of the drying process and were found in the range 50 – 800 µm. SEM measurement also confirmed this observation. Less foamed samples show lower shrinkage but higher compressive strength. A shrinkage of as low as 7.8% was observed for the sample dried at 110ºC but it increased significantly to 29.3% when dried at 180ºC. The compressive strength of the 110ºC's sample was 5.72 MPa at 43.6% porosity and it decreased to 4.57 MPa at 50.4% porosity when foamed at 180ºC. These results have opened a novel preparative way for porous ceramics especially alumina-based porous materials designed for biomedical applications.

Satellite events

Workshop

Welcome

Workshop organised by European Integrated Project NAPOLYDE (Nano-structured polymer deposition processes for mass production of innovative systems for energy production & control and for smart devices) and the European Networks of Excellence NAPOLYNET and NANOFUN-POLY

Organisers

James Rohan, Tyndall National Institute, Cork, Ireland,

Frederic Sanchette, CEA, Grenoble, France,

Mircea Modreanu, Tyndall National Institute, Cork, Ireland,

Emmanuel Scolan, CSEM, Neuchatel, Switzerland,

Clara Silvestre, Institute of Chemistry and Technology of Polymers, Naples, Italy

Jose Kenny, ECNP and University of Perugia, Italy

Sponsors

ARCELORMITTAL, Belgium

Programme

Monday, 15 September

Opening & Plenary Session

Czochralski Award Ceremony
Monday morning, 15 September, 10:00
Small Hall (237)

Lunch break
Monday afternoon, 15 September, 12:30
Inner Courtyards

Optical Spectroscopy Tutorials
Monday afternoon, 15 September, 14:00
Room 123
Chair: James Rohan, Emmanuel Scolan

14:00 Invited oral

Optical spectroscopy: from experimental measurements to band structure determination

Mircea Modreanu

University College Cork, Tyndall National Institute (TYNDALL), Lee Maltings, Prospect Row, Cork, Ireland

e-mail: mircea.modreanu@tyndall.ie

UV-VIS-NIR Spectrophotometry and Spectroscopic ellipsometry (SE) are two non-destructive and versatile characterization techniques that have applications in many different fields. These optical characterization techniques are well established in the semiconductor, flat panel display, optical coatings, data storage, telecommunication, chemical and biological applications, for demanding research or industrial quality control applications.

In this tutorial an overview of the principles and instrumentation for UV-VIS-NIR Spectrophotometry and Spectroscopic ellipsometry will be presented.

Typical information's that can be extracted from these two optical characterization techniques are:

* Optical constants and film thickness

* Optical band gap and interband transitions

* Surface or interfacial roughness

* Chemical composition or intermixing

* Crystallinity (polymorphs identification)

* Micro-porosity

* Anisotropy or birefringence

General rules for building optical models with a more details discussion for the case of spectroscopic ellipsometry are presented. Several examples of functional oxides will be also discussed.

15:00 Invited oral

Infra red Spectroscopic Ellipsometry analysis of nano structured thin films in polymers and semiconductors.

Jean-Louis Stehlé, Dorian Zahorski

SOPRA SA, 26 Pierre Joigneaux, Bois-Colombes 92270, France

e-mail: jeanlouis.stehle@sopra-sa.com

Infra red spectroscopic ellipsometry (IRSE) has been developped for semiconductors and dopants characterization. The Drude tail in Mid IR enables to quantify the dose of active dopants, their mobility, the depth and the sheet resistance. In case of polymers with nanometer thickness, the IRSE enables to measure not only the thickness but also the refractive index, N and k absorption coefficient, without the need for Kramers Kronig assumptions. The N and k in the IR range are linked to the dielectric value for lowK and can be measured with the density or porosity of the layer. The sensibility to very thin films will be shown as well as the recognition of the interlayer SiO2 under highK HfAlOx layers. new application for porous layers will be presented.

Coffee break
Monday afternoon, 15 September, 16:00

Poster session

Monday & Wednesday
Monday afternoon, 15 September, 16:30
Main Hall

Tuesday, 16 September

Fundamentals
Tuesday morning, 16 September, 9:00
Room 123
Chair: James Rohan, Christophe Le Pen

9:00 Oral

NAPOLYDE, an European Integrated Project concerning NAno-structured POLYmer DEposition processes for mass production of innovative systems for energy production & control for smart devices.

Patrick Choquet[1], Christophe Le pen[2]

1. *CRP Gabriel Lippmann (CRP-GL), 41 rue du Brill, Belvaux L4422, Luxembourg* **2.** *ARCELORMITTAL Liege research and development, Bd de colonster, B57, Liège 4000, Belgium*

e-mail: choquet@lippmann.lu

Polymer thin films are of high interest in various industries mainly due to their low cost, low thermal load, light weight, flexibility and transparency. Recent studies are showing that polymeric film with controlled nanoscale features can provide systems with radically new chemical or physical properties (i.e. mechanical protection, super-hydrophobicity, antireflectivity, etc…). In traditional sectors, such as large scale steel and glass surface manufacturing, coil coating, dip coating and spray techniques are fully industrialized with high throughput processes. However, they all lead to high thickness, without mastering the nanostructure itself. Therefore, merging nanoscale precision with mass production constraints is a key challenge to open the door to new generations of high added value products.

NAPOLYDE project, supported by the European Commission brings together over 20 to innovative SME's with research and academic centers.The overall goal of this Integrated Project is to develop new technologies and processes with full control of the nanoscale for mass-production of new highly innovative products, integrating such size dependant properties. The NAPOLYDE key challenge is to bridge the gap between nano-scale precision and mass production requirements in the field of thin film polymer deposition. The overall objectives are the development of new process technologies: wet (sol-gel, sonochemistry or self assembly) and dry deposition processes (plasma CVD, sputtering, …) and to provide nanolayering, nanoclustering and nanotexturing of organic thin films in mass production. It includes also measurement instruments and design tools to control these deposition technologies at industrial scale (in-situ continuous characterization tools, simulation models…) and the scale-up methodologies and know-how to support new technologies introduction inside industrial processing chains.

9:30 Invited oral

Coating Flat and Curved Surfaces by Nanoparticles Using Ultrasound and Microwave Radiations

Aharon Gedanken

Bar-Ilan University, Ramat-Gan 52900, Israel

e-mail: gedanken@mail.biu.ac.il

Abstract *(up to 200 words)*

- Both Ultrasound and MW radiations were employed to coat flat and curved surfaces of Polymers, glass, textiles and metals by a variety of nanoparticles. We will present a few examples and explain why the nanoparticles adhere very well to the surface of the substrate. Most of the examples will concentrate on the antibacterial nanoparticles. We will present evidence that coating glass surfaces with nanoparticles of MgF_2 prevent the development of biofilms of two types of bacteria.
- Combining MW and ionic liquids for the fabrication of nanomaterials will be discussed and a special emphasis will be devoted to metal fluoride nanoparticle.

10:00 Invited oral

Plasma nanolayering, nanoclustering and nanotexturing: challenges for future processes for mass production.

Patrice Raynaud, Richard Clergereaux, Yvan Segui, Nicolas Gherardi, Bernard Despax

Université Toulouse, LAboratoire PLAsma et Conversion d'Energie (LAPLACE), 118 Route de Narbonne, Toulouse 31062, France

e-mail: patrice.raynaud@laplace.univ-tlse.fr

It is well known, Polymeric films with controlled nanoscale features (thickness, porosity, roughness, surface structures or inclusions such as nanoparticles) can provide systems with radically new chemical or physical properties. Among them, barrier, mechanical protection, super-hydrophobicity, antireflectivity, conductivity, antimicrobial, antifouling are identified as being the most relevant. Moreover, the miniaturization of functional micro devices will be reached by the manipulation on the nanoscale of polymer thin films.

Plasma tools are now highly involved in the development of new technologies and processes with full control over the nanoscale for the mass production of new highly innovative products integrating such size dependant properties enabling innovation.

Three main fields have been investigated and succinctly described below: nanolayering, nanoclustering and nanotexturing.

Nanolayering is presented as a multi nano-layering deposition of successive polymeric layer for combining different physical and chemical properties can be achieved by PECVD (high density plasma, pulsed plasma or capacitive plasma): nanolayering of different organic thin films (SiOxCyHz, CFx, CHx) .

Nanoclustering can be a PECVD/sputtering co-deposition : sputtering of a material (Pt, Ag, …) to provide nanoclusters imbedded in polymeric matrix deposited from monomer such as SiOxCyNz, CFx, CHx, ….

Nano-texturing is a surface patterning process which allows to design a topography tailored to the specific application : i.e. super-hydrophobicity …

This presentation will give a large overview of plasma processes which can be achieved to reach scientific (phenomenon understanding, control of final properties, plasma and surface diagnostics …) and industrial (high speed processes, on line control, repeatability,…) targets. In that way plasma reactors, diagnostics tools and results will be described, explained and linked to final properties to be reached.

Coffee break

Tuesday morning, 16 September, 10:30
Main Hall

Applications

Tuesday morning, 16 September, 10:50
Room 123
Chair: Patrick Choquet, Patrice Raynaud

10:50 Oral

Development of transparent thin film to improve corrosion protection of steel

Christophe Le pen, Alain Daniel

ARCELORMITTAL Liege research and development, Bd de colonster, B57, Liège 4000, Belgium

e-mail: christophe.lepen@arcelormittal.com

The corrosion behavior of silica thin film with different compositon deposited by PECVD on steel was investigated in a 3.5% NaCl solution at ambient temperature. Potentiodynamic polarization tests, electrochemical impedance spectroscopy (EIS) and scanning electron microscopy (SEM) were the techniques applied to

characterize the corrosion behavior. In parallel, the composition and the structure of such thin film were analysis by several technique (IR, thickness, optical properties, AES, XPS, WCA) and correlate to the corrosion resistance of the film.

11:10 Invited oral

Microbattery technology overview and associated multilayer encapsulation process

Raphaël Salot, Steve Martin, Sami Oukassi, Messaoud Bedjaoui, Jennifer Ubrig

CEA (LITEN), 17 rue des Martyrs, Grenoble 38054, France

e-mail: raphael.salot@cea.fr

Important technological innovations emerged during the past decade in the field of MEMS. Current development programmes dedicated to MEMS are mainly focussed on the technology necessary to fabricate and implement MEMS. Nevertheless, their energy supply and management appear to be, by comparison, neglected. Indeed, available MEMS require “hardwire” connection for either power or communication. Integration of power source with the MEMS to obtain an autonomous or remote system appears to be a challenging task of major interest in the MEMS field.

Lithium microbatteries with different positive electrode materials (V_2O_5, $LiCoO_2$, TiOS) in association with a solid electrolyte (LiPONB) and a lithium negative electrode are very promising energy storage systems that can fit all the applications requirements. One of the challenge of the technology is related to the fact that lithium microbatteries are easily degraded in atmosphere. Indeed, these devices require encapsulation with a barrier material, which exhibits extremely low permeation rates for water vapour and oxygen. To obtain such a high barrier, we chose to direct our studies on layers deposited by plasma-enhanced chemical vapour deposition (PECVD), and more particularly on amorphous materials like silicon oxide (SiOx) and silicon nitride (SiNx).

Both the active layers of the microbattery architecture and the multilayer encapsulation stack will be discussed.

11:40 Oral

Nanostructured sol-gel surfaces

Emmanuel Scolan, Véronique Monnier, Raphaël Pugin

Centre Suisse d'Electronique et de Microtechnique (CSEM), Jaquet-Droz 1, Neuchâtel 2002, Switzerland

e-mail: esn@csem.ch

Sol-gel processes are very adapted and versatile to deposit layers with controlled homogeneity, thickness, porosity and associated surface structures. A specific route has been explored for the preparation of sol-gel nanostructured surfaces with high specific area, controlled porosity, and optical size dependant properties.

Our preparation approach based on a leaching process was developed for alumina based coatings [Tadanaga, *J. Am. Ceram. Soc.*, 1997]. Alumina based spin- or dip-coated films on a large variety of substrates are annealed and dipped in boiling water. SEM observations show the formation of surface structures resulting from successive dissolution-precipitation mechanisms of the initial alumina-based film. Characteristic sizes of these structures (distance between spines, texture depth) can be easily tuned by adjusting different process parameters.

Moreover, the formulation can be changed to induce chemical composition, morphology and properties modifications of the final films: doping with TiO_2 for photocatalytic applications, hierarchical morphologies, increased film thickness and surface area.

Antireflective and wettability effects due to these nanostructures are currently studied and seem to be promising. Samples of such “hot-water-treated” alumina based coated glass have been optically characterised in the visible and near infra-red range. The reflection spectrum at normal incidence demonstrates a significant reduction of intensity for wavelengths in the range [400 – 1200 nm].

Moreover, the nanostructured surfaces are highly hydrophilic and therefore exhibit very interesting antifogging properties. If the nanostructures surfaces are silanised with fluorinated agents, the surface energy of the coating can be drastically reduced. Large superhydrophobic surfaces have been obtained exhibiting high water contact angle with highly mobile drops.

12:00 Oral

Hydrophobic thin films with controlled surface roughness made by the sol gel method

Sebastian Kamps

Siemens AG, Guenther-Scharowsky-Str. 1, Erlangen 91058, Germany

e-mail: sebastian.kamps.ext@siemens.com

Sebastian Kamps[1]

Florian Eder[1], Anett Berndt[1], Prof. Dr. W. Ensinger[2]

For several years already coating of surfaces with functional films has been a common method to improve their usability, durability or optical appearance. Even for house-hold use, there is a broad range of products providing easy-to-clean, anti-fouling, or anti-static functionality on the applied surfaces. This boom of functional coatings was due to the fact, that the raw materials were available in large quantities at low costs and the final coating layers were easy to apply and showed a long term effect.

For some applications, like anti-icing, it might become important to introduce a certain structure or roughness into the functional layer to increase its efficiency. In the case of super-hydrophobic surfaces it is well known from the lotus leaf, that a combination of a complex micro- and nano-structure together with a hydrophobic surface functionality leads to super-hydrophobic effect with water-contact angles > 150°.

Various attempts by many research groups have been made to copy this example from nature. It was possible to reproduce this effect on various substrates by wet- or plasma-processes. Still there are obstacles to overcome regarding the layers mechanical durability, hydrolytic stability or cost-efficient applicability on large or complex shaped surfaces.

Therefore the aim of this thesis is to find materials and processes allowing the deposition of coatings with very low surface energies, reasonable production and application costs and a good mechanical stability and durability. Various ways of structurization will be used while focussing on the simplicity of the process. Special attention will be given to the generation of functional surfaces with a double-roughness. The final functionality will be generated by applying organo-functional polysiloxanes with perflourinated groups according to the sol gel method.

12:20 Oral

Fabrication of superhydrophobic surfaces with controlled topography and chemistry

Nicolas Blondiaux, Ana-Maria Popa, Mona Klein, Emmanuel Scolan, Raphaël Pugin

Centre Suisse d'Electronique et de Microtechnique (CSEM), Jaquet-Droz 1, Neuchâtel 2002, Switzerland

e-mail: nbx@csem.ch

Superhydrophobic surfaces have been receiving increasing research interest in recent years since they may be useful for many applications such as the fabrication of self-cleaning and anti-icing surfaces or the design or micro-fluidic channels with reduced liquid-flow slippage. Since superhydrophobicity arises from both surface topography and surface chemistry, a wide library of structured surfaces having well-defined surface chemistries has been developed.

Controlled nanostructures have been fabricated in silicon by first making a structured polymer thin film (by polymer demixing or block-copolymer self assembly) and then transferring the structures in the underlying substrate using deep reactive ion etching (DRIE). The structures can be tuned first via the polymer self-assembly step which allows the control of the lateral size of the structures (from tens of nanometers to tens of micrometers) and their type (pits or pillars). Second, via the DRIE step which allows the control of the depth of the structures. To investigate the effect of nanostructuring on wettability, we focused on pillar arrays obtained combining polymer demixing and DRIE. The lateral size of the structures was 400nm and their depth was ranging from 200nm to 4μm. Other structures of 80nm in lateral size were also realized using self organized block copolymer micelles films as a mask and the depth of the structures reached 200nm.

Hydrophobic surfaces with controlled contact-angle hysteresis have been fabricated by either silanizing or plasma-coating the surfaces. The wettability of each surface has been characterized by measuring the water contact angles (advancing and receding) and the rolling angle. These tunable nanostructured surfaces with well controlled surface chemistries allow the differentiation between different wetting concepts: the superhydrophobic modes (eg. Cassie-Baxter vs Wenzel); the dynamic contact-angle hysteresis and finally the self-cleaning properties (low rolling-off angles).

Lunch break

Tuesday afternoon, 16 September, 12:40
Inner Courtyards

Characterisation

Tuesday afternoon, 16 September, 14:00
Room 123
Chair: Clara Silvestre, Mircea Modreanu

14:00 Oral

characterization of barrier layer and porous materials by Ellipsometry porosimetry

Jean-Louis Stehlé, Dorian Zahorski

SOPRA SA, 26 Pierre Joigneaux, Bois-Colombes 92270, France

e-mail: jeanlouis.stehle@sopra-sa.com

Barrier layers are very important for the protection, reliability and life time of the polymers embeded in photovoltaic or OLED or electronic layers as well as for food packaging. these barrier layers are usually multiple with alternate organic and inorganic materials deposited by PE CVD process. The ability to stop the moisture and oxygen penetration must be assessed. The new ellipsometry porosimetry (EP) technique measures the penetration of solvent, in this case water, in the pores of the layers as BET does for adsorption and desorption cycles.

This presentation will disclose the way the EP works at atmospheric pressure under room temperature and what are the limitations in term of sensitivity to moisture content and the permeability measurements. The barrier layer maybe deposited on a porous layer on a substrate which will change its optical thickness when the moisture diffuses through the inter-connexions of the pores. The diffusion factor of porous layers can be measured by EP.

14:20 Oral

Nanostructured materials as seen by Small Angle Scattering

Sigrid Bernstorff

Sincrotrone Trieste, Strada Statale 14, km 163.5, in AREA Science Park, Trieste 34012, Italy

e-mail: bernstorff@elettra.trieste.it

Small-Angle X-ray Scattering (SAXS) is a well-established and widely used nondestructive technique for the characterization of non-crystalline or partly ordered materials. SAXS provides structural information in the size range between about 1 and a few hundred nm, and can be applied to a huge variety of systems: from semiconductors and metal alloys to polymers, from colloids to micelles and micro-emulsions, and from porous media to liquid crystals.
Grazing-incidence small-angle X-ray scattering (GISAXS) measurements are sensitive to both the surface morphology and the internal structure of films, and provide information both about lateral and normal ordering at a surface or inside a thin film. Possible applications

include thin polymer films, and nanoparticles at interfaces or on surfaces. As a result, GISAXS provides an excellent complement to more conventional nanoscale structural probes such as atomic force microscopy and transmission electron microscopy
The full potential of these techniques is realized when using a synchrotron source (high photon flux, strong beam collimation and choice of wavelength in order to avoid fluorescence or to perform anomalous measurements) and when patterns are recorded with low-noise, fast two-dimensional detectors. Microbeam applications as well as in-situ and real-time studies of e.g. nanoparticle formation and growth in the (sub)millisecond range are possible. Several examples of rapidly evolving research areas will be presented in order to highlight the possibilities of the SAXS and GISAXS techniques.

14:40 Invited oral

NANOFUN-POLY: The European Network of Excellence on Multifunctional Nanostructured Polymers and Nanocomposites

Jose M. Kenny

University of Perugia, Pentima Bassa, Terni 05100, Italy

e-mail: jkenny@unipg.it

The European Network of Excellence NANOFUN-POLY has been generated to become the European reference for Multifunctional Nanostructured Polymers and Nanocomposite Materials. This objective has been reached through a trans-disciplinary partnership of 120 scientists combining excellence in different scientific areas. Applications that benefit from NANOFUN-POLY concern strategic industrial sectors which can be competitive only by using advanced technologies: optoelectronics and telecommunications, packaging, agriculture, building construction, automotive and aerospace, biomaterials, etc.

The main deliverable of the NANOFUN-POLY project is the foundation of the European Centre for Nanostructured Polymers – ECNP – which develops a Joint Program of Activities aimed at structuring, shaping and promoting research on nanostructured polymers and nanocomposites. The integrating activities include sharing of research facilities/tools/platforms, a joint management of the participants' knowledge portfolio, staff mobility and exchanges and the use of electronic communication tools to support interactive working. In addition, NANOFUN-POLY and ECNP perform a joint programme of research, developing new research programmes and sharing platforms for common use.

Finally, activities designed to spread excellence are performed through a joint programme for training researchers and PhD students. This include the International PhD Program on Materials Nanotechnology and the European Master on Polymer Nanotechnologies. Other dissemination and communication activities include transfer technology and raising public awareness and understanding of science.

The final objective is the consolidation of a lasting integrated organisation of European researchers, well connected with the rest of the world and able to lead research, education and technology transfer in nanostructured polymers and their nanocomposites.

15:10 Invited oral

Polymer nanocomposites from functionalized carbon nanotubes

Luca Valentini

Civil and Environmental Engineering Department, University of Perugia, Pentima Bassa, Terni 05100, Italy

e-mail: mic@unipg.it

Carbon nanotubes (CNTs) are crystalline, tubular, carbon structures with extraordinary mechanical, chemical, optical and electrical properties. In this regard the possibility to realize a fully integrated nanotube-reinforced polymer system represents a promise for the preparation of composite materials with outstanding mechanical and multi-functional features. It is the aim of this work to consider the approaches to chemical functionalization of CNTs and to account for the advances that have been produced so far in the processing of polymer nanocomposites.

Coffee break

Tuesday afternoon, 16 September, 15:40
Main Hall

Parallel Session

Tuesday afternoon, 16 September, 16:00
Chair: Aharon Gedanken, Jose Kenny

16:00 Invited oral

Coordination Action: NMP3-CA-2008-218331-NaPolyNet Setting up research-intensive clusters across the EU on characterization of polymer nanostructures

Clara Silvestre

Istituto di Chimica e Tecnologia dei Polimeri (ICTP-CNR), via Campi Flegrei, 34, Napoli 80078, Italy

e-mail: silvestre@ictp.cnr.it

On the First of April the new project "NaPolyNet" is started. It is a 36 month project involving 15 partners from 10 European countries. The objective are: 1) to network at regional, national and international level with experts on the characterization of polymer nanostructured materials in the field of packaging, textiles and membranes, bridging the gap between scientific and engineering approaches for the improved understanding of the structure-performance correlation in polymer devices; 2) to facilitate transnational access to important and unique equipment and to train young scientists and SMEs technologists; 3) to harmonize the work necessary for new standards in the field of characterization of polymer nanostructures for packaging, textiles and membranes. NaPolyNet will also focus on latest findings for managing the safety implications of polymer nanostructure along the life-cycle of those products. The activities are grouped into 7 work-packages (WP). After setting up the procedures for managing the project, the team will map the competences in the different field of characterization of polymer nanostructures and will set up an European Open Laboratory (EOL) open to outside the consortium partners incorporating the best and novel characterization methodologies and expertises. The EOL will allow average trained users of equipment for thermal, structural, morphological, mechanical characterization to produce reliable data on nanostructured materials and correctly interpret them. An international Workshop is planned on processing-structure-dynamics-and-properties of polymer nanostructures in order to further support development and design of intrinsically safe nanomaterials. The last part of the project will be dedicated to harmonize the work for preparation of new standards for polymeric nanomaterials characterization and to overcome barriers to the industrial application of polymer nanostructured materials especially in SMEs.

16:30 Oral

Structure development during melt crystallization of isotactic polypropylene modified with clay and hydrocarbon resin

Donatella Duraccio, Sossio Cimmino, Clara Silvestre

Istituto di Chimica e Tecnologia dei Polimeri (ICTP-CNR), via Campi Flegrei, 34, Napoli 80078, Italy

e-mail: duraccio@ictp.cnr.it

The influence of a based montmorillonite (MMT) clay on the structure, morphology and crystallization behaviour of iPP is investigated. A low molecular mass hydrocarbon resin, containing hydroxyl and acid groups, suitable to interaction through hydrogen bonding with the polar surface of the clay, was also added to iPP/clay system with the aim to increase the compatibility between iPP and clay and then to improve the performance of such nanocomposites. The results clearly indicate that the phase structure, morphology and isothermal and non isothermal crystallization behaviours of iPP, iPP/clay and iPP/TR/clay are depending on preparation conditions and composition.

It was found that the crystallization conditions dictate the phase structure of the materials: for iPP/TR blend and ternary systems, the higher cooling rate crystallization process preserves the homogeneity of the amorphous phase inhibiting the liquid-liquid phase separation process between iPP and TR. This separation occurs, conversely, when the samples are cooled from the melt at low cooling rate.

The principal finding of this work is that for the ternary system in the condition of isothermal crystallization used the TR in iPP/TR/cay system is able to establish interaction through hydrogen bonding with the polar surface of the clay, providing the lost of clay crystallographic regularity (clay exfoliation). The presence of the third component, miscible or partially miscible with iPP opens a new field of investigation with the analysis of the processes of intercalation of clay by iPP, and the two processes of phase separation that can be observed: liquid-liquid separation and liquid-solid separation due to iPP crystallization. In dependence on crystallization conditions and composition these processes can be in competition and their control offers great possibility to determine the morphology and hence the properties of the resulting material.

16:50 Oral

Molecular fractal surfaces analysis with spectroscopic ellipsometry

Frédéric Ferrieu[1], Jean-Philippe Piel[2], Jean-Louis Stehlé[2], Adrien Danel[3]

1. *STMicroelectronics, 850 rue Jean Monnet, Crolles CEDEX 38926, France* **2.** *SOPRA SA, 26 Pierre Joigneaux, Bois-Colombes 92270, France* **3.** *CEA-LETI-MINATEC (MINATEC), 17 rue des Martyrs, Grenoble 38054, France*

e-mail: jeanlouis.stehle@sopra-sa.com

It is known for years that surface adsorption/desorption can be studied by in Situ Spectroscopic Ellipsometry (SE). The physical adsorption of water or other small adsorbate molecules species on the surface of non-porous materials, gives rise to a Type II isotherms which can be measurerd with sufficient accuracy by SE. The paper reports on recent highlights of this promising application of SE as interpretated with the fractal description of surfaces. The adsorption theories including the effect of fractal properties of thin films surfaces have been recently reviewed and corresponding models can be specifically applied to SE analysis. Within the concept of the surface fractal properties, the study of surface adsorption provides interesting parameters such as dimensionality and surface energy parameters to be correlated with other instrumental observations. Some examples are presented and discussed.

17:10 Oral

Microfabrication of thin film microbatteries

Sami Oukassi, Steve Martin, Raphaël Salot

CEA (LITEN), 17 rue des Martyrs, Grenoble 38054, France

e-mail: sami.oukassi@cea.fr

During the last decades, recent advances have been achieved in the field of the thin film microbatteries. Major efforts have been carried out on the encapsulation of such devices, given the sensitive aspect of most of materials present on the active stack (lithium containing layers).

It is presented in this work recent achievements concerning thin film encapsulation of metallic lithium negative electrode. In the context of this study, encapsulation stack includes polymer and dielectric layers combined in such way to optimize barrier performances of the whole structure towards oxygen and water vapor permeation.

The first part of this work is dedicated to the description of the barrier stack architecture and properties. A second part presents the application of a microfabrication process to the metallic lithium negative electrode and barrier stack so as to have very small features (100x100 µm² patterns). The microfabrication process includes several steps of photolithography and etching (dry and wet) blocks, which allowed reaching the targeted critical dimensions. These results put in evidence the success of patterning functional metallic lithium. It demonstrates the feasibility of energy sources miniaturization which is an important issue in the field of autonomous and wireless sensor networks.

Wednesday, 17 September

Parallel Session

Wednesday morning, 17 September, 9:00
Room 123
Chair: Ulrich Schubert, Christophe Le Pen

9:00 Invited oral

Bioactive Surfaces

Jas Pal Badyal

Surface Innovations Ltd, Wolsingham DL133HH, United Kingdom

e-mail: j.p.badyal@surface-innovations.com

Over the years, several methods have been developed to coat solid surfaces for biotechnological applications. Success has primarily been achieved by using wet chemical methods employing solvents, or strong acid / base media, some of which are becoming increasingly unacceptable due to environmental and safety concerns. An alternative approach is to employ non-isothermal plasmachemical processing. This technology offers many potential benefits including low energy consumption, absence of solvents, minimal waste, rapid treatment times, ambient temperatures, applicability to a whole host of different substrate materials, and control of surface functionality. Specific examples will be given including high throughput and low-cost technological solutions for preparing re-writable DNA microarrays, protein chips, antibacterial surfaces, thermo-responsive coatings for tissue engineering, and substrates for rapid cell growth.

9:30 Oral

Self-cleaning surfaces

Jerome Gavillet

CEA-Grenoble (CEA-GRE), 17 Rue des martyrs, Grenoble 38054, France

e-mail: jerome.gavillet@cea.fr

The liquid repellency of a surface is principally governed by a combination of its chemical nature and topographical microstructure. Although flat low surface energy materials can often exhibit high water contact angle values, this is not normally sufficient to yield super-hydrophobicity (description reserved for materials upon which water drops move spontaneously across horizontal or near horizontal surfaces). In order for this behaviour to occur, the difference between advancing and receding contact angles (hysteresis) must be minimal. Effectively, the hysteresis can be regarded as the force required to move a liquid droplet across the surface; i.e. in the case of little or no hysteresis, very little force is required to move a droplet, hence it rolls off easily. Theoretical studies for idealised rough hydrophobic surfaces predict that contact angle hysteresis initially increases with surface roughness, until eventually a maximum value is reached; greater roughness scales beyond this lead to a fall due to the formation of a composite interface (liquid unable to completely penetrate the surface). The latter can be described by the Cassie-Baxter state, where the inherent surface roughness causes air to become trapped in voids (i.e. prevents liquid from wicking). Hence low contact angle hysteresis can be achieved by substrate roughening to produce a composite interface.

Low surface energy polymers form an important class of thin coatings. Such coatings are widely used for a broad variety of ‘anti’-applications like anti-wetting, anti-fogging or anti-fouling. They are important for microelectronics, textile, optical and even medical applications. Such polymer coatings have surface energies that are much lower than those of traditional solids and lower than that of water and even oil. Thus, even if oil were spilled on a low surface energy polymer film, it would not spread out to cover the surface, but the oil would form droplets instead, which could easily be removed.

9:50 Oral

Plasma deposition of hydrocarbon films containing platinum nanoclusters

Elena Dilonardo[1], Antonella Milella[1], Fabio Palumbo[2], Riccardo D'Agostino[1], Francesco Fracassi[1]

1. *Università degli studi di Bari, Dip. Chimica, Via E. Orabona 4, Bari 70126, Italy* **2.** *Institute of Inorganic Methodologies and of Plasma (IMIP-CNR), Bari 70126, Italy*

e-mail: ellylamoretta@hotmail.it

Nowadays there is much interest in nanocomposites films consisting of metal nanoparticles embedded in polymeric matrix because they offer interesting electronic, optical and catalytic properties due to their very small dimensions. As result, various approaches have been used to incorporate metal nanoparticles into polymers. In this contribution a one-step plasma deposition process is described to obtain an uniform dispersion of small platinum nano-clusters throughout a thin hydrocarbon matrix (Pt/CH_X films). These composite films have been deposited by simultaneous plasma-enhanced chemical vapour deposition (PECVD) of ethylene (C_2H_4) and argon (Ar) gas mixtures and RF sputtering of a platinum target. Characterization of platinum-containing plasma-polymerized ethylene films has been realized using X-ray Photoelectron Spectroscopy (XPS), Fourier Transform Infra-Red spectroscopy (FTIR), UV-Vis spectroscopy, Atomic Force Microscopy (AFM), Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM). An *in situ* plasma diagnostic technique, Optical Emission Spectroscopy (OES), has been used to correlate the chemical composition of the plasma with the amount of metal embedded in the deposited film. A comprehensive study on the effect of different plasma parameters (RF power, deposition time, flow rate of gasses) on the chemical composition and structure of the film will be presented. Results show that platinum content in the coating can be carefully controlled by changing the RF power and the monomer flow rate. In particular TEM images confirm that platinum aggregates in nanoclusters in crystalline form distributed uniformly in the material. Furthermore the porosity due to the columnar film growth, together with the nanodispersion of the metal clusters, can be advantageously used for catalytic applications.

10:10 Oral

Mesoscopic objects, porous layers and nanocomposites - possibilities of sol-gel chemistry

Ireneusz Piwoński

University of Łódź, Department of Chemical Technology and Environmental Protection, Pomorska 163, Łódź 90-236, Poland

e-mail: irek@uni.lodz.pl

Sol-gel as versatile technique commonly used in materials’ engineering offers the broad possibility of preparation of many metal oxides, composites, organic-inorganic hybrids and other materials in a form of mesoscopic objects (fibers, nanorodes, nanoparticles) as well as thin structured films, porous materials and nanocomposites.

In this approach illustration of these possibilities is presented. Silica nanorodes prepared with the use of various templates is shown as an example of the synthesis of elongated ceramic materials.

Another part concerns the preparation of titania and zirconia systems in the form of nonporous or porous ultrathin layers deposited in dip-coating procedure. The material morphology including porosity level and pore-size was controlled by application of appropriate type and concentration of surfactants or polymer beads which served as template. These types of materials may be applied as sensors, catalysts, low-*k* materials, photonic crystals, etc.

Furthermore, the synthesis of nanocomposite systems based on titania or alumina containing hard ceramic nanoparticles (Al_2O_3, ZrO_2) is presented. Application of nanoparticles considerably enhances the mechanical and tribological properties of the material.

Last part of this study is devoted to the preparation of titania nanoparticles, which are considered as promising material in such applications as solar energy conversion, photocatalysis, biomedical systems etc. Here, titania nanoparticles were prepared and their size was investigated using microscopic techniques.

In all experiments mainly Atomic Force Microscopy (AFM) was used as flexible technique of surface and nanoobject imaging.

Coffee break

Wednesday morning, 17 September, 10:30
Main Hall

Parallel Session

Wednesday morning, 17 September, 11:00
Room 123
Chair: Jas Pal Badyal, Emmanuel Scolan

11:00 Invited oral

Sol-Gel and Polymer Films with Incorporated Inorganic Nanoparticles

Ulrich Schubert, Miroslava Malenovska, Philipp Heinz, Marie-Alexandra G. Neouze

Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9, Wien 1060, Austria

e-mail: uschuber@mail.zserv.tuwien.ac.at

Sol-gel thin films with incorporated metal oxide or metal nanoparticles can be prepared by controlled post-synthesis treatment of inorganic gels containing covalently bonded metal complexes. To this end, the precursors for the metal particles and the host phase are tethered by means of an organic group. This results in the homogeneous dispersion of the metal compound during sol-gel processing. Nanocomposites are then obtained by thermal, photochemical or chemical post-synthesis treatment of the gels by which the organic tether is removed and/or the metal ions are de-coordinated with concomitant growth of the metal oxide or metal particles. While this method was previously developed for composite powders, the development of composite films required modifications to render the particle-forming step compatible with film properties (e.g., adhesion etc.). Several examples will be demonstrated, such as silica films on glass substrates with homogeneously dispersed Pt, Au or Ag nanoparticles, Ag nanoparticles in the outer shell of multishell inorganic-organic hybrid sub-micron particles, or Ag particles in nanotextured alumina films.

Polymeric films with highly dispersed inorganic clusters as nanosized building blocks were prepared from pre-formed metal oxide/alkoxide clusters of the general formula $M_xO_y(OH/OR)_v(carboxylate)_w$ with unsaturated carboxylate ligands. Polymerization of small proportions of the clusters with organic co-monomers results in hybrid polymers in which the clusters crosslink the polymer chains. The properties of the new hybrid materials originate from a combination of nanofiller and crosslinking effects in addition to the intrinsic properties of the base polymer and the inorganic cluster.

11:30 Oral

Waveguide nanostructuring for biosensing applications

Bernard Wenger, Ana-Maria Popa, Stéphanie Pasche, Emmanuel Scolan, Guy Voirin, Raphaël Pugin

Centre Suisse d'Electronique et de Microtechnique (CSEM), Jaquet-Droz 1, Neuchâtel 2002, Switzerland

e-mail: bernard.wenger@csem.ch

Optical biosensors have now proved to be sensitive and reliable devices as proved by the numerous commercial devices available. Label free biosensing systems are very interesting in the fields of research, drug discovery and point of care applications but they can suffer from a lack of sensitivity for the detection of small molecules. Nanostructuration is an elegant approach to lower the limit of detection by increasing the sensitive surface area. The optical sensing technique WIOS developed at CSEM, which is based on evanescent wave refractometry, has been modified following two different strategies to enhance the sensitivity: 1) formation of quasi-periodic nanostructures in silica by deep reactive ion etching using an etch mask made of self-assembled polymer micelles and 2) deposition of thin mesoporous films of nanoparticles.

With the appropriate choice of the polymer layer self assembly parameters and etching conditions, the silica layer is nanostructured in nano-pillars or nano-holes form. The samples were tested with the WIOS[1] instrument and the results show that the presence of a residual SiO_2 layer can hinder drastically the effect of the increased surface area. Careful control of the deposited layer and the etching conditions lead to an appreciable improvement for the non-specific adsorption of bovine serum albumin (BSA). Using the second approach, different sensing layers made of various metal oxides stabilized by a photo-crosslinkable polymer or sintered at high temperature have been compared. Improvements have been observed for non-specific adsorption of BSA. Finally, the nanostructured sensing surfaces were tested in a biosensor environmental application for the specific recognition of pesticides and antibiotics in water samples using adapted immunoassays.

[1] Wavelength-Interrogated Optical Sensing

11:50 Invited oral

Architecture and composition influence on the properties of some smart polymeric materials designed as matrices in drug delivery systems

Cornelia A. Vasile, Raluca P. Dumitriu, Gina-Gabriela Bumbu

Petru Poni Institute of Macromolecular Chemistry of the Romanian Academy, Aleea Grigore Ghica Voda 41A, Iasi, Romania

e-mail: cvasile@icmpp.ro

Variable architecture polymeric materials that can respond with a change in conformation to relevant stimuli action, such as temperature, pH, ionic strength, biological molecules are of considerable interest for a wide range of applications because of their sensitivities to the modification in environmental conditions. Variable architecture polymeric materials, have been as developed covering interpolymeric complexes, graft copolymers and hydrogels constituted from natural and synthetic polymers which offer unique properties such as, responsiveness to temperature and/or pH, biodegradability, specificity, and biocompatibility.

By combining a temperature-sensitive polymer/monomer usually N-isopropylacrylamide with one pH-sensitive in different architectures, dual/multiple-responsive materials can be obtain. The poly(N-isopropyl acryl amide) (PNIPAM) or hydroxypropyl cellulose (HPC) as thermoresponsive component were used.

Graft copolymers, interpolymeric complexes and blends of PNIPAM with carboxymethylcellulose (CMC) exhibit “thermothickening”. Enzymatic degradation is influenced by molecular interactions in the studied system.

Interpolymeric complexes of PNIPAM with a dicarboxylic copolymer as maleic acid-*alt*-vinylacetate have a compact structure similar with those of PNIPAM with hydroxypropylcellulose, their stability depends on chemical nature and environmental conditions (pH, temperature). Graft copolymers of PNIPAM with dicarboxylic copolymer as maleic acid-*alt*-vinyl acetate also exhibit a very strong “thermothickening” effect.

The interpolymeric complexes and hydrogels of PNIPAM with alginate or chitosan behave as “smart” dual-responsive materials with transition temperature/pH values close to the physiological ones.

This new class of interpolymeric complexes, graft copolymers and hydrogels can sense environmental changes in the physiological range and has found usefulness in drug delivery . Kinetics of the loading and release of some drugs has been evaluated.

12:20 Oral

Plasma deposition of organosilicon polymer thin films with embedded nanosilver for prevention of microbial adhesion

Claire Saulou[1], Bernard Despax[1], Muriel Mercier-Bonin[2], Philippe Marcus[3], Sandrine Zanna[3], Patrice Raynaud[1]

1. *Laboratoire Plasma et Conversion d'Energie (LAPLACE), 118 Route de Narbonne, Toulouse 31062, France* **2.** *Laboratoire d'Ingénierie des Systèmes Biologiques et des Procédés (LISBP), 135 Avenue de Rangueil, Toulouse 31077, France* **3.** *Ecole Nationale Supérieure de chimie de Paris (ENSCP), 11 rue P. et M. Curie, Paris 75005, France*

e-mail: claire.saulou@insa-toulouse.fr

The project is focused on the plasma deposition of thin films (~100 nm) containing silver nanoparticles embedded in a polymeric matrix, on stainless steel. Silver has been chosen for its broad-spectrum antimicrobial properties and stainless steel AISI 316 L because of its extensive use in agro-food equipments and in biomedical devices. Nevertheless, a strong and specific microorganism adhesion was previously demonstrated on this surface. To avoid microbial adhesion, stainless steel surfaces were coated with plasma-mediated nanocomposite films. The process originality relies on a dual strategy associating Ag target sputtering and plasma polymerization in argon-HMDSO plasma, using an asymmetrical RF discharge (13.56 MHz). The film properties (Ag content, surface energy…) can be controlled through changes of the operating conditions (flow rate, RF power…). Polymeric matrix with or without Ag content have been analysed by FTIR. The presence of Si-H, Si-O-Si, Si-$(CH)_n$-Si and C-H groups was established. The silver atomic compositions, evaluated by XPS, were in the range 0-20%. To determine the anti-adhesive efficiency, detachment experiments were performed in a shear stress flow chamber. The maximal detachment efficiency was achieved with the polymeric matrix, thus confirming its anti-adhesive properties, probably due to a surface energy modification. Silver antimicrobial effect is assumed to be related to Ag^+ ion progressive release from the embedded particles (resulting from metallic silver preliminary oxidation). The Ag^+ release kinetics was confirmed by ICP-MS measurements: a maximal release was reached after 2 day-contact time. In parallel, film toxicity was evaluated: a significant decrease in cell viability was observed for the maximal silver composition of 20%. From an engineering point of view, film properties (thickness, silver content, hydrophilic/hydrophobic properties) have now to be optimized. The film stability will be also particularly investigated.

12:40 Oral

Development of a hybrid PECVD/PVD process for nanocomposite thin films synthesis: application to copper-silica layers

Alain Daniel[1], Christophe Le pen[1], François Reniers[2]

1. *ARCELORMITTAL Liege research and development, Bd de colonster, B57, Liège 4000, Belgium* **2.** *Université Libre de Bruxelles, Analytical and Interfacial Chemistry (ULB), Boulevard du Triomphe, Brussels 1050, Belgium*

e-mail: alain.daniel@arcelormittal.com

Nanocomposite coatings offer a wide range of functionalities for steel industry: aesthetic, superhardness, low friction coefficient, anticorrosion, self-healing, optical filters, hydrophilicity, … Sol-gel techniques are often used to obtain this kind of materials.

Here a hybrid process which combines Plasma Enhanced Chemical Vapour Deposition (PECVD) and sputtering is developed to produce nanocomposite thin films on steel. The work describes the synthesis of layers based on a silica matrix and copper oxide clusters. The influence of some process parameters on the coating composition, such as the precursor flowrate and the power, is evaluated.

This work shows that by using the hybrid process it is possible to manage the quantity of sputtered metal inside a silica-like matrix from a copper or copper oxide film to a pure organosilicon matrix. The thin films are characterized by SEM, X-Ray Fluorescence, X-Ray Diffraction and FTIR measurements.

The process flexibility could allow us to develop various silica based coatings just by replacing the metallic target with the appropriate one.

Lunch break

Wednesday afternoon, 17 September, 13:00
Inner Courtyards

No session

Wednesday afternoon, 17 September, 14:00
Room 123

Coffee break

Wednesday afternoon, 17 September, 15:30
Main Hall

Joint Poster Session 2

Wednesday afternoon, 17 September, 16:00
Main Hall

Posters

Monday, 15 September

Poster session

Monday & Wednesday
Monday afternoon, 15 September, 16:30
Main Hall

16:30 Poster W1

Structural and morphological study of hydroxyapatite grown by chemical methods on different substrates

Toma Stoica, Tionica Stoica[2], Adrian Slav[2], Crina-Elena Anastasescu[1], Mihai Anastasescu[1], Madalina Nicolescu[1], Adelina Ianculescu[3], Mariuca Gartner[1], Maria Zaharescu[1]

1. *Instituite of Physical Chemsitry (ICF), Splaiul Independentei 202, Bucharest 060021, Romania* **2.** *National Institute for Materials Physics, Bucharest- Magurele 010555, Romania* **3.** *University Politehnica of Bucharest, Polizu 1-7, Bucharest, Romania*

e-mail: canastasescu@icf.ro

Many efforts have been done in order to obtain biocompatible materials (e.g. bone substitutes) with special properties (corrosion and mechanical resistance). Biocompatible materials are composed of a ceramic layer deposited on a metallic substrate. Titanium dioxide is often used as an interface layer material to increase the adhesion of the bio-material (hydroxiapatite in our case) to the metallic substrate.

Thus, in this paper, three kinds of hydroxyapatite (HA)-based films, deposited on different substrates (Si, TiO_2 and HA) are presented. The first two types of samples consisting of HA/TiO_2/Si and a mixture of (HA - TiO_2)/Si with different TiO_2 content are deposited by sol-gel and dipping method. The third type, composed of HA coatings are chemical growth from solution, by so-called Simulated Body Fluid method, which simulate the chemical environment in which the HA coatings are supposed to be used. The X-ray diffraction (XRD), Fourier transformed infra red spectroscopy (FTIR), Spectroscopic Ellipsometry (SE) and Atomic Force Microscopy (AFM) were used to investigate the growth and crystallization conditions of the films and to adjust the HA growth (adherence, stability and compatibility) *in vivo*. The obtained films are homogeneous and crack-free with various porosities (0-49%), wide range of refractive indices and accordingly, with the band gap in the broad range of 3.9 - 9.8 eV. Unlike, the SBF films are thinner (around 200-300 A) and non-porous. From the morphologic point of view, it has been observed the formation of HA-based films with a fine granular structure and with a grain diameter of the order of hundreds of nm for both HA-TiO_2 and SBF films. The RMS roughness depends on the substrate and the deposition method and has values from few nm up to tens nm.

This work pointed out that besides sol-gel, the chemical growth from solution is also a suitable method, even better for the deposition of the nanostructured films on different substrates.

16:30 Poster W2

Hydroxiapatite films on Ti and TiO_2 for biological applications

Tionica Stoica[2], Toma Stoica[2], Adrian Slav[2], Mihai Anastasescu[1], Mihai Stoica[1], Stefania Petrescu[3], Mariuca Gartner[1]

1. *Instituite of Physical Chemsitry (ICF), Splaiul Independentei 202, Bucharest 060021, Romania* **2.** *National Institute for Materials Physics, Bucharest- Magurele 010555, Romania* **3.** *Institute for Biochemistry of Romanian Academy, Splaiul Independentei, Bucharest, Romania*

e-mail: manastasescu@icf.ro

Hydroxyapatite (HAp) - $Ca_{10}(PO_4)_6(OH)_2$ - is one of the most investigated materials for bone implants due to its suitable chemical composition and morphology which is very similar with mineralized bones of human tissues. Recently, it was reported that the biocompatible hydroxyapatite granules were successfully employed to fill the bone defects and that these defects were faster restored with HA granules of smaller diameters, in the micrometer scale.

Under these circumstances, the aim of this work was to find the optimal conditions regarding both deposition and annealing conditions for obtaining HAp coatings of tailored thickness, roughness, porosity and bioactivity. By using the sol–gel method, amorphous as well as crystalline coatings can be obtained with a very good control of the composition and stoichiometry. Spectroscopic ellipsometry in combination with Atomic Force Microscopy was used to characterize the structural and morphological properties of the HAp films deposited on Titanium and Titania buffer layers. Thus, it was found that the HAp films deposited directly on Ti are thicker, more porous, and exhibit surface deposits as well as pits. The films obtained by using a buffer layer of TiO_2 between the substrates and HAp, are thinner, less porous, with a uniform granular structure which was consistently characterized. For all samples, a low value of the annealing temperature determines the lowering of the surface roughness and porosity.

The bioactivity tests performed with osteoblast/osteosarcoma cells evidenced a good correlation between the densities of the primar cells and the composition of the layers. The highest cell density was observed on the HA samples with two layers. The studied HAp films exhibit a good mechanical stability leading to the cell adherence and normal proliferation on the tested surfaces. No cell morphological changes occur.

16:30 Poster W3

Coloured DLC nanolayers

Frantisek Cerny, Vladimir Jech, Svatava Konvickova, Rudolf Dvorak

Czech Technical University in Prague, Faculty of Mechanical Engineering (CTU), Technicka 4, Prague 16607, Czech Republic

e-mail: Frantisek.Cerny@fs.cvut.cz

Coloured DLC (Diamond-Like Carbon) nanolayers were prepared by PACVD (Plasma Assisted Chemical Vapour Deposition) method as decorative coatings on stainless steel sheet. Microhardness of the substrate/coating systems obtained was determined by nanoindentation. The coatings were hard and adherent. Rather attractive DLC coatings of different colours can be produced simply by controlling the coating thickness.

16:30 Poster W4

Novel Precursors in the Synthesis of Mesoporous Silica-Titania Films

Nicola K. Huesing, Joachim H. Koehler

Ulm University, Albert-Einstein-Allee 47, Ulm 89081, Germany

e-mail: nicola.huesing@uni-ulm.de

For different fields of applications, e.g. in sensing, catalysis, etc., doping of mesostructured silica films with metal oxides is of high importance for the compensation of the rather inert character of pure silica. In this approach, the focus lies on the preparation of titania-doped silica films, which can be used for photocatalysis or for catalyzing epoxidation reactions depending on the incorporated amount of titania. There are several routes for the preparation of catalytically active mesoporous silica films, e.g. post-treatment to incorporate active species after the porous silica-matrix was prepared. However, problems such as pore-blocking and an inhomogeneous distribution of the metal constitutes a big problem. Another possible way is the direct synthesis by mixing an alkoxysilane e.g. tetraethyl-orthosilicate (TEOS) with the titanium-analogue tetraethyl-orthotitanate (TEOT), which although won´t work in this case since hydrolysis and condensation rates of the silica and titania sources differ strongly and titania would precipitate in the sol.

For the preparation of mesostructured silica-titania films with a variable Si/Ti-ratio, the complexation of the titanium alkoxide precursor to the structure-directing agent, e.g. Brij56 has been reported previously. In this approach, the Ti-content is directly connected to the amount of surfactant and cannot be varied to a large extent. In this work, a novel more flexible approach is described based on the application of a preformed single-source precursor (SSP). This precursor was prepared from 3-acetyl-6-triethoxysilylhexane-2-one coordinated to titanium tetraisopropoxide. Applying this SSP in an evaporation-induced self-assembly process allows to deliberately tune the composition of the final film up to a Si : Ti ratio of 1. All materials are characterized by TEM, SAXS, XRD and nitrogen sorption. The potential and disadvantages of this approach are discussed in detail.

16:30 Poster W5

Three dimensional substrates for Microbatteries

Arockia Vimal Jeyaseelan, James F. Rohan

University College Cork, Tyndall National Institute (TYNDALL), Lee Maltings, Prospect Row, Cork, Ireland

e-mail: vimal.arockia@tyndall.ie

There has been an increasing interest in recent years for lithium ion microbatteries for microelectromechanical systems (MEMs) integrated devices on silicon substrates. These thin film energy sources may be patterned and integrated on chip to match the specific requirements of the system. Minimising the footprint of such devices while maintaining the capacity and current drain capability is desirable to maximise the integration per substrate. One of the techniques that may be employed while utilising standard thin film battery materials is to structure the substrate prior to active materials deposition. This increases the quantity of available active material and the surface area for current drain while maintaining the optimised planar active layer thickness in the same footprint area. This paper describes lithographic techniques for patterning planar substrates to achieve microbattery materials compatible 3 D nickel substrates for sequential deposition of active battery materials. A single spin negative photoresist is used to achieve 90 µm height. After patterning, nickel is electroplated on the substrates from a low stress nickel sulfamate bath to a maximum of 90 µm. The sidewall angle achieved is in the range 6-9° yielding a thinner nickel feature at the surface level than at the base which is a key parameter to facilitate subsequent active battery materials deposition by vacuum deposition techniques. Aspect ratios of 1.5 to 1 have been achieved and the surface area may be doubled using this process by comparison with planar electrodes.

16:30 Poster W6

Sol-gel synthesis and functionalisation of multi-layered template-structured silica films on glass substrate

Tetyana Levchenko, Yuri Plyuto

Institute of Surface Chemistry NAS of Ukraine, 17 General Naumov, Kyiv 03164, Ukraine

e-mail: levchtat@i.com.ua

The goal of present work was to clarify how the way of preparation of the multi-layered template-structured silica films influences their structure and accessibility with respect to doping dye molecules.

Multi-layered silica films on glass slides were prepared by dip-coating technique using sol-gel precursor (reagents molar composition was 1 $Si(OC_2H_5)_4$: 22 C_2H_5OH : 5 H_2O : 0.004 HCl : 0.096 $CH_3(CH_2)_{15}N^+(CH_3)_3Br^-$). The dip-coated silica films were calcined in air at 400 ºC for 1 h to complete condensation of siloxane oligomers into silica framework and to remove the template. Two alternative preparation routes that differ in the sequence of dip-coating and calcination steps were applied. The adsorption of Methylene Blue dye from $5 \cdot 10^{-5}$ M aqueous solution was studied in order to examine accessibility of pores in the developed multi-layered silica films.

It has been found out that in the case of preparation route which includes reiteration of dip-coating and calcination steps, only the pores of the top silica layer appeared to be accessible to dye molecules. In contrast, when the preparation route includes successive dip-coatings accomplished by calcination of the final multi-layered film, all pores were found to be accessible. This is due to formation of the pores which occurs *via* simultaneous removal of the template over the whole thickness of the multi-layered silica film.

One can observe that dip-coating over the top of uncalcined film results in multi-layered films of different thickness and surface uniformity depending on the intervals between dip-coatings. This could be caused by variation of hydrophilic-hydrophobic properties upon drying and ageing of the as-synthesised template-doped silica film. If each dip-coating step was accomplished with calcination for the template removal, no difference in dip-coating of the successive layers were observed although the developed multi-layered films appeared to be less promising for further functionalisation.

16:30 Poster W7

Characterized of self-assembled monolayers (SAMs) on polymer substrate comparative with silicon substrate for E.coli detection

Carmen Moldovan, Carmen Mihailescu, Dana Stan

National Institute for Research and development in Microtechnologies (IMT-Buchares), P.O.Box 38-160, Bucharest 023573, Romania

e-mail: carmen.moldovan@imt.ro

In order to develop a plat surface for the printing anti – E.coli O157:H7 polyclonal antibody used in microarray technology and immunosensors, the substrates are coated with thick layer of gold and are functionalized with self-assembled monolayer technique. In experiment are two types of substrates: one is formatted with silicon substrate and other is formatted with polymer substrate. One of the most important points in the design of an immunosensor and a microarray is the choice of immobilization method. Recently, self –assembled monolayers (SAMs) generated by adsorption of alcanethiols on gold have been the subject of extensive research. These techniques will allow the study of the adsorption of proteins to different SAMs formed on the gold surfaces. In this work, the cyclic voltammetry and spectroscopy technique (Spectroscopic Ellipsometry, FTIR, Raman) have been utilized for surfaces characterization. The vibration molecule frequencies of the thiol monolayer can be detected with infrared spectroscopy (FTIR-ATR). Activation method included NHS/EDC for coupled SAM with an affinity purified polyclonal antibody to *E. coli* O157:H7 made in Goat. For microarray detection the anti-E. coli O157:H7 polyclonal antibody was labeled with fluorescein isothiocyanate (FITC).

The samples for microarray were prepared using anti-E. coli polyclonal antibody (KPL) in PBS (Sigma) in serial dilutions to determine optimal working concentrations. In the present study we report two substrates, silicon and polymer who are functionalized with different SAMs in order to immobilize efficient the anti-E O157:H7 polyclonal purified antibody.

This experimental study was revealed the necessity to investigate each step taking into account in the same time the factors that influence the chemistry of the surface and the further interactions as well.

The realisation of an e-coli sensor is envisaged and the comparison between the two substrates is achieved.

16:30 Poster W8

Core-shell and raspberry-like nanocomposites based on hybrid silica nanoparticles and on a functional polycarbazole polymer

Anna Peled, Vadim Kotlyar, Jean-Paul Lellouche

Bar Ilan University, Ramet-Gan 52900, Israel

e-mail: aniapeled@yahoo.com

Preparation of inorganic particle / organic polymer nanocomposites is challenging nanotechnological problem in terms of morphology control. However, preparation of nanocomposites from hard inorganic nanoparticles and functional conducting polymers can lead to development of remarkable materials with synergistic inorganic-organic properties. These novel nanocomposites may found practical application in stable sensory coatings, corrosion protection and electrode materials for organic photovoltaics.

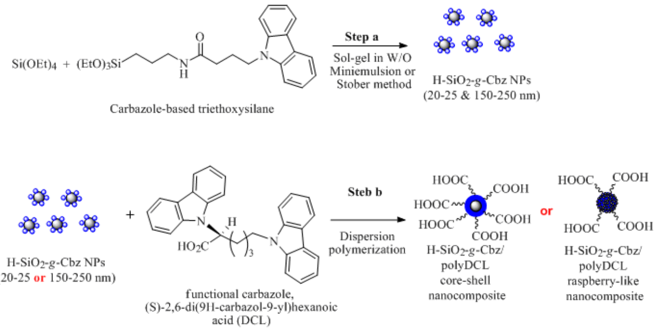

Figure. Fabrication of core-shell and raspberry-like hybrid silica/polycarbazole nanocomposites

In this poster, we describe preparation of triethoxysilane-carbazole anchoring group and their incorporation into hybrid silica nanoparticles (20-25 & 150-250 nm), **Figure**. The hybrid silica nanoparticles with carbazole-anchoring groups were used for the preparation of hybrid silica/functional polycarbazole nanocomposite materials by chemical oxidative polymerization, **Figure**. Resulting nanocomposites were extensively characterized by TEM, SEM, HR-SEM, FT-IR, XPS and elemental analysis. They showed distinct core-shell and raspberry-like morphologies. The main conclusion of our study is that hybrid silica with anchoring carbazole groups on the surface is a critical factor (besides the many ones which were investigated) for morphology control at a nanometric scale.

16:30 Poster W9

Amorphous hydrocarbon film deposition in plasma assisted CVD process: competition between deposition and erosion

Richard Clergereaux[1], Freddy Gaboriaux[1], Aref Slim[1], Jean-Louis Stehlé[2], Dorian Zahorski[2], Patrice Raynaud[1]

1. *Université Toulouse, LAboratoire PLAsma et Conversion d'Energie (LAPLACE), 118 Route de Narbonne, Toulouse 31062, France*
2. *SOPRA SA, 26 Pierre Joigneaux, Bois-Colombes 92270, France*

e-mail: patrice.raynaud@laplace.univ-tlse.fr

Amorphous hydrocarbon film deposition in a DECR Multipolar Microwave Plasma takes place from two deposition mechanisms: Hydrocarbon species sticking and film erosion by hydrogen formed in the discharge. This last mechanism leads to the formation of volatile species such as C_xH_y that can be dissociated and modify the film deposition process. For example, in CH_4 plasma, it appears that the discharge is modified during the first minutes of the process. Indeed, excited volatile species can be observed by optical emission spectroscopy such as C_2. As the probability of recombination in plasma volume is low, these species can not be created from the reactor walls. To simulate this competition between deposition and erosion on the reactor walls, the process on uncooled substrate was analyzed by in-situ spectroscopic ellipsometry. From the evolution of ellipsometric angles, it appears that erosion is highly dependant on the substrate temperature. Indeed, above 100°C, erosion is more important than deposition process – leading to the decrease of the film thickness – although the sticking coefficients are not affected in this range of temperature. Moreover, from the analysis of ellipsometric spectra, the evolution of the film structure will be shown. Then, during the first deposition times, the discharge is highly modified (volatile species formation and dissociation) inducing an evolution of the film structure for controlled processes (i.e. at substrate temperature fixed). This evolution will then be analyzed by spectroscopic ellipsometry and compared to those of the discharge from optical emission spectroscopy.

16:30 Poster W10

Environmental analysis by lca approach applied to plasma and sol-gel deposition processes

Andrea Terenzi, Giovanni Lelli, Roberto Petrucci

MDP Materials Design and Processing Srl (MDP), Loc. Pentima Bassa, 21, Terni 05100, Italy

e-mail: andrea.terenzi@mdpsrl.it

LCA is a relatively new methodology to evaluate the environmental impact of products and processes. This methodology is principally based on the approach "from cradle to grave" because the flow of resources involved in the process or product analysed is followed during their entire life cycle.

In this work LCA methodology is applied to deposition processes for nanostructured coating. The work was performed in the frame of NAPOLYDE project and the main objective was to analyse the efficiency of the new technologies developed in the project from an environmental point of view. Two main technologies was analysed in this work, the first one is based on plasma and the second one is based on sol-gel approach.

In order to evaluate the efficiency of the new technology developed in the frame of NAPOLYDE, a comparative study was performed. In the first part of the typical plasma and sol-gel processes were analysed, in the second part of the work have been analysed deposition process to obtain similar functionality of the coating but using the technologies developed in NAPOLYDE. Finally the results in terms of environmental impact have been compared in order to analyse the environmental efficiency of these new technologies.
The results show that the new technologies does not influence the total environmental load or in some case improve the environmental impact of the processes. But in general the properties of the coating are significantly improved. A really important contribution is given by the abatement systems; in fact in the new processes nanostructured coating have been produced and in this case it is very important the minimization of the emissions in terms of nanoparticles.

16:30 Poster W11

PECVD ion exchange membrane for Proton Exchange Membrane Fuel Cell

Jessica Thery, Steve Martin, Lucie Jodin
CEA (LITEN), 17 rue des Martyrs, Grenoble 38054, France
e-mail: theryjessica@gmail.com

Proton Exchange Membrane (PEM) fuel cells deliver high power density and offer the advantage of low weight and volume, compared to other fuel cells. The PEM fuel cell present a Membrane Electrode Assembly (MEA) architecture corresponding to a proton conductive membrane sandwiched between two catalytic electrodes. Platinum and its alloys are mainly used as the catalyst and Nafion® as the proton conductive material. It is now clear that the emergence of PEMFC as a leading low carbon energy solution for applications in transport, stationary and portable power??? requires strong performances improvement of the key fuel cell material components (catalysts and proton conductive membrane) as well as new solutions to overcome integration limitations. Directing our works towards an industry-compatible material processing method, we developed a PECVD ion conductive membrane with proton conductivity values of the same order than the one of Nafion®. The membrane is made of a CF backbone with carboxylic functions providing a proton conductive pattern. The XPS analysis indicate the presence of many fluorated species (mainly CF_2-CF_2 and CF_3-CF_2) and C-O / C=O bonds. The proportion of C-O and C=O bonds influences strongly the proton conductivity and can be adjusted through the process parameters (See figure 1). For a conductivity of ~ 100 mS/cm, an ionic exchange capacity of 2.1 meq/g was measured. This PECVD membrane was tested integrated in a fuel cell stack. Open circuit voltages around 900 mV were measured for a 12µm thick membrane. Despite the elevated proton conductivity, the performances of the fuel cells with this PECVD membrane are disappointing. However, we observed that interfaces improvement (through annealing treatments, composite zones at the interfaces) improve the fuel cell performances (See figure 2). We will present the conductivity measurement and comparison with the one of Nafion® membranes and fuel cell performances will be discussed.
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List of Participants

Mehmet Acet
mehmet.acet@uni-due.de
- Duisburg-Essen University, Experimental Physics
  Lotharstr. 1, Duisburg D-47048, Germany

Magdalena Aflori
maflori@icmpp.ro
- Petru Poni Institute of Macromolecular Chemistry of the Romanian Academy
  Aleea Grigore Ghica Voda 41A, Iasi, Romania

Jonathan Agbenyega
a.olfers@elsevier.com
- Elsevier Ltd.
  Radarweg 29, Amsterdam 1043NX, Netherlands

Wha-Seung Ahn
whasahn@inha.ac.kr
- Inha University-Dept.Chem.Eng
  253 Yonghyun-Dong, Nam-Gu, Incheon 402-751, Korea, South

Camelia Alexandru
bratuelenacamelia@yahoo.com
- ICPE-CA-Bucharest
  313 Splaiul Unirii, Bucharest 74204, Romania

Ahmed Al-Jumaily
ahmed.al-jumaily@aut.ac.nz
- Institute of Biomedical Technologies, Auckland University of Technology (AUT)
  AUT City Campus, Auckland 1142, New Zealand

Rui M. Almeida
rui.almeida@ist.utl.pt
- Instituto Superior Técnico
  Lisboa 1049-001, Portugal

Ramon A. Alvarez-Puebla
ramon.alvarez@uvigo.es
- University of Vigo
  Campus Universitario Lagoas-Marcosende Vigo Spain, Vigo 36310, Spain

Crina-Elena Anastasescu
canastasescu@icf.ro
- Instituite of Physical Chemsitry (ICF)
  Splaiul Independentei 202, Bucharest 060021, Romania

Mihai Anastasescu
manastasescu@icf.ro
- Instituite of Physical Chemsitry (ICF)
  Splaiul Independentei 202, Bucharest 060021, Romania

Rostislav A. Andrievskiy
ara@icp.ac.ru
- Russian Academy of Sciences, Institute of Problems of Chemical Physics (IPCP RAS)
  Institutskii pr., 18, Chernogolovka 142432, Russian Federation

Olena R. Andriyevskaya
era@ipms.kiev.ua
- Institute for Problems of Materials Science, National Academy of Sciences of Ukraine
  Krzizanovsky, Kyiv 38(044), Ukraine

Mariusz Andrzejczuk
mandrzejczuk@inmat.pw.edu.pl
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

Elias Aperathitis
eaper@physics.uoc.gr
- Microelectronics Research Group, Institute of Electronic Structure and Laser, Foundation for Research and Technology – Hellas, P.O. Box 1527, 71110 Heraklion, Crete, Greece
  P.O. Box 1527, Heraklion 71110, Greece

Sonja Aškrabić
sonask@phy.bg.ac.yu
- Institute of Physics (IF)
  Pregrevica 118, Belgrade 11080, Serbia

Georgios I. Athanasopoulos
atgeorge@ucy.ac.cy
- University of Cyprus (UCY)
  Kallipoleos Avenue, Nicosia 1678, Cyprus

Stefan F. Awietjan
stefan_a@wp.pl
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

Yuriy Azhniuk
azhn@ukrpost.net
- Institute of Electron Physics, Ukr. Nat. Acad. Sci.
  Universytetska Str., Uzhhorod 88017, Ukraine

Beata Backiel-Brzozowska
bbb@pb.edu.pl
- Bialystok Technical University, Institut of Civil Engineering
  Wiejska 45E, Białystok 15-351, Poland

Jas Pal Badyal
j.p.badyal@surface-innovations.com
- Surface Innovations Ltd
Wolsingham DL133HH, United Kingdom

Armelle Baeza
baeza@univ-paris-diderot.fr
- Paris Diderot University, Laboratoire de Cytophysiologie et Toxicologie cellulaire
case 70 73, 2 Place Jussieu, Paris cedex 05, Paris 75251, France

Sina Baghbani kordmahale
sina_baq.k@aut.ac.ir
- Amirkabir University of Technology (AUT)
Hafez, Tehran 15914, Iran

Mihaela Baibarac
barac@infim.ro
- National Institute for Materials Physics
Bucharest- Magurele 010555, Romania

Anna Bajorek
anna.bajorek@us.edu.pl
- University of Silesia, August Chełkowski Institute of Physics, Department of Solid State Physics
Uniwersytecka 4, Katowice 40-007, Poland

Natalya Baklanova
baklanova@solid.nsc.ru
- Institute for Solid State and Mechanical Chemistry of RAS
Novosibirsk 630090, Russian Federation

Sergey V. Balakhonov
Balakhonov@inorg.chem.msu.ru
- M.V. Lomonosov Moscow State University
Vorobyevy gory, Moscow 119992, Russian Federation

Ioan Baltog
ibaltog@infim.ro
- National Institute for Materials Physics
Bucharest- Magurele 010555, Romania

Hanna Bandarenka
vitaly51@mail.ru
- Belarusian State University of Informatics and Radioelectronics (BSUIR)
P.Brovka str. 6, Minsk 220000, Belarus

Pedro Barquinha
pmcb@fct.unl.pt
- Materials Science Department, CENIMAT-IxN and CEMOP-UNINOVA, FCT-UNL
Campus da Caparica, Caparica, Caparica 2829-516, Portugal

Michel W. Barsoum
barsoumw@drexel.edu
- Drexel University
3141 Chestnut St, Philadelphia 19104, United States

Muhammad Bashouti
M.Bashouti@gmail.com
- Technion
Technion, Haifa 32000, Israel

Nina Baumjohann
nina.baumjohann@web.de
- HiNanoAnalytics Network
Heisenbergstasse 11, Münster 48149, Germany

Jan Becker
beckerja@uni-mainz.de
- Johannes Gutenberg Universität, Institut für Physikalische Chemie
Jakob Welder Weg, 11, Mainz 55128, Germany

Paulina Bednarek
bednarek@ch.pw.edu.pl
- Warsaw University of Technology, Faculty of Chemistry
Noakowskiego 3, Warszawa 00-664, Poland

Irina Belan
belanira@ipms.kiev.ua
- Institute for Problems of Materials Science, National Academy of Sciences of Ukraine
Krzizanovsky, Kyiv 38(044), Ukraine

Ludovic Bellot-Gurlet
bellot-gurlet@glvt-cnrs.fr
- Lab Dynamique Interaction et Reactivite, CNRS and Univ Paris VI (LADIR)
2 rue Henry Dunant, Thiais 94320, France

Ciceron A. Berbecaru
berbecaru2ciceron@yahoo.com
- University of Bucharest, Faculty of Physics
Bucharest-Magurele p.o.box mg-11, Bucharest 76900, Romania

Vesna I. Berec
vesnaber@gmail.com
- Institute of Physics (IF)
Pregrevica 118, Belgrade 11080, Serbia

Christian Berendsen
cbe@smb.dk
- Scandinavian MicroBiodevices ApS (SMB)
Farum 3520, Denmark

Sigrid Bernstorff
bernstorff@elettra.trieste.it
- Sincrotrone Trieste
Strada Statale 14, km 163.5, in AREA Science Park, Trieste 34012, Italy

Danilo Bersani
danilo.bersani@fis.unipr.it
- Dipartimento di Fisica, Università
Viale G.P. Usberti 7/a, Parma 43100, Italy

Rémy Besson
Remy.Besson@univ-lille1.fr
- Laboratoire de Métallurgie Physique et Génie des Matériaux (LMPGM)
Université de Lille 1, Villeneuve d'Ascq 59655, France

Havazelet Bianco Peled
bianco@tx.technion.ac.il
- Technion Israel Institute of Technology Dept. of Chemical Engineering
Technion City, Haifa 32000, Israel

Christophe Bichara
xtof@cinam.univ-mrs.fr
- Centre de Recherche en Matière Condensée et Nanosciences (CRMCN-CNRS)
Campus de Luminy, case 913, Marseille 13288, France

Anna Biedunkiewicz
anna.biedunkiewicz@ps.pl
- Szczecin University of Technology, Institute of Materials Engineering
Szczecin 70-310, Poland

Jens-Peter Biethan
biethan@hfe.tu-darmstadt.de
- Darmstadt University of Technology, Department of High Frequency Electronics
Merckstr. 25, Darmstadt 64283, Germany

Monika Bil
mbil@meil.pw.edu.pl
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
Wołoska 141, Warszawa 02-507, Poland

Johannes H. Bitter
j.h.bitter@uu.nl
- Inorganic Chemistry and Catalysis, Utrecht University
Sorbonnelaan 16, Utrecht 3584CA, Netherlands

Monserrat Bizarro
monserrat@iim.unam.mx
- Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico (UNAM)
A.P. 70-360, México 04510, Mexico

Yuri V. Blagoveschenskiy
yuriblag@imet.ac.ru
- Baikov Institute of Metallurgy and Material Science, RAS (IMET)
49, Leninsky prospect, Moscow 119991, Russian Federation

Juliette Blanchard
juliette.blanchard@upmc.fr
- Laboratoire de réactivité de Surface, CNRS UPMC (LRS)
4 place Jussieu, casier 178, Paris 75252, France

Peter Blomqvist
pbl@smb.dk
- Scandinavian Micro Biodevices
Gammelgårdsvej 87c, Farum 3520, Denmark

Nicolas Blondiaux
nbx@csem.ch
- Centre Suisse d'Electronique et de Microtechnique (CSEM)
Jaquet-Droz 1, Neuchâtel 2002, Switzerland

Anna Boczkowska
abocz@meil.pw.edu.pl
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
Wołoska 141, Warszawa 02-507, Poland

Emiliano Bonera
emiliano.bonera@unimib.it
- University of Milano-Bicocca, Department of Materials Science
via Cozzi 53, Milano 20125, Italy

Guillaume Bonnefont
guillaume.bonnefont@insa-lyon.fr
- MATEIS
Jean Capelle, Villeurbanne 69621, France

Magali Bonne
magali.bonne@etu.univ-poitiers.fr
- LACCO
UMR CNRS 6503,, Poitiers ESIP, France

Elisabetta Borsella
elisabetta.borsella@ismn.cnr.it
- Istituto per lo Studio dei Materiali Nanostrutturati (ISMN-CNR)
Monterotondo, Roma I-00016, Italy

Michał A. Borysiewicz
mbory@ite.waw.pl
- Institute of Electron Technology (ITE)
al. Lotników 32/46, Warszawa 02-668, Poland

Malika Boualleg
malika.boualleg@cpe.fr
- Chimie, Catalyse, Polymère, Procédé, UMR CNRS CPE UCBL (CCPP)
43 bd du 11 Nov. 1918, Villeurbanne 69616, France

Michael Bowker
bowkerm@Cardiff.ac.uk
- Cardiff University
School of Chemistry, Park Place, Cardiff CF103AT, United Kingdom

Francesco Branda
branda@unina.it
- Department of Materials & Production Engineering, University of Naples "Federico II" (DIMP-CRIB)
Piazzale Tecchio, 80, Napoli 80125, Italy

Michael Bredol
bredol@fh-muenster.de
- Fachhochschule Münster
Stegerwaldstraße 39, Steinfurt 48565, Germany

Reiner Brings
reiner.brings@jobinyvon.de
- Horiba Jobin Yvon
Paris 91165, France
- Horiba Jobin Yvon GmbH
Hauptstr. 1, Unterhaching 82008, Germany

Iegor Brodnikovskyi
bregor@ya.ru
- Institute for Problems of Materials Science
3, Krzhizhanovsky, Kyiv 03142, Ukraine

Natalia Bukrina
bookr@mail.ru
- Institute of Stregth Physics and Materials Science of SB RAS
Tomsk, Russian Federation

Hervé Bulou
herve.bulou@ipcms.u-strasbg.fr
- Institut de Physique et Chimie des Materiaux de Strasbourg, UMR7504, CNRS - ULP
23, rue du Loess, BP 43, Strasbourg CEDEX 2 67034, France

Bogusław Burak
comef@comef.com.pl
- COMEF
Kalinowa 41, Katowice, Katowice 40-750, Poland

Kurt H. Buschow
k.h.j.buschow@uva.nl
- Van der Waals-Zeeman Institute Univ. of Amsterdam
Valckenierstraat 65, Amsterdam NL-1018XE, Netherlands

Joanna Cabaj
joanna.cabaj@pwr.wroc.pl
- Wroclaw University of Technology, Faculty of Chemistry
Smoluchowskiego 23, Wrocław 50-372, Poland

Valeria Califano
valeriacalifano@hotmail.com
- INFM - Coherentia
Via Cinthia, Napoli 80125, Italy

Andrzej Calka
andrzej_calka@uow.edu.au
- University of Wollongong
Wollongong NSW, Australia
- Faculty of Enginneering, University of Wollongong
Wollongong NSW 2522, Australia

Enrique Camarillo
cgarcia@fisica.unam.mx
- Universidad Nacional Autónoma de México-Instituto de Física (IFUNAM)
Circuito exterior s/n ciudad universitaria, México 04330, Mexico

Ranieri Cancedda
ranieri.cancedda@unige.it
- University of Genova
Genova 16126, Italy

Andres Cantarero
cantarer@uv.es
- University of Valencia
PO Box 22085, Valencia 46071, Spain

Aldo Capobianchi
aldo.capobianchi@ism.cnr.it
- CNR-ISM
Roma 00016, Italy

Valérie Caps
valerie.caps@ircelyon.univ-lyon1.fr
- Institut de recherches sur la Catalyse et l'Environnement de Lyon (IRCELYON)
2, avenue Albert Einstein, Villeurbanne 69626, France

Manuel Cardona
M.Cardona@fkf.mpg.de
- Max-Planck-Institut FKF
Heisenbergstr. 1, Stuttgart D70569, Germany

Xavier Carrier
xavier.carrier@upmc.fr
- Laboratoire de Réactivité de Surface (UPMC-CNRS)
4 place Jussieu, case 178, Paris 75252, France

Elti Cattaruzza
cattaruz@unive.it
- Physical Chemistry Dept, Università Ca' Foscari Venezia
Dorsoduro 2137, Venezia I-30123, Italy

Józef Cebulski
cebulski@univ.rzeszow.pl
- University of Rzeszow, Institute of Physics
  Rejtana 16, Rzeszów 35-310, Poland

Ondřej Černohorský
oce@razdva.cz
- Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical Engineering, Department of Physical Electronics
  Brehova str. 7, Prague 115 19, Czech Republic
- Czech Academy of Sciences, Institute of Photonics and Electronics
  Chaberská 57, Prague 18251, Czech Republic

Frantisek Cerny
Frantisek.Cerny@fs.cvut.cz
- Czech Technical University in Prague, Faculty of Mechanical Engineering (CTU)
  Technicka 4, Prague 16607, Czech Republic

Rachman Chaim
rchaim@technion.ac.il
- Technion - Israel Institute of Technology, Dept. of Materials Engineering
  Haifa 32000, Israel

Paul R. Chalker
pchalker@liv.ac.uk
- The University of Liverpool (UOL)
  Oxford Street, Liverpool L697ZD, United Kingdom

Catalina Natalia Cheaburu
duncaty@icmpp.ro
- Petru Poni Institute of Macromolecular Chemistry of the Romanian Academy
  Aleea Grigore Ghica Voda 41A, Iasi, Romania

Guoping Chen
Guoping.CHEN@nims.go.jp
- National Institute for Materials Science
  Ibaraki 305-0047, Japan

Si Chen
bt03chsi@chestud.chalmers.se
- Chalmers University of Technology
  Göteborg S-412 96, Sweden

Leonid I. Chernyshev
chern@ipms.kiev.ua
- Frantsevich Institute for Problems of Materials Science (IPMS)
  3, Krzhizhanivsky Str., Kiev 03680, Ukraine

Emilia Choinska
choinska.emilia@gmail.com
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

In-Sun Cho
cis005@snu.ac.kr
- Seoul National University, Department of Materials Science and Engineering (MSE, SNU)
  San 56-1, Sillim-dong, Gwanak-gu, Seoul 151-744, Korea, South

Patrick Choquet
choquet@lippmann.lu
- CRP Gabriel Lippmann (CRP-GL)
  41 rue du Brill, Belvaux L4422, Luxembourg

Taejun Cho
taejun@daejin.ac.kr
- Daejin University (TJCHO)
  Sundan11-1, Pocheon 487-711, Korea, South

Habibullah A. Chowdhury
chowdhh2@mail.dcu.ie
- School of Mechanical and Manufacturing Engineering, Dublin City University
  Dublin Dublin9, Ireland

Tadeusz Chudoba
chudoba@unipress.waw.pl
- Polish Academy of Sciences, Institute of High Pressure Physics (UNIPRESS)
  Sokolowska 29/37, Warszawa 01-142, Poland

Tomasz Ciach
ciach@ichip.pw.edu.pl
- Warsaw University of Technology, Faculty of Chemical Engineering
  Warynskiego 1, Warsaw 00-645, Poland

Gabriela Ciobanu
gciobanu03@yahoo.co.uk
- Technical University from Iasi (UTI)
  Bd.D.Mangeron 63, Iasi 700050, Romania

Fabrizio Cleri
fabrizio.cleri@univ-lille1.fr
- Institute for Electronics and Nanotechnology
  Lille 60069, France

Jacinto Cortés-Pérez
jacop@correo.unam.mx
- Universidad Nacional Autónoma de México, Facultad de Estudios Superiores Aragón, CTA (UNAM)
  Av. Rancho Seco S/N, col. impulsora, Cd. Nezahualcoyotl, Edo. de México, México 57130, Mexico

Luís C. Costa
kady@ua.pt
- Physics Department (UA)
  Campus Universitario, Aveiro 3810-193, Portugal

Corneliu M. Craciunescu
craciunescucm@yahoo.com
- Politehnica University of Timisoara (UPT)
  Bd. Mihai Viteazul 1, Timisoara 300222, Romania

Manuel Cruz-Yusta
manuel.cruz@aidico.es
- Asociación Investigación Industrias de Construcción (AIDICO)
  Parque Tecnológico Valencia, Valencia 46980, Spain

Paweł Czuma
comef@comef.com.pl
- COMEF
  Kalinowa 41, Katowice, Katowice 40-750, Poland

Paul Dalton
dalton@soton.ac.uk
- University of Southampton
  Southampton SO167PX, United Kingdom
- Shanghai Jiao Tong University (SJTU)
  Shanghai 200030, China

Alain Daniel
alain.daniel@arcelormittal.com
- ARCELORMITTAL Liege research and development
  Bd de colonster, B57, Liège 4000, Belgium

Moshe P. Dariel
dariel@bgu.ac.il
- Ben-Gurion University of the Negev, Department of Materials Engineering (BGU)
  Beer-Sheva 84105, Israel

Geta David
geta_david2000@yahoo.com
- Technical University from Iasi (UTI)
  Bd.D.Mangeron 63, Iasi 700050, Romania

Anne M. Davidson
anne.davidson@upmc.fr
- Universite Pierre et Marie Curie
  Place Jussieu, Bat F Boite 39, Paris 75252, France

Luis Antonio S. De Almeida Prado
L.Prado@tuhh.de
- Technical University Hamburg-Harburg (TUHH)
  Denickestr. 15, Hamburg 21073, Germany

Damien P. Debecker
damien.debecker@uclouvain.be
- Université catholique de Louvain, unité de catalyse et chimie des matériaux divisés (UCL)
  Croix du Sud, 2/17, Louvain-la-Neuve 1348, Belgium

Santiago De Bernardi-Martín
debernardi@us.es
- Universidad de Sevilla (USE)
  Sevilla 41012, Spain

Fatemeh Dehghan Nayeri
f.d.nayeri@gmail.com
- Laser Resaerch Center Paya Partov Co.
  Tehran 14665576, Iran

Annick P. Dejaegere
annick@igbmc.fr
- University Louis Pasteur
  Strasbourg, France

Sasanka Deka
sasanka.deka@unile.it
- Scuola Superiore ISUFI
  Distretto Tecnologico ISUFI, Via per Arnesano Km.5, Lecce 73100, Italy
- National Nanotechnology Laboratory of CNR-INFM (NNL)
  via per Arnesano Km 5, Lecce 73100, Italy

Alejandra De la Vega
delavega@tuhh.de
- Technical University Hamburg-Harburg (TUHH)
  Denickestr. 15, Hamburg 21073, Germany

Daniela D'Elia
daniela.delia@ensmp.fr
- Ecole Nationale des Mines de Paris
  Paris 75272, France

Christoph Dellago
Christoph.Dellago@univie.ac.at
- University of Vienna, Faculty of Physics
  Boltzmanngasse 5, Wien 1090, Austria

Brian Derby
brian.derby@manchester.ac.uk
- University of Manchester - School of Materials Science - Materials Science Centre
  grosvenor street, Manchester M1 7HS, United Kingdom

Grzegorz Dercz
gdercz@op.pl
- University of Silesia, Institute of Material Science
  Bankowa 12, Katowice 40-007, Poland

Ida-Dunja Desnica Frankovic
ddesnica@irb.hr
- RUDJER BOSKOVIĆ INSTITUTE
  BIJENIČKA C. 54, Zagreb 10 000, Croatia

Uros V. Desnica
desnica@irb.hr
- Rudjer Boskovic Institute
Bijenicka cesta 54, Zagreb HR-10000, Croatia

Elena Dilonardo
ellylamoretta@hotmail.it
- Università di Bari, Dip. Chimica
Bari 70124, Italy

Antonela Dima
antonela.dima@liv.ac.uk
- The University of Liverpool (UOL)
Oxford Street, Liverpool L697ZD, United Kingdom

Henryk Dłużewski
emrs@lot-oriel.de
- L.O.T. Oriel
Im Tiefen See 58, Darmstadt 64293, Germany

Romuald Dobosz
rdobosz@inmat.pw.edu.pl
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
Wołoska 141, Warszawa 02-507, Poland

Witold Dobrowolski
dobro@ifpan.edu.pl
- Polish Academy of Sciences, Institute of Physics
al. Lotników 32/46, Warszawa 02-668, Poland

Zorana D. Dohcevic-Mitrovic
zordoh@phy.bg.ac.yu
- Institute of Physics (IF)
Pregrevica 118, Belgrade 11080, Serbia

Pavel Dorozhkin
dorozhkin@ntmdt.ru
- NT-MDT Co.
Build. 100, Zelenograd Moscow 124482, Russian Federation

Kathrin Dorr
k.doerr@ifw-dresden.de
- Institut fuer Metallische Werkstoffe, IFW
Dresden, Germany

Timothy Douglas
douglas@mkg.uni-kiel.de
- Dresden University of Technology
Mommsenstr. 4, Dresden D 01-062, Germany
- Christian-Albrechts-Universität Kiel
Kiel 24098, Germany

Rui Dou
rui.dou@postgrad.manchester.ac.uk
- University of Manchester - School of Materials Science - Materials Science Centre
grosvenor street, Manchester M1 7HS, United Kingdom

Józef Dresner
inbox@eurotek.com.pl
- EUROTEK INTERNATIONAL
Al. Lotników 32/46, Warsaw 02-668, Poland

Peter S. Dubinin
Dubinin-2005@yandex.ru
- Siberian Federal University (SFU)
Krasnoyarskii rabochii 95, Krasnoyarsk 660095, Russian Federation

Ida O. Dulińska-Molak
idad@meil.pw.edu.pl
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
Wołoska 141, Warszawa 02-507, Poland

Lucia Dumitrescu
lucia.dumitrescu@gmail.com
- Transilvania University of Brasov, Centre Product Design for Sustainable Development
Eroilor 29, Brasov 500036, Romania

Raluca P. Dumitriu
rdumi05@yahoo.com
- Petru Poni Institute of Macromolecular Chemistry of the Romanian Academy
Aleea Grigore Ghica Voda 41A, Iasi, Romania

Carlos A. Duque
cduque_echeverri@yahoo.es
- Universidad de Antioquia (UA)
Calle-67-N-53-108, Medellín 05001000, Colombia

Donatella Duraccio
duraccio@ictp.cnr.it
- Istituto di Chimica e Tecnologia dei Polimeri (ICTP-CNR)
via Campi Flegrei, 34, Napoli 80078, Italy

Vladimir P. Dyakonov
dyakon@ifpan.edu.pl
- Polish Academy of Sciences, Institute of Physics
al. Lotników 32/46, Warszawa 02-668, Poland

Takashi Ehara
ehara@isenshu-u.ac.jp
- Ishinomaki Senshu University
Ishinomaki 986-8580, Japan

Miroslawa El Fray
mirfray@ps.pl
- Szczecin University of Technology, Polymer Instiute
  Pulaskiego 10, Szczecin 70-322, Poland

Ilze Elksnite
zicans@ktf.rtu.lv
- Riga Technical University (RTU)
  Azenes St. 14/24, Riga LV-1048, Latvia

Klaus Ellmer
ellmer@helmholtz-berlin.de
- Helmholtz Centre Berlin for Materials and Energy
  Glienicker Str. 100, Berlin D-14109, Germany

Szilvia Eosoly
szilvia.eosoly2@mail.dcu.ie
- School of Mechanical and Manufacturing Engineering, Dublin City University
  Dublin Dublin9, Ireland

William Erhabor
grpinvestment@yahoo.com
- University of Johannesburg
  Kingsway, Johannesburg 2006, South Africa
- Judith motors (JM)
  58 anderson street, Johannesburg 2000, South Africa

Yuri Estrin
yuri.estrin@eng.monash.edu.au
- School of Physics and Materials Engineering, Monash University
  Melbourne, Australia
- CSIRO Division of Materials Science and Engineering
  Private Bag 33, Clayton South MDC, Melbourne 3169, Australia

Paul Everitt
info@goodfellow.com
- Goodfellow Cambridge Limited
  Ermine Business Park, Huntingdon PE296WR, United Kingdom

Alexander V. Evteev
Alexander.Evteev@newcastle.edu.au
- The University of Newcastle
  University Drive, Newcastle 2308, Australia

Wojciech R. Fabianowski
wofab@ch.pw.edu.pl
- Warsaw University of Technology, Faculty of Chemistry
  Noakowskiego 3, Warszawa 00-664, Poland

Dariusz Fabjanowicz
inbox@eurotek.com.pl
- EUROTEK INTERNATIONAL
  Al. Lotników 32/46, Warsaw 02-668, Poland

Paweł Falkowski
falkowski@ch.pw.edu.pl
- Warsaw University of Technology, Faculty of Chemistry
  Noakowskiego 3, Warszawa 00-664, Poland

Gilbert Fantozzi
gilbert.fantozzi@insa-lyon.fr
- Laboratoire de Physique de la matière (LPM)
  INSA, 7 avenue capelle, Lyon 69621, France

Marek A. Faryna
nmfaryna@imim-pan.krakow.pl
- Polish Academy of Sciences, Institute of Metallurgy and Materials Sciences (IMIM PAN)
  Reymonta 25, Kraków 30-059, Poland

Daniele Fausti
d.fausti@rug.nl
- Zernike Institute for Advanced Materials
  Nijenborgh 4, Groningen 9747AG, Netherlands

Jarosław Ferenc
jferenc@inmat.pw.edu.pl
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

Janusz D. Fidelus
jdf@unipress.waw.pl
- Polish Academy of Sciences, Institute of High Pressure Physics (UNIPRESS)
  Sokolowska 29/37, Warszawa 01-142, Poland

Paweł Figiel
pfigiel@ps.pl
- Szczecin University of Technology, Institute of Materials Engineering
  Szczecin 70-310, Poland

Izabela Firkowska
firkowska@caesar.de
- center of advanced european studies and research (caesar)
  Ludwig-Erhard-Allee 2, Bonn 53175, Germany

Edwin Flikkema
edf@aber.ac.uk
- University of Aberystwyth (UWA)
  Aberystwyth SY233BZ, United Kingdom

Tadeusz Florczak
t.florczak@neostrada.pl
- Ośrodek Innowacyjno-Wdrożeniowy Tekoma-OIW Sp. z o.o (TEKOMA-OIW)
  Pyszniańska 8, Warszawa 02-829, Poland

Anton Fojtík
ftk@fjfi.cvut.cz
- Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical Engineering, Department of Physical Electronics
  Brehova str. 7, Prague 115 19, Czech Republic

Naum Frage
nfrage@bgu.ac.il
- Ben-Gurion University of the Negev
  P.O.Box 653, Beer-Sheva 84105, Israel

Isabella R. Franchini
isabella.franchini@unile.it
- National Nanotechnology Laboratory of CNR-INFM (NNL)
  via per Arnesano Km 5, Lecce 73100, Italy
- Scuola Superiore ISUFI
  Distretto Tecnologico ISUFI, Via per Arnesano Km.5, Lecce 73100, Italy

Jan Franc
franc@karlov.mff.cuni.cz
- Charles University, Institute of Physics (FU UK)
  Ke Karlovu 5, Prague 121 16, Czech Republic

Affouard Frederic
frederic.affouard@univ-lille1.fr
- Universite des Sciences et Techniques de Lille CNRS (USTL)
  cite scientifique Villeneuve d'Ascq, Lille 59655, France

Sławomir Fryszak
prevac@prevac.eu
- Prevac sp. z o.o.
  Raciborska 61, Rogów 44-362, Poland

Hideo Fukumura
d6821004@edu.kit.ac.jp
- Kyoto Institute of Technology
  Kyoto 606-8585, Japan

Masahiro Funahashi
funahashi@chembio.t.u-tokyo.ac.jp
- The University of Tokyo
  Bunkyo-ku, Tokyo 113-8655, Japan

Alison M. Funston
afunston@unimelb.edu.au
- The Univeristy of Melbourne (UNIMELB)
  Grattan Street, Melbourne 3052, Australia

Urszula R. Gabriel
ugabri@ps.pl
- Szczecin University of Technology, Institute of Materials Engineering
  Szczecin 70-310, Poland

Melanie Gaillet
webmaster@jobinyvon.fr
- Horiba Jobin Yvon
  Paris 91165, France

Anne Galarneau
anne.galarneau@enscm.fr
- Institut Charles Gerhardt
  CC15, Place eugène Bataillon, Montpellier 34095, France

Paola Gallo
gallop@fis.uniroma3.it
- Physics Department, University Roma Tre
  Via della vasca navale 84, Roma 00146, Italy

Perla E. Garcia-Casillas
perlaelviagarcia@yahoo.com
- Universidad Autonoma de Ciudad Juarez
  Ave. del Charro 450 Norte, Juarez 32360, Mexico
- Universidad Autónoma de Cd. Chihuahua
  Ave. Escorza y Venustiano Carranza s/n, Chiuahua 3100, Mexico

Ille C. Gebeshuber
gebeshuber@iap.tuwien.ac.at
- Institut fuer Allgemeine Physik, Vienna University of Technology (IAP)
  Wiedner Hauptstrasse 8-10/134, Wien 1040, Austria
- Austrian Center of Competence for Tribology (ACCT)
  Viktor Kaplan-Strasse 2, Wiener Neustadt 2700, Austria

Wojtek Gebicki
wojtg@if.pw.edu.pl
- Warsaw University of Technology, Faculty of Physics
  Koszykowa 75, Warszawa 00-662, Poland

Aharon Gedanken
gedanken@mail.biu.ac.il
- Bar-Ilan University
  Ramat-Gan 52900, Israel

Mohamed Nawfal Ghazzal
g_nawfel@yahoo.fr
- Laboratoire de chimie et méthodologie pour l'environnement (LCME)
  Rue Victor Demange, Metz 57500, France
- Metz University
  Victor Demange, Saint-Avold 57500, France

Florin Gherendi
florin.gherendi@infim.ro
- National Institute for Lasers, Plasma and Radiation Physics (INFLPR)
  Bucharest- Magurele 077125, Romania

Jacques Ghijsen
jacques.ghijsen@fundp.ac.be
- University of Namur, Laboratoire Interdisciplinaire de Spectroscopie Electronique (LISE)
  61 rue de Bruxelles, Namur 5000, Belgium

Ioannis Giapintzakis
giapintz@ucy.ac.cy
- University of Cyprus (UCY)
  Kallipoleos Avenue, Nicosia 1678, Cyprus

Mike Gibbs
m.r.gibbs@sheffield.ac.uk
- University of Sheffield, Department of Engineering Materials
  Mappin Street, Sheffield S1 3JD, United Kingdom

Marti Gich
marti.gich@saint-gobain.com
- Saint-Gobain Recherche (SGR)
  39, Quai Lucien-Lefranc, Aubervilliers 93303, France

Michael Giersig
giersig@helmholtz-berlin.de
- Helmholtz Centre Berlin for Materials and Energy
  Glienicker Str. 100, Berlin D-14109, Germany

Harald Giessen
giessen@physik.uni-stuttgart.de
- University of Stuttgart, Institute of Physics
  Pfaffenwaldring 57, Stuttgart D-70569, Germany

David S. Ginley
david_ginley@nrel.gov
- National Renewable Energy Laboratory (NREL)
  1617 Cole Blvd, Denver 80401, United States

George Gnesin
geognesin@yandex.ru
- Institute for Problems of Materials Science, National Academy of Sciences of Ukraine
  Krzizanovsky, Kyiv 38(044), Ukraine
- Institute for Problems in Materias Science (IPMS)
  3, Krzhizhanivsky Str., Kiev 03680, Ukraine

Morgan Gohin
morgan.gohin@polytechnique.edu
- Physique de la Matière Condensée, Ecole Polytechnique, CNRS
  Palaiseau 91128, France

Maria J. Gomes
mjesus@fisica.uminho.pt
- University of Minho (UM)
  Campus de Gualtar, Braga 4710057, Portugal

Gonçalo Gonçalves
gpg@fct.unl.pt
- Materials Science Department, CENIMAT-IxN and CEMOP-UNINOVA, FCT-UNL
  Campus da Caparica, Caparica, Caparica 2829-516, Portugal

Agustin R. González-Elipe
arge@icmse.csic.es
- Instituto de Ciencia de Materiales de Sevilla (ICMSE)
  Avda. Americo Vespucio, 49, Sevilla 41092, Spain

Krzysztof M. Górny
kgorny@us.edu.pl
- University of Silesia, Institute of Physics
  Uniwersytecka 4, Katowice 40-007, Poland

Tomasz Goryczka
goryczka@us.edu.pl
- University of Silesia, Institute of Materials Science
  12, Bankowa Str., Katowice 40-007, Poland

Roland Goschke
goschke@atomicforce.de
- ATOMIC FORCE GmbH
  Hauptstrasse 161, Mannheim 68-259, Germany

Christine Goyhenex
goyhenex@ipcms.u-strasbg.fr
- Institut de Physique et Chimie des Materiaux de Strasbourg, UMR7504, CNRS - ULP
  23, rue du Loess, BP 43, Strasbourg CEDEX 2 67034, France

Jacek D. Grabarczyk
jacek.grabarczyk@p.lodz.pl
- Technical University of Lodz, Institute of Materials Science and Engineering
  1/15 Stefanowskiego, Łódź 90-924, Poland

Salvatore Grasso
GRASSO.Salvatore@nims.go.jp
- NIMS National Institute for Material Science (NIMS)
  Ibaraki 305-0047, Japan, Tukuba 3050047, Japan

Thomas J. Graule
thomas.graule@empa.ch
- Empa, Swiss Federal Laboratories for Materials Testing and Research, High Performance Ceramics
  Ueberlandstrasse 129, Dübendorf 8600, Switzerland

Eva Gregorová
eva.gregorova@vscht.cz
- Institute of Chemical Technology (VSCHT)
  Technicka 5, Prague 16628, Czech Republic

Anastasia V. Grigorieva
anastasia@inorg.chem.msu.ru
- M.V. Lomonosov Moscow State University
  Vorobyevy gory, Moscow 119992, Russian Federation

Larisa Grigorjeva
lgrig@latnet.lv
- Institute of Solid State Physics, University of Latvia
  8 Kengaraga, Riga LV-1063, Latvia

Kacper Grodecki
kgrod@tlen.pl
- Uniwersytet Warszawski, Wydział Fizyki
  ul. Pasteura 7, Warszawa 02-093, Poland
- Institute of Electronic Materials Technology (ITME)
  Warszawa 01919, Poland

Valentina Grossi
valentina.grossi@aquila.infn.it
- Università dell'Aquila, Dipartimento di Fisica
  Via Vetoio, L'Aquila I-67010, Italy

Michael Grünwald
michael.gruenwald@univie.ac.at
- University of Vienna, Faculty of Physics
  Boltzmanngasse 5, Wien 1090, Austria

Fabien Guillemot
fabien.guillemot@inserm.fr
- Laboratoire de biomatériaux et réparation tissulaire
  Université Victor Segalen Bordeaux 2, case postale 45, 146 rue Léo-Saignat, Bordeaux 33076, France

Georgy V. Gursky
gursky@eimb.ru
- Engelhardt Institute of Molecular Biology RAS (EIMB)
  Vavilova 32, Moscow 119991, Russian Federation

Katarzyna Gutowska
gutka@inmat.pw.edu.pl
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

Daniel Guyomar
daniel.guyomar@insa-lyon.fr
- LGEF-INSA-Lyon
  8 rue de la physique, Lyon 69621, France

Amir Habib
amir.habib@arcs.ac.at
- Austrian Research Centers GmbH (ARC)
  Wien 2444, Austria

Branka Hadzic
branka@phy.bg.ac.yu
- Institute of Physics (IF)
  Pregrevica 118, Belgrade 11080, Serbia

Shabnam Hajiesmaili
shabnam.hajesmaili@gmail.com
- CNRS, ULP, Laboratoire des Matériaux, Surfaces et Procédés pour la Catalyse (LMSPC)
  25 rue Becquerel, Strasbourg 67087, France

Amer Hakki
amerhakki@iftc.uni-hannover.de
- Leibniz University Hannover, Institute of Technical Chemistry
  Callinstrasse 3, Hannover 30167, Germany

Maria Hammer
maria.hammer@physik.uni-wuerzburg.de
- University of Würzburg, Experimental Physics VI
  Am Hubland, Würzburg 97074, Germany

Won Suk Han
wshan1@skku.edu
- School of Advanced Materials Science and Engineering Sungkyunkwan University (SKKU)
  300 Cheoncheon-dong, Jangan-gu, Suwon, Suwon 440-746, Korea, South

Mohammad M. Haque
masuqul2003@yahoo.com
- Kyungpook National University (KNU)
  Daegu 702-701, Korea, South

Lothar A. Heinrich
Lothar.Heinrich@marcotech.de
- HiNanoAnalytics Network
  Heisenbergstasse 11, Münster 48149, Germany

Marcin K. Heljak
marcin.heljak@gmail.com
- Faculty of Materials Science and Engineering
  Woloska, Warsaw 02-507, Poland
- Queensland University of Technology (QUT)
  Queensland 4001, Australia

Ernie W. Hill
e.w.hill@manchester.ac.uk
- The University of Manchester, Centre for Mesoscience and Nanotechnology (CMN)
  Oxford Road, Manchester M13-9PL, United Kingdom

Masahiro Hirano
m-hirano@lucid.msl.titech.ac.jp
- Tokyo Institute of Technology (TIT)
  Ookayama, Meguro-ku, Tokyo, Tokyo 152-8550, Japan

Alexeys Hmelovs
ahmelov@ktf.rtu.lv
- RTU, SMI
Riga, Azenes str. 14/24, Riga LV-1048, Latvia

Jean-Francois Hochepied
hochepied@ensmp.fr
- Laboratoire de Systemes Colloidaux dans le Processus Industriels (SCPI), Ecole des Mines de Paris
Paris F - 75272, France

Goetz Hoffmann
m.schaefer@schaefer-tec.com
- Schaefer Technologie GmbH
Morfelder Landstrasse 33, Langen 63225, Germany

Jan Holnicki-Szulc
holnicki@ippt.gov.pl
- Polish Academy of Sciences, Institute of Fundamental Technological Research (IPPT PAN)
Świętokrzyska 21, Warszawa 00-049, Poland

Hadi Hosseinzadegan
hadiinfo@ieee.org
- University of Tehran (UT)
North-Kargar, Tehran 14395-731, Iran

Gabriela Hristea
ghristea@icpe-ca.ro
- ICPE-CA-Bucharest
313 Splaiul Unirii, Bucharest 74204, Romania

Tung-Ching Huang
htc.eo92g@nctu.edu.tw
- Department of Photonics, Institute of Electro-Optical Engineering, National Chiao Tung Univ
Hsinchu 30050, Taiwan

Cs Hwang
hwang-cs@etri.re.kr
- Electronics and Telecommunication Research Institute (ETRI)
161 Gajeong-Dong, Daejeon 305-350, Korea, South

Iuliia V. Iermolaieva
yermolayeva@isc.kharkov.ua
- Institute for Single Crystals NAS of Ukraine (ISC)
60 Lenin Ave., Kharkov 61001, Ukraine

Milko N. Iliev
miliev@uh.edu
- University of Houston, Texas Center for Superconductivity and Advanced Materials
Houston, TX 77204, United States

Henning Immink
immink@uni-bonn.de
- Univ.Bonn
Bonn, Germany

Mariella Ippolito
m.ippolito@caspur.it
- CASPUR
via dei Tizii 6b, Roma 00185, Italy

Nataly V. Isaeva
Felix-2001@mail.ru
- Moscow State Academy of Fine Chemical Tecnology by M. V. Lomonosov
Vernadskogo pr., 86, Moscow 119571, Russian Federation

Masashi Ishii
ISHII.Masashi@nims.go.jp
- National Institute for Materials Science (NIMS)
1-2-1 Sengen, Tsukuba 305-0047, Japan

Simona Ispas
simona.ispas@lcvn.univ-montp2.fr
- Laboratoire des Colloides, Verres et Nanomateriaux, Univ Montpellier II (LCVN)
Place Eugene Bataillon, Montpellier 34095, France

Manabu Ito
manabu.ito@toppan.co.jp
- Toppan Printing Co., Ltd
4-2-3 Takanodai-Minami, Sugito, Saitama 345-8508, Japan

Mile Ivanda
ivanda@irb.hr
- Ruđer Bošković Institute
Bijenička 54, Zagreb 10000, Croatia

Tatjana Ivanova
zicans@ktf.rtu.lv
- Riga Technical University (RTU)
Azenes St. 14/24, Riga LV-1048, Latvia

Radoslaw M. Iwankiewicz
iwankiewicz@tuhh.de
- Technical University Hamburg-Harburg (TUHH)
Denickestr. 15, Hamburg 21073, Germany

Ali Jaafar
ali.jaafar@ipcms.u-strasbg.fr
- Institut de Physique et Chimie des Materiaux de Strasbourg, UMR7504, CNRS - ULP
23, rue du Loess, BP 43, Strasbourg CEDEX 2 67034, France

Zbigniew Jaegermann
bioceramika@neostrada.pl
- Institute of Glass, Ceramics, Refractory and Construction Materials (ISC)
  Postepu 9, Warszawa 02-676, Poland

Janusz Jaglarz
pujaglar@cyfronet.krakow.pl
- Cracow University of Technology, Institute of Physics (PK)
  Podchorążych 1, Kraków 30-084, Poland

Ignacy Jakubowicz
ignacy.jakubowicz@sp.se
- SP Technical Research Institute of Sweden (SP)
  Brinellgatan 4, Boras 50115, Sweden

Izabela M. Janowska
izabela.janowska@ecpm.u-strasbg.fr
- Euroepan Laboratory for Catalysis and Surface Sciences, ELCASS (CNRS-ULP)
  25 rue Becquerel, Strasbourg 67087, France

Tomasz Jaroszewicz
t_jaroszewicz@o2.pl
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

Marcin Jedyński
jedynski@ippt.gov.pl
- Military University of Technology, Institute of Optoelectronics (IOE)
  Kaliskiego 2, Warszawa 00-908, Poland

Arockia Vimal Jeyaseelan
vimal.arockia@tyndall.ie
- University College Cork, Tyndall National Institute (TYNDALL)
  Lee Maltings, Prospect Row, Cork, Ireland

Jose Jimenez Jimenez
jjimenez@uma.es
- Universidad de Malaga (UMA)
  Campus Teatinos, Malaga E29071, Spain

Melanie Johnson
mel.johnson@ualberta.ca
- University of Alberta (U of A)
  ECERF, University of Alberta, Edmonton T6G 2V4, Canada

Đorđe M. Jovanović
djordje@phy.bg.ac.yu
- Institute of Physics (IF)
  Pregrevica 118, Belgrade 11080, Serbia

Jarosław Judek
jerryj@if.pw.edu.pl
- Warsaw University of Technology, Faculty of Physics
  Koszykowa 75, Warszawa 00-662, Poland
- Institut d'Electronique, de Microélectronique et de Nanotechnologie (IEMN)
  cité scientifique, Lille 59655, France

Stefan Jurga
stjurga@amu.edu.pl
- Macromolecular Physics Department, Faculty of Physics, Adam Mickiewicz University (AMU)
  Umultowska 85, Poznań 61-614, Poland

Ali Kachmar
kachmar@quantix.u-strasbg.fr
- Institut de Chimie (CNRS/ULP)
  4, rue Blaise Pascal, Strasbourg 67000, France
- Institut de Physique et Chimie des Materiaux de Strasbourg, UMR7504, CNRS - ULP
  23, rue du Loess, BP 43, Strasbourg CEDEX 2 67034, France

Michał Kaczmarek
michal.kaczmarek@fh-muenster.de
- Fachhochschule Muenster
  Stegerwaldstrasse 39, Münster 48565, Germany

Rafal Kajka
rafal.kajka@ilot.edu.pl
- Instytut Lotnictwa (ILOT)
  Al. Krakowska 110/114, Warszawa 02-256, Poland

Jerzy Kaleta
pawel.gasior@pwr.wroc.pl
- Politechnika Wrocławska (PWR)
  Wybrzeże Wyspiańskiego, Wrocław 50-370, Poland

Beata Kalska-Szostko
kalska@uwb.edu.pl
- University of Białystok, Institute of Chemistry
  Hurtowa 1, Białystok 15-399, Poland

Eliana Kamińska
eliana@ite.waw.pl
- Instytut Technologii Elektronowej (ITE)
  al. Lotników 32/46, Warszawa 02-668, Poland
- Polish Academy of Sciences, Institute of Physics
  al. Lotników 32/46, Warszawa 02-668, Poland
- Institute of Molecular Physics, Polish Academy of Sciences
  Smoluchowskiego 17, Poznań 60-179, Poland

Weekyung Kang
wkang@ssu.ac.kr
- Dept. of Chemistry, Soongsil University
  511, Sangdo-dong, Dongjak-ku, Seoul 156-743, Korea, South

Svetlana Karitskaya
sv.karitskaya@rambler.ru
- Urals State Technical University (USTU-UPI)
  Mira,19, Ekaterinburg 620002, Russian Federation

Małgorzata Karolus
karolus@us.edu.pl
- University of Silesia, Institute of Material Science
  Bankowa 12, Katowice 40-007, Poland

Jarosław Kaszewski
jaroslavuss@wp.pl
- Szczecin University of Technology, Institute of Chemical and Environment Engineering
  Szczecin 70-322, Poland

Grzegorz Kaszyński
kaszynski@ight.com.pl
- IGHT s.c.
  Marszałkowska 80, Warszawa 00-517, Poland

Takayoshi Katase
katase@lucid.msl.titech.ac.jp
- Materials and Structures Laboratory, Tokyo Institute of Technology (TOKYOTECH)
  R3-1, 4259 Nagatsuta, Midori-ku, Yokohama, JAPAN, Kanagawa 226-8503, Japan
- Japan Science and Technology Agency, Tokyo Institute of Technology (JST)
  R3-1, 4259 Nagatsuta, Midori-ku, Yokohama, Kanagawa 226-8503, Japan
- Garaduate School of Enginnering, Nagoya University (NAGOYAU)
  Nagoya university, Furo-cyo, Chikusa-ku, Nagoya, Japan, Nagoya 464-8603, Japan
- Frontier Reserch Center, Tokyo Institute of Technology (FRC)
  R3-1, 4259 Nagatsuta, Midori-ku, Yokohama, Kanagawa 226-8503, Japan

Nicolas Keller
nkeller@chimie.u-strasbg.fr
- CNRS, ULP, Laboratoire des Matériaux, Surfaces et Procédés pour la Catalyse (LMSPC)
  25 rue Becquerel, Strasbourg 67087, France

Valérie Keller-Spitzer
vkeller@chimie.u-strasbg.fr
- CNRS, ULP, Laboratoire des Matériaux, Surfaces et Procédés pour la Catalyse (LMSPC)
  25 rue Becquerel, Strasbourg 67087, France

Krzysztof Kempa
kempa@bc.edu
- Boston College (BC)
  Chestnut Hill, Boston, MA 02467, United States

Tamara Kharlamova
kharlamova@catalysis.ru
- Boreskov Institute of Catalysis (BIC)
  pr. akad. Lavrentieva, 5, Novosibirsk 630090, Russian Federation

Igor V. Khobta
hobta_igor@ipms.kiev.ua
- Institute for Problems of Materials Science
  3, Krzhizhanovsky, Kyiv 03142, Ukraine

Wolfgang Kiefer
wolfgang.kiefer@mail.uni-wuerzburg.de
- Institut für Physikalische Chemie
  Am Hubland, Würzburg 97074, Germany

Ewa Kijeńska
ewakijenska@gmail.com
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

Konstantin Kikoin
konstk@post.tau.ac.il
- Tel Aviv University (TAU)
  Ramat Aviv, Tel Aviv 69787, Israel

Dong-Kuk Kim
kimdk@knu.ac.kr
- Kyungpook National University, Department of Chemistry
  Daegu 702-701, Korea, South

Dong Wook Kim
dong0414@snu.ac.kr
- Seoul National University, Department of Materials Science and Engineering (MSE, SNU)
  San 56-1, Sillim-dong, Gwanak-gu, Seoul 151-744, Korea, South

Hyo Sung Kim
hyosunglove@hanmail.net
- Inha University, School of Materials science and engineering
  253 Yong Hyun Dong, Nam Ku, Incheon 402-751, Korea, South

Jun Tak Kim
taks@kut.ac.kr
- Korea University of Technology and Education
  Cheonan 330-708, Korea, South

Kyungrae Kim
kr0314@ssu.ac.kr
- Soongsil University, Depr. of Chemistry
  511, Sangdo-dong, Dongjak-ku, Seoul 156-743, Korea, South

Giora Kimmel
kimmel@bgu.ac.il

- Institutes for Applied Research, Ben Gurion University of the Negev
  Beer-Sheva 84105, Israel
- Universitat Rovira i Virgili (URV)
  Av. Països Catalans, 26, Tarragona 43007, Spain

Sang Ho Kim
shkim@kut.ac.kr

- Korea University of Technology and Education
  Cheonan 330-708, Korea, South

Tae ok Kim
koeugeun@kimm.re.kr

- Korea Institute of Machinery and Materials (KIMM)
  Busan 305-343, Korea, South
- School of Mechanical Engineering Pusan National University
  Busan 607-735, Korea, South

George Kiriakidis
kiriakid@iesl.forth.gr

- PEML IESL (FORTH)
  100, N. Plastira str, Heraklion 70013, Greece
- Physics Dpt, Univ. of Crete
  PO Box 1527, Heraklion 71409, Greece

Aneta Kisielewska
anetailik@uni.lodz.pl

- University of Łódź, Department of Chemical Technology and Environmental Protection
  Pomorska 163, Łódź 90-236, Poland

Masaaki Kitano
hp_kitano@newkast.or.jp

- Kanagawa Academy of Science and Technology (KAST)
  3-2-1 Sakado, Takatsu-ku, Kawasaki 213-0012, Japan

Ulrich Kneser
ulrich.kneser@uk-erlangen.de

- University Erlangen
  Erlangen 91054, Germany

Erich Kny
erich.kny@arcs.ac.at

- Austrian Research Centers Seibersdorf (ARCS)
  Seibersdorf A-2444, Austria

Hisatoshi Kobayashi
kobayashi.hisatoshi@nims.go.jp

- National Institute for Materials Science (NIMS)
  1-2-1 Sengen, Tsukuba 305-0047, Japan

Joachim H. Koehler
joachim.koehler@uni-ulm.de

- Ulm University
  Albert-Einstein-Allee 47, Ulm 89081, Germany

Wim Koelewijn
wkoelewijn@scanco.ch

- Scanco Medical AG
  Fabrikweg 2, Bruettisellen 8306, Switzerland

Hyejin Ko
tototo24@naver.com

- Kyunghee university (KHU)
  Suwon 449-701, Korea, South

Justyna Kokoszka
j.kokoszka@poczta.fm

- AGH University of Science and Technology, Faculty of Materials Science and Ceramics (AGH UST)
  Mickiewicza 30, Kraków 30-059, Poland

Aleksandra Kolano-Burian
olak@imn.gliwice.pl

- Institute of Nonferrous Metals
  Sowińskiego 5, Gliwice 44-100, Poland

Irina V. Kolesnik
kolesnik@inorg.chem.msu.ru

- Faculty of Materials Science, Moscow State University
  Lenin Hills, Moscow 119992, Russian Federation

Nataliia Konig
sem_kob@ipms.kiev.ua

- Institute for Problems of Materials Science, National Academy of Sciences of Ukraine
  Krzizanovsky, Kyiv 38(044), Ukraine

Katarzyna Konopka
kako@inmat.pw.edu.pl

- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

Milan J. Konstantinovic
mkonstan@sckcen.be

- Belgian Nuclear Research Centre-Centre d'Etude de l'Energie nucléaire (SCKCEN)
  Boeretang 200, Mol 2400, Belgium

Javad Koohsorkhi
javadkoohsorkhi@yahoo.com

- University of Tehran (UT)
  North-Kargar, Tehran 14395-731, Iran

Jari J. Koskinen
jari.koskinen@vtt.fi

- VTT (VTT)
  Biologinkuja 7, Otaniemi, Espoo 02044, Finland

Marek Kostecki
mkostecki@meil.pw.edu.pl
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
Wołoska 141, Warszawa 02-507, Poland

Radmila Kostic
radmila.kostic@phy.bg.ac.yu
- Institute of Physics (IF)
Pregrevica 118, Belgrade 11080, Serbia

Mariya H. Kostova
mariya.kostova@ww.uni-erlangen.de
- University of Erlangen-Nürnberg, Glass and Ceramics
Martenstr.5, Erlangen 91058, Germany

Gerasimos A. Kourouklis
gak@gen.auth.gr
- General Department of Physics and Mathematics, Polytechnic School, Aristotle University of Thessaloniki, GR-54124 Thessaloniki, Greece
Thessaloniki GR-54124, Greece

Agnieszka Kowalczyk
hoch@lot-oriel.de
- L.O.T. Oriel
Im Tiefen See 58, Darmstadt 64293, Germany

Bożena Koziarska-Glinka
inbox@eurotek.com.pl
- EUROTEK INTERNATIONAL
Al. Lotników 32/46, Warsaw 02-668, Poland

Larisa E. Kozlova
kozlova@imag.kiev.ua
- Institute of Magnetism, NAS of Ukraine
36-B Vernadsky str., Kiev 03142, Ukraine

Rafal Kozubski
rafal.kozubski@uj.edu.pl
- Jagiellonian University, Institute of Physics (IF UJ)
Reymonta 4, Kraków 30-059, Poland

Artem Kozyrev
kozyrev-a@list.ru
- V. Bakul Institute for Superhard Materials NAS of Ukraine
2, Autozavodska str., Kiev 04074, Ukraine

Carl E. Krill III
carl.krill@uni-ulm.de
- Ulm University, Institute of Micro and Nanomaterials
Albert-Einstein-Allee 47, Ulm 89081, Germany

Michael Krisch
krisch@esrf.fr
- European Synchrotron Radiation Facility
Grenoble, France

Maciej Krystian
maciej.krystian@arcs.ac.at
- Austrian Research Centers Seibersdorf (ARCS)
Seibersdorf A-2444, Austria

Oleksandra S. Kryzhanovska
alexkryzh@isc.kharkov.ua
- Institute for Single Crystals NAS of Ukraine (ISC)
60 Lenin Ave., Kharkov 61001, Ukraine

Hanna J. Krztoń
hkrzton@imz.pl
- Institute for Ferrous Metallurgy (IMZ)
Karola Miarki, Gliwice 44-100, Poland

Martyna A. Kucharska
kucharska@ichip.pw.edu.pl
- Warsaw University of Technology, Faculty of Chemical and Process Engineering
L.waryńskiego 1, Warszawa 00-645, Poland

Andrzej Kudelski
akudel@chem.uw.edu.pl
- University of Warsaw, Department of Chemistry
Pasteura 1, Warsaw, Warszawa 02-093, Poland

Alexey V. Kulik
alexey.v.kulik@gmail.com
- Baltic State Technical University (BSTU)
1st Krasnoarmeyskaya st. 1, Saint-Petersburg 190005, Russian Federation

Victor I. Kulik
victor.i.kulik@gmail.com
- Baltic State Technical University (BSTU)
1st Krasnoarmeyskaya st. 1, Saint-Petersburg 190005, Russian Federation

Sumeet Kumar
sumeet.kumar.iitk@gmail.com
- Università degli Studi del Piemonte Orientale (DISTA)
Via V. Bellini 25/G., Alessandria 15100, Italy

Hideya Kumomi
kumomi.hideya@canon.co.jp
- Canon Inc.
3-30-2 Shimomaruko, Ohta-ku, Tokyo 146-8501, Japan

Izabela S. Kunce
iza_kunce@tlen.pl
- Military University of Technology, Faculty of Advanced Technology and Chemistry
  Kaliskiego 2, Warszawa 00-908, Poland

Dominik Kurzydłowski
d.kurzydlowski@student.uw.edu.pl
- Uniwersytet Warszawski, Wydział Chemii
  Warszawa, Poland

Krzysztof J. Kurzydlowski
kjk@inmat.pw.edu.pl
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

Tomasz Kurzynowski
tomasz.kurzynowski@pwr.wroc.pl
- Politechnika Wrocławska (PWR)
  Wybrzeże Wyspiańskiego, Wrocław 50-370, Poland

Magdalena Kwiatkowska
magdalena.kwiatkowska@ps.pl
- Szczecin University of Technology, Institute of Materials Science and Engineering
  Piastow 19, Szczecin 70-310, Poland

Olha Kyryliv
okyryliv@yahoo.com
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

Sergij M. Lakiza
sergij_lakiza@ukr.net
- Institute for Problems of Materials Science, National Academy of Sciences of Ukraine
  Krzizanovsky, Kyiv 38(044), Ukraine

Holger Lange
holger.lange@physik.tu-berlin.de
- Institut für Festkörperphysik, TU Berlin
  Hardenbergstr. 36, Berlin 10623, Germany

Tetyana V. Laptyeva
lapteva@mail.fti.ac.donetsk.ua
- National Academy of Sciences of Ukraine, A.Galkin Donetsk Institute for Physics & Technology (DonPTI NASU)
  Roza Luxemburg 72, Donetsk 83114, Ukraine

Hon Kit Lau
ckcklau@gmail.com
- The Hong Kong Polytechnic University (HK, PolyU)
  Hung Hom, Hong Kong, Hong Kong

Siew H. Lau
shlau@xradia.com
- Xradia Inc
  5052 Commercial Circle, Concord 94520, United States

Nenad Ž. Lazarević
nesalazarevic@gmail.com
- Institute of Physics (IF)
  Pregrevica 118, Belgrade 11080, Serbia

Zorica Lazarevic
Zorica.lazarevic@phy.bg.ac.yu
- Institute of Physics (IF)
  Pregrevica 118, Belgrade 11080, Serbia

Laurent A. Lebrun
laurent.lebrun@insa-lyon.fr
- INSA Lyon LGEF (INSALGEF)
  8 rue de la Physique, Villeurbanne 69621, France

Marc J. Ledoux
ledoux@ecpm.u-strasbg.fr
- European Laboratory for Catalysis and Surface Sciences, ELCASS (CNRS-ULP)
  25 rue Becquerel, Strasbourg 67087, France

Ji Eun Lee
happyching@hanmail.net
- Kyungpook National University, Department of Chemistry
  Daegu 702-701, Korea, South

Ki-Rim Lee
kirimi84@gmail.com
- Sungkyunkwan University, Institute of Basic Science, Department of Chemistry
  300 ChunChun-dong JangAn-Gu, Suwon 440-746, Korea, South

Jozef Lelatko
jlelatko@us.edu.pl
- University of Silesia, Institute of Material Science
  Bankowa 12, Katowice 40-007, Poland

Monika Lelonek
monika.lelonek@marcotech.de
- HiNanoAnalytics Network
  Heisenbergstasse 11, Münster 48149, Germany

Peter Lemmens
p.lemmens@tu-bs.de
- Inst. Condensed Matter Physics (IPKM)
  Mendelssohnstr. 3, Braunschweig 38108, Germany

Marcin K. Leonowicz
mkl@inmat.pw.edu.pl
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
Wołoska 141, Warszawa 02-507, Poland

Christophe Le pen
christophe.lepen@arcelormittal.com
- ARCELORMITTAL Liege research and development
Bd de colonster, B57, Liège 4000, Belgium

Ed Lester
edward.lester@nottingham.ac.uk
- University of Nottingham
Nottingham, United Kingdom

Elena V. Levchenko
elena.levchenko@newcastle.edu.au
- The University of Newcastle
University Drive, Newcastle 2308, Australia

Tetyana Levchenko
levchtat@i.com.ua
- Institute of Surface Chemistry NAS of Ukraine
17 General Naumov, Kyiv 03164, Ukraine

Malgorzata Lewandowska
malew@inmat.pw.edu.pl
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
Wołoska 141, Warszawa 02-507, Poland

Renata Lewandowska
renata.lewandowska@jobinyvon.fr
- Horiba Jobin Yvon
Rue de Lille, Villeneuve d'Ascq 59650, France

Małgorzata Lewandowska-Szumieł
mszumiel@ib.amwaw.edu.pl
- Medical University of Warsaw, Department of Biophysics and Human Physiology
Chałubińskiego 5, Warszawa 02-004, Poland

Daniel Lewandowski
daniel.lewandowski@pwr.wroc.pl
- Wroclaw University of Technology, Institute of Materials Science and Applied Mechanics (PWr - IMMT)
Smoluchowskiego 25, Wrocław 50-370, Poland

Efthymios P. Liarokapis
eliaro@central.ntua.gr
- National Technical University of Athens (NTUA)
Heroon Polytechneiou 9, Athens 157 80, Greece

Kuo-Feng Lin
xia117.eo94g@nctu.edu.tw
- Department of Photonics, Institute of Electro-Optical Engineering, National Chiao Tung Univ
Hsinchu 30050, Taiwan

Chia-Chang Liu
lcceric90@yahoo.com.tw
- National Yang Ming University
Taipei 112-21, Taiwan

Wai Kit Li
07900613r@polyu.edu.hk
- Department of Applied Physics and Materials Research Centre,The Hong Kong Polytechnic University
Hung Hom, Kowloon, Hong Kong 00-852, China

Jose-Manuel Lloris
manolo.lloris@aidico.es
- Asociación Investigación Industrias de Construcción (AIDICO)
Parque Tecnológico Valencia, Valencia 46980, Spain

Mariajose López-Tendero
mlopezt@aidico.es
- Asociación Investigación Industrias de Construcción (AIDICO)
Parque Tecnológico Valencia, Valencia 46980, Spain

Heinrich Lothar
monika.lelonek@marcotech.de
- HiNanoAnalytics Network
Heisenbergstasse 11, Münster 48149, Germany

Nelson Lou
nelson@cemes.fr
- CEMES-CNRS (CEMES-CNRS)
29, rue Jeanne Marvig, Toulouse F31055, France

Guy Lucazeau
guy.lucazeau@lepmi.inpg.fr
- Grenoble Institute of Technology, Laboratoire d'électrochimie et de physicochimie des matériaux (LEPMI-CNRS)
1130 rue de la piscine BP75, Grenoble 38402, France

Nikolay Lyakhov
lyakhov@solis.nsc.ru
- Institute for Solid State and Mechanical Chemistry of RAS
Novosibirsk 630090, Russian Federation

Viktor Lyashenko
gasta1@yandex.ru
- Kremenchuk State Polytechnical University
Kremenchuk, Ukraine

Mirosław Mączka
m.maczka@int.pan.wroc.pl
- Institute of Low Temperature and Structure Research, Polish Academy of Sciences
  P.Ne 1410, Wrocław 50-950, Poland

Siavash Mahdavi
sia@complexmatters.com
- University College London (UCL)
  20 Gordon Street, London WC1H, United Kingdom

Sayani Majumdar
sayani.majumdar@utu.fi
- Abo Akademi University, Department of Physics
  Porthansgatan 3, Turku 20500, Finland
- Wihuri Physical Laboratory, University of Turku (UTU)
  Vesilinnantie 5, Turku 20014, Finland

Malgorzata Makowska-Janusik
m.makowska@ajd.czest.pl
- Institute of Physics, Jan Dlugosz University
  Al. Armii Krajowej 13/15, Częstochowa 42200, Poland

Philippe Makowski
philippe.makowski@mpikg.mpg.de
- Max Planck Institute of Colloids and Interfaces (MPIKGF)
  Research Campus Golm, Potsdam 14424, Germany

Przemyslaw Malinowski
malin77@o2.pl
- Warsaw University, Faculty of Chemistry
  Pasteura 1, Warszawa 02-093, Poland

Iwona E. Malka
imalka@wat.edu.pl
- Military University of Technology, Faculty of Advanced Technology and Chemistry
  Kaliskiego 2, Warszawa 00-908, Poland

Corrado Mandoli
corrado.mandoli@uniroma2.it
- Universita di Roma 'Tor Vergata'
  Roma 00133, Italy

Sellaperumal Manivannan
ksmaniphysics@yahoo.com
- Kyung Hee University
  Dongdaemoon-Ku, Seoul 130-701, Korea, South

Inderchand Manjubala
i.manjubala@mpikg.mpg.de
- Max Planck Institute of Colloids and Interfaces (MPIKGF)
  Research Campus Golm, Potsdam 14424, Germany

Eric Marceau
eric.marceau@upmc.fr
- Laboratoire de réactivité de Surface, CNRS UPMC (LRS)
  4 place Jussieu, casier 178, Paris 75252, France

Augusto Marcelli
marcelli@lnf.infn.it
- °Laboratori Nazionali Frascati INFN (INFN)
  Via E. Fermi 40, Frascati 00044, Italy

Michał Marchewka
marmi@univ.rzeszow.pl
- University of Rzeszow
  Rejtana 16 A, Rzeszów 35-310, Poland

Aurelian Marcu
marcu@ifin.nipne.ro
- National Institute for Lasers Plasma and Radiation Physics (INFLPR)
  Atomistilor 111, Bucharest -, Romania

Marcin Marczak
mm@if.pw.edu.pl
- Warsaw University of Technology, Faculty of Physics
  Koszykowa 75, Warszawa 00-662, Poland
- Institut d'Electronique de Microelectronique et de Nanotechnologie, UMR CNRS 8520 (IEMN)
  BP 60069 - Cité scientifique-avenue Poincaré, Villeneuve d'Ascq 59652 Cedex, France

Michele Marrocco
michele.marrocco@casaccia.enea.it
- ENEA
  via Anguillarese 301, Roma 00123, Italy

Rodrigo F. Martins
rm@uninova.pt
- Centro de Investigacao em Materiais (CENIMAT/ Fac)
  Campus Caparica, Caparica 2829-516, Portugal

Steve Martin
steve.martin@cea.fr
- CEA (LITEN)
  17 rue des Martyrs, Grenoble 38054, France

Marcin Masłowski
m.maslowski@poczta.onet.pl
- Technical University of Łódź, Faculty of Chemistry, Institute of Polymer and Dye Technology (PŁ)
  Stefanowskiego 12/16, Łódź 90-924, Poland

Carlo Massobrio
Carlo.Massobrio@ipcms.u-strasbg.fr
- Institut de Physique et Chimie des Materiaux de Strasbourg, UMR7504, CNRS - ULP
  23, rue du Loess, BP 43, Strasbourg CEDEX 2 67034, France

Masahiko Matsubara
Masahiko.Matsubara@LCVN.univ-montp2.fr
- Université Montpellier II, Laboratoire des Colloïdes, Verres et Nanomatériaux (LCVN)
  place Eugène Bataillon, Montpellier 34095, France

Kosuke Matsuzaki
matsuzaki@lucid.msl.titech.ac.jp
- Materials and Structures Laboratory, Tokyo Institute of Technology
  Mailbox R3-1, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan

Alessandro Mattoni
alessandro.mattoni@dsf.unica.it
- CNR-INFM SLACS and Dipartimento di Fisica, Università di Cagliari
  Cittadella Universitaria, Monserrato (Cagliari) I-09042, Italy

Wojciech Maziarz
nmmaziar@imim-pan.krakow.pl
- Polish Academy of Sciences, Institute of Metallurgy and Materials Sciences (IMIM PAN)
  Reymonta 25, Kraków 30-059, Poland

Saiful A. Mazlan
saiful.mazlan2@mail.dcu.ie
- School of Mechanical and Manufacturing Engineering, Dublin City University
  Dublin Dublin9, Ireland

Jose Menendez
jose.menendez@asu.edu
- Arizona State University, Department of Physics and Astronomy
  Tempe, AZ 85287-1504, United States

Sebastien Mercier
mercier@lpmm.univ-metz.fr
- Laboratoire de Physique et de mécanique des matériaux, UMR CNRS 7554 (LPMM)
  Ile du Saulcy, Metz 57045, France

Remo Merijs Meri
zicans@ktf.rtu.lv
- Riga Technical University (RTU)
  Azenes St. 14/24, Riga LV-1048, Latvia

Alexander G. Milekhin
milekhin@thermo.isp.nsc.ru
- Institute of Semiconductor Physics SB RAS
  Lavrentjeva 13, Novosibirsk 630090, Russian Federation

Donats Millers
dmillers@latnet.lv
- Institute of Solid State Physics, University of Latvia
  8 Kengaraga, Riga LV-1063, Latvia

Seiichi Miyazaki
semiya@hiroshima-u.ac.jp
- Hiroshima University, Graduate School of Advanced Sciences of Matter (HU-ADSM)
  Higashi-Hiroshima 1-3-1, Higashi-Hiroshima 739-8530, Japan

Adnen Mlayah
Adnen.Mlayah@cemes.fr
- CEMES-CNRS (CEMES-CNRS)
  29, rue Jeanne Marvig, Toulouse F31055, France

Nuru R. Mlyuka
nmlyuka@yahoo.com
- Uppsala University, Department of Engineering Sciences, The Angstrom Laboratory
  Uppsala SE-75121, Sweden
- University of Dar es Salaam, Physics Department
  Dar es Salaam 35063, Tanzania

Maryla Moczulska
maryla.moczulska@gmail.com
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland
- EMPA, Materials Science and Technology, Laboratory for Advanced Fibers
  Lerchenfeldstrasse 5, St.Gallen 9014, Switzerland

Mircea Modreanu
mircea.modreanu@tyndall.ie
- University College Cork, Tyndall National Institute (TYNDALL)
  Lee Maltings, Prospect Row, Cork, Ireland

Carmen Moldovan
carmen.moldovan@imt.ro
- National Institute for Research and development in Microtechnologies (IMT-Buchares)
  P.O.Box 38-160, Bucharest 023573, Romania

Carla Molteni
carla.molteni@kcl.ac.uk
- King's College London (KCL)
  Strand, London WC2R2LS, United Kingdom

Karine Molvinger
karine.molvinger@enscm.fr
- Institut Charles Gerhardt
  CC15, Place eugène Bataillon, Montpellier 34095, France

Francesco Montalenti
francesco.montalenti@unimib.it
- University of Milano-Bicocca, Department of Materials Science
  via Cozzi 53, Milano 20125, Italy

Henryk Morawiec
morawiec@us.edu.pl
- University of Silesia, Institute of Materials Science
  12, Bankowa Str., Katowice 40-007, Poland

Rodrigo Moreno
rmoreno@icv.csic.es
- Consejo Superior de Investigaciones Cientificas ICV (ICV-CSIC)
  Kelsen nº5, Madrid 28049, Spain

Karina Morgenstern
morgenstern@fkp.uni-hannover.de
- Universität Hannover, Institut für Festkörperphysik (FKP)
  Appelstrasse 2, Hannover D-30167, Germany

Kiyotaka Mori
kiyotaka.mori@eu.panasonic.com
- Panasonic
  Cambridge CB30GL, United Kingdom

Aziz Moro
ginternazionale@yahoo.com
- University of Johannesburg
  Kingsway, Johannesburg 2006, South Africa

Olga Morozova
om@polymer.chph.ras.ru
- Institute of Chemical Physics RAS (ICP)
  Kosygin St., 4, Moscow 119991, Russian Federation

Ignacy Mościcki
moscicki@ntinstruments.com
- IGHT s.c.
  Marszałkowska 80, Warszawa 00-517, Poland
- NT-MDT Europe BV (NT-MDT)
  De Pinckart 54, Nuenen 5674CC, Netherlands

Piotr Moszczyński
moszczu@gmail.com
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

Adrian M. Motoc
amotoc@imnr.ro
- National Institute for Nonferrous and Rare Metals (IMNR)
  102 Biruintei Blvd., Pantelimon 077145, Romania

Mac Mugumaoderha Cubaka
mac.mugumaoderhacubaka@fundp.ac.be
- University of Namur (FUNDP)
  rue de Bruxelles 61, Namur 5000, Belgium

Steven Mullens
steven.mullens@vito.be
- Flemish Institute for Technological Research (VITO)
  Boeretang 200, Mol 2400, Belgium

Paul Mulvaney
mulvaney@unimelb.edu.au
- The University of Melbourne
  School of Chemistry, Parkville, VIC, Melbourne 3010, Australia

Shankar Muthukonda Venkatakrishnan
Shankar.Muthukonda@ecpm.u-strasbg.fr
- CNRS, ULP, Laboratoire des Matériaux, Surfaces et Procédés pour la Catalyse (LMSPC)
  25 rue Becquerel, Strasbourg 67087, France

Marek Muzyk
muzyk@inmat.pw.edu.pl
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

Andrzej Mycielski
mycie@ifpan.edu.pl
- Polish Academy of Sciences, Institute of Physics
  al. Lotników 32/46, Warszawa 02-668, Poland

Kiyotaka Nakajima
nakajima.k.ae@m.titech.ac.jp
- Materials and Structures Laboratory, Tokyo Institute of Technology
  4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan

Takaaki Nakamura
m7621022@edu.kit.ac.jp
- Kyoto Institute of Technology
  Kyoto 606-8585, Japan

Urszula Narkiewicz
urszula.narkiewicz@ps.pl
- Szczecin University of Technology, Institute of Chemical and Environment Engineering
  Szczecin 70-322, Poland

Lívia Naszályi Nagy
lnaszalyi@mail.bme.hu
- Budapest University of Technology and Economics, Department of Physical Chemistry and Materials (BME)
  Budafoki út 6-8., Budapest 1111, Hungary
- Institut Européen des Membranes
  Montpellier 34095, France

Christoph Neinhuis
christoph.neinhuis@tu-dresden.de
- Technische Universität Dresden, Institut für Botanik
  Zellescher Weg 20b, Dresden 01069, Germany

Marie-Alexandra G. Neouze
mneouze@mail.zserv.tuwien.ac.at
- Vienna Technical University
  9, Getreidemarkt, Wien 1040, Austria

Wai Fong Ng
07900582r@polyu.edu.hk
- The Hong Kong Polytechnic University (HK, PolyU)
  Hung Hom, Hong Kong, Hong Kong

Katarzyna Niespodziana
katarzyna.niespodziana@put.poznan.pl
- Poznań Technical University
  pl. Marii Skłodowskiej-Curie 5, Poznań 60-965, Poland

Tadeusz Niezgoda
niezgoda@onet.pl
- Military University of Technology (WAT)
  Kaliskiego 2, Warszawa 00-908, Poland

Jun Hong Noh
perfect3@snu.ac.kr
- Seoul National University, Department of Materials Science and Engineering (MSE, SNU)
  San 56-1, Sillim-dong, Gwanak-gu, Seoul 151-744, Korea, South

Emmanuel S. Nolot
emmanuel.nolot@cea.fr
- CEA-LETI-MINATEC (MINATEC)
  17 rue des Martyrs, Grenoble 38054, France

Filip Novotny
filip.novotny@fjfi.cvut.cz
- Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical Engineering, Department of Physical Electronics
  Brehova str. 7, Prague 115 19, Czech Republic

Yoichi Ogo
y-ogo@lucid.msl.titech.ac.jp
- Tokyo Institute of Technology
  Yokohama 226-8502, Japan

Toshiharu Ohnuma
ohnuma@criepi.denken.or.jp
- Central Research Institute of Electric Power Industry (CRIEPI)
  Tokyo 201-8511, Japan

Mihaela A. Olaru
olaruma@icmpp.ro
- Petru Poni Institute of Macromolecular Chemistry of the Romanian Academy
  Aleea Grigore Ghica Voda 41A, Iasi, Romania

Wiesława Olesińska
olesin-w@sp.itme.edu.pl
- Institute of Electronic Materials Technology (ITME)
  Wólczyńska 133, Warszawa 01-919, Poland
- University of Silesia
  Katowice, Poland

Dariusz Oleszak
daol@inmat.pw.edu.pl
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

Agnieszka Opalińska
agnieszka@unipress.waw.pl
- Polish Academy of Sciences, Institute of High Pressure Physics (UNIPRESS)
  Sokolowska 29/37, Warszawa 01-142, Poland
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

Ana Maria Oprea
aoprea@icmpp.ro
- Petru Poni Institute of Macromolecular Chemistry of the Romanian Academy
  Aleea Grigore Ghica Voda 41A, Iasi, Romania

Sukyas Ordanyan
ceramic-department@yandex.ru
- StPSTI (STPSTI)
  Moskovsky, 26, Saint-Petersburg 190013, Russian Federation

Barbara D. Ostrowska
bostrowska@gmail.com
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

Sami Oukassi
sami.oukassi@cea.fr
- CEA (LITEN)
  17 rue des Martyrs, Grenoble 38054, France

Willi Pabst
pabstw@vscht.cz
- Institute of Chemical Technology (VSCHT)
  Technicka 5, Prague 16628, Czech Republic

Olivier Pagès
pages@univ-metz.fr
- Université Paul Verlaine, Laboratoire de Physique des Milieux Denses (LPMD)
  1 Bd. Arago, Metz 57000, France

Thierry Pagnier
thierry.pagnier@lepmi.inpg.fr
- LEPMI
  1130 rue de la Piscine, Saint Martin d'Hères 38402, France

Jonghoo Paik
jhpaik@kicet.re.kr
- Korea Institute of Ceramic Engineering and Technology (KICET)
  , Gasang-Dong, Geumcheon-Gu, Seoul 153023, Korea, South

Pier Luca Palla
pierluca.palla@dsf.unica.it
- CNR-INFM SLACS and Dept of Physics, University of Cagliari
  Cittadella Universitaria di Monserrato, Dept of Physics, University of Cagliari, Cagliari I-09042, Italy

Roman Pampuch
roman.pampuch@neostrada.pl
- AGH University of Science and Technology, Department of Ceramics Technology (AGH)
  Kraków, Poland

Magdalena Parlinska-Wojtan
magdalena.parlinska@empa.ch
- Empa Materials Science and Technology (Empa)
  Überlandstrasse 129, Dübendorf 8600, Switzerland

Krzysztof Parlinski
krzysztof.parlinski@ifj.edu.pl
- Polish Academy of Sciences, Institute of Nuclear Physics (IFJ PAN)
  Radzikowskiego 152, Kraków 31-342, Poland
- Pedagogical University, Institute of Technics
  Podchorążych 2, Kraków 30-084, Poland

Piotr Patoka
patoka@caesar.de
- Max Planck Institute of Colloids and Interfaces (MPIKGF)
  Research Campus Golm, Potsdam 14424, Germany
- center of advanced european studies and research (caesar)
  Ludwig-Erhard-Allee 2, Bonn 53175, Germany

Novica Paunović
npaun@phy.bg.ac.yu
- Institute of Physics (IF)
  Pregrevica 118, Belgrade 11080, Serbia

Zbigniew Pędzich
pedzich@agh.edu.pl
- AGH University of Science and Technology, Faculty of Materials Science and Ceramics (AGH UST)
  Mickiewicza 30, Kraków 30-059, Poland

Niculina Peica
n.peica@fz-juelich.de
- Central Division of Analytical Chemistry, Research Center Juelich (ZCH)
  Leo-Brandt Strasse., Jülich 52425, Germany

Anna Peled
aniapeled@yahoo.com
- Bar Ilan Universiry
  Ramet-Gan 52900, Israel

Yan Pennec
yan.pennec@univ-lille1.fr
- Institute for Electronics and Nanotechnology
  Lille 60069, France

Celine Perego
celine.perego@ifp.fr
- IFP
  Lyon 69390, France

Celeste M. Pereira
cpereira@inegi.up.pt
- Instituto de Engenharia Mecânica e Gestão Industrial (INEGI)
  Rua Doutor Roberto Frias, 378, Porto 4200Porto, Portugal

Luis Pereira
lmnp@fct.unl.pt
- Materials Science Department, CENIMAT-IxN and CEMOP-UNINOVA, FCT-UNL
  Campus da Caparica, Caparica, Caparica 2829-516, Portugal
- Electronics Department, University of Barcelona
  C\ Martí i Franqu?s, Barcelona 08028, Spain

Giorgio Perez
perez@mlib.cnr.it
- Institute of the Study of Nanostructured Materials (ISMN-CNR)
  Monterotondo, Monterotondo (RM) I-00016, Italy

Krzysztof Perkowski
kperkowski@ch.pw.edu.pl
- Warsaw University of Technology, Faculty of Chemistry
  Noakowskiego 3, Warszawa 00-664, Poland

Maria Pervolaraki
pervolaraki@ucy.ac.cy
- University of Cyprus (UCY)
  75 Kallipoleos Avenue, Nicosia 1678, Cyprus

Tamara Petkova
tpetkova@bas.bg
- Institute of Electrochemistry and Energy Systems (IEES)
  Acad.G.Bonchev str.Bl.10, Sofia 1113, Bulgaria

Plamen Petkov
p.petkov@uctm.edu
- Uniersity of Chemical Technology and Metallurgy (UCTM)
8, Kl.Ohridsky Blvd, Sofia 1756, Bulgaria

Oleksander S. Petukhov
asp@ipms.kiev.ua
- Institute for Problems in Materias Science (IPMS)
3, Krzhizhanivsky Str., Kiev 03680, Ukraine

Fabio Pezzoli
fabio.pezzoli@mater.unimib.it
- University of Milano-Bicocca, Department of Materials Science
via Cozzi 53, Milano 20125, Italy

Rudolf Pfeiffer
rudolf.pfeiffer@univie.ac.at
- University of Vienna, Faculty of Physics
Boltzmanngasse 5, Wien 1090, Austria

Cuong Pham-Huu
cuong.lcmc@ecpm.u-strasbg.fr
- CNRS, ULP, Laboratoire des Matériaux, Surfaces et Procédés pour la Catalyse (LMSPC)
25 rue Becquerel, Strasbourg 67087, France

Karine Philippot
karine.philippot@lcc-toulouse.fr
- Laboratoire de Chimie de Coordination (LCC)
205 route de Narbonne, Toulouse 31077, France

Adam Piątek
afriday@interia.eu
- University of Silesia, Institute of Physics
Uniwersytecka 4, Katowice 40-007, Poland

Roman Pielaszek
roman@pielaszek.net
- Polish Academy of Sciences, Institute of High Pressure Physics (UNIPRESS)
Sokolowska 29/37, Warszawa 01-142, Poland

Véronique Pierron-Bohnes
vero@ipcms.u-strasbg.fr
- Institut de Physique et Chimie des Materiaux de Strasbourg, UMR7504, CNRS - ULP
23, rue du Loess, BP 43, Strasbourg CEDEX 2 67034, France

Bożena Pietrzyk
bozena.pietrzyk@p.lodz.pl
- Technical University of Lodz, Institute of Materials Science and Engineering
1/15 Stefanowskiego, Łódź 90-924, Poland

Monika Pilz
Monika.Pilz@sintef.no
- SINTEF (SINTEF)
Forskingsveien 1, Oslo N-0314, Norway

Aron Pinczuk
aron@phys.columbia.eu
- Columbia University
New York, NY 10027, United States

Krzysztof Piskorski
kpisk@ite.waw.pl
- Institute of Electron Technology (ITE)
al. Lotników 32/46, Warszawa 02-668, Poland

Robert R. Piticescu
rpiticescu@imnr.ro
- Institute for Non-ferrous and Rare Metals
102 Biruintei Blvd., Pantelimon 73957, Romania

Roxana M. Piticescu
roxana@imnr.ro
- National Institute for Nonferrous and Rare Metals (IMNR)
102 Biruintei Blvd., Pantelimon 077145, Romania

Ireneusz Piwoński
irek@uni.lodz.pl
- University of Łódź, Department of Chemical Technology and Environmental Protection
Pomorska 163, Łódź 90-236, Poland

Antoni Planes
toni@ecm.ub.es
- Universitat de Barcelona, Departament d'Estructura i Constituents de la Materia
Barcelona 08028, Spain

Arie J. Plomp
a.j.plomp@uu.nl
- Inorganic Chemistry and Catalysis, Utrecht University
Sorbonnelaan 16, Utrecht 3584CA, Netherlands

Christopher J. Plummer
Christopher.plummer@epfl.ch
- Ecole Polytechnique Federale de Lausanne (EPFL)
Ecublens, Lausanne 1015, Switzerland

Malgorzata M. Pociask
pociask@univ.rzeszow.pl
- University of Rzeszow, Institute of Physics
Rejtana 16, Rzeszów 35-310, Poland

Boaz Pokroy
bpokroy@seas.harvard.edu
- Harvard University
12 Oxford Street, Cambridge, MA 02138, United States

Jacek Polit
polijack@univ.rzeszow.pl
- University of Rzeszow, Institute of Physics
Rejtana 16, Rzeszów 35-310, Poland

Laura A. Poole-Warren
L.Poolewarren@unsw.edu.au
- University of New South Wales (UNSW)
Sydney 2052, Australia

Madalina L. Popescu
mpopescu@imnr.ro
- National Institute for Nonferrous and Rare Metals (IMNR)
102 Biruintei Blvd., Pantelimon 077145, Romania

Zoran V. Popovic
zoran.popovic@phy.bg.ac.yu
- Institute of Physics (IF)
Pregrevica 118, Belgrade 11080, Serbia

Oleg Posudievsky
posol@inphyschem-nas.kiev.ua
- L.V.Pisarzhevsky Institute of Physical Chemistry of the National Academy of Sciences of Ukraine
prospect Nauki 31, Kiev 03028, Ukraine

Annegret Potthoff
Annegret.Potthoff@ikts.fraunhofer.de
- Fraunhofer IKTS (IKTS)
Winterbergstraße 28, Dresden 01277, Germany

Nicoleta Preda
nicol@infim.ro
- National Institute for Materials Physics
Bucharest- Magurele 010555, Romania

Roger Proksch
roger@rasy.com
- Asylum Research
Santa Barbara, CA 93117, United States

Judita Puišo
judita.puiso@ktu.lt
- Kaunas University of Technology, Department of Physics
Studentu 50, Kaunas, Lithuania
- Kaunas University of Technology, Institute of Physical Electronics
Savanoriu 271, Kaunas LT-3009, Lithuania

Lluís Pujadas
lpujadas@ascamm.com
- Fundació Privada Ascamm (LLUIS)
Av. Universitat Autònoma,23, Barcelona 08290, Spain

Ryszard Pyrz
rp@ime.aau.dk
- Aalborg University (AAU)
Pontoppidanstræde 101, Aalborg 9220, Denmark

Anna Pytel
anna.pytel@ichp.pl
- Industrial Chemistry Research Institute (ICRI)
Rydygiera 8, Warszawa 01-793, Poland

Taras M. Radchenko
Taras.Radchenko@gmail.com
- Institute for Metal Physics, N.A.S.U.
36 Vernadsky Boulevard, Kyiv 03142, Ukraine

Marko Radović
marrad@phy.bg.ac.yu
- Institute of Physics (IF)
Pregrevica 118, Belgrade 11080, Serbia

Michael Raghunath
bierm@nus.edu.sg
- National University of Singapore (NUS)
Singapore, Singapore

Andrey V. Ragulya
ragulya@ipms.kiev.ua
- Institute for Problems of Materials Science
3, Krzhizhanovsky, Kyiv 03142, Ukraine

Anant K. Ramdas
akr@physics.purdue.edu
- Purue University, Department of Physics
525 Northwestern Avenue, West Lafayette 47907-2036, United States

Jing Rao
jing.rao@tyndall.ie
- University College Cork, Tyndall National Institute (TYNDALL)
Lee Maltings, Prospect Row, Cork, Ireland

Jean-Yves Raty
jyraty@ulg.ac.be
- University of Liege (ULg)
B5, Liège 4000, Belgium

Patrice Raynaud
patrice.raynaud@laplace.univ-tlse.fr
- Université Toulouse, LAboratoire PLAsma et Conversion d'Energie (LAPLACE)
118 Route de Narbonne, Toulouse 31062, France

Ian M. Reaney
I.M.Reaney@sheffield.ac.uk
- Sheffield University
Brook Hill, Sheffield S37HF, United Kingdom

Maximilian Reismann
Reismann@Physik.RWTH-Aachen.de
- Institute of Physics IA, RWTH Aachen University
  Sommerfeldstraße 14, Aachen 52074, Germany

Maria W. Richert
mrichert@edu.pl
- AGH University of Science and Technology (AGH)
  al. Mickiewicza 30, Kraków 30-059, Poland

Enrique Rodriguez Castellon
castellon@uma.es
- Universidad de Malaga (UMA)
  Campus Teatinos, Malaga E29071, Spain

David J. Rogers
d.j.rogers@nanovation.com
- Nanovation
  103 bis rue de Versailles, Orsay, Orsay 91400, France

James F. Rohan
james.rohan@tyndall.ie
- University College Cork, Tyndall National Institute (TYNDALL)
  Lee Maltings, Prospect Row, Cork, Ireland

Anabela G. Rolo
arolo@fisica.uminho.pt
- University of Minho (UM)
  Campus de Gualtar, Braga 4710057, Portugal

Maja Romcevic
romcevic@phy.bg.ac.yu
- Institute of Physics (IF)
  Pregrevica 118, Belgrade 11080, Serbia

Nebojsa Romcevic
romcevi@phy.bg.ac.yu
- Institute of Physics (IF)
  Pregrevica 118, Belgrade 11080, Serbia

Gil Rosenman
gilr@eng.tau.ac.il
- Tel Aviv University (TAU)
  Ramat Aviv, Tel Aviv 69787, Israel

Marcin Rosinski
ninmar@inmat.pw.edu.pl
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

Zbigniew Roslaniec
zbigniew.roslaniec@ps.pl
- Technical University of Szczecin, Institute of Materials Science and Engineering (TUS)
  Piastów 19, Szczecin 71-310, Poland

Jerome Rouquette
jerome@lpmc.univ-montp2.fr
- Institut Charles Gerhardt
  CC15, Place eugène Bataillon, Montpellier 34095, France

Carme Rovira
crovira@pcb.ub.es
- Parc Científic de Barcelona (PCB)
  Baldiri Reixac 10-12, Barcelona 08028, Spain
- Institució Catalana de Recerca i Estudis Avançats (ICREA)
  Passeig Lluís Companys 23, Barcelona 08018, Spain
- Institut Químic de Sarrià. Universitat Ramon Llull (IQS-URL)
  Via Augusta, Barcelona 08017, Spain

Riccardo Ruggerone
riccardo.ruggerone@epfl.ch
- Ecole Polytechnique Federale de Lausanne (EPFL)
  Ecublens, Lausanne 1015, Switzerland

Vladimir Rumyantsev
info@virial.ru
- VIRIAL Ltd. (VIRIAL)
  Engelsa, 27, St-Petersburg 194156, Russian Federation

Agnieszka Rytel
emrs@inmat.pw.edu.pl
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

Witold Rzodkiewicz
rzodki@ite.waw.pl
- Institute of Electron Technology (ITE)
  al. Lotników 32/46, Warszawa 02-668, Poland

Tomek Rzysko
tomek.rzysko@renishaw.com
- Renishaw Plc
  Szyszkowa 34, Warsaw 02-285, Poland

Ivo Safarik
ivosaf@yahoo.com
- Institute of Systems Biology and Ecology (USBE)
  Na Sadkach 7, Ceske Budejovice 37005, Czech Republic

Yoshio Sakka
SAKKA.Yoshio@nims.go.jp
- National Institute of Advanced Industrial Science and Technology (AIST)
  sukuba Central 2-1-D811, 1-1-1 Umezono, Tsukuba, Ibaraki, Tukuba 305-8568, Japan

Yutaka Sakurai
ysakurai@toyama-nct.ac.jp
- Toyama National College of Technology
  13 Hongo, Toyama 939-8630, Japan

Philip S. Salmon
P.S.Salmon@bath.ac.uk
- University of Bath, Department of Physics
Claverton Down, Bath BA27AY, United Kingdom

Raphaël Salot
raphael.salot@cea.fr
- CEA (LITEN)
17 rue des Martyrs, Grenoble 38054, France

Francisco M. Sánchez
fsanchez@iim.unam.mx
- Universidad Nacional Autonoma de Mexico-Centro de Ciencias Aplicadas Desarrollo Tecnologico (CCADET)
Circuito Ext. S/N Ciudad Universitaria Coyoacan, México 70-186, Mexico

Antonio Javier Sanchez-Herencia
ajsanchez@icv.csic.es
- Consejo Superior de Investigaciones Cientfificas (ICV)
Cº Valdelatas, SN, Madrid 2809, Spain

Ie Sangyub
phantom7@empal.com
- Korea Institute of Science and Technology, Material Science and Technology Division
39-1 Hawolgok-dong, Wolsong-gil 5, Seongbuk-gu, Seoul 136-791, Korea, South

Claire Saulou
claire.saulou@insa-toulouse.fr
- Laboratoire Plasma et Conversion d'Energie (LAPLACE)
118 Route de Narbonne, Toulouse 31062, France

Rachel E. Saunders
Saunders.rachel@gmail.com
- University of Manchester - School of Materials Science - Materials Science Centre
grosvenor street, Manchester M1 7HS, United Kingdom

Serhiy A. Savchuk
savchuk@chnu.cv.ua
- Chernivtsi National University (ChNU)
2 Kotsubinsky Str., Chernivtsi 58012, Ukraine

Tommaso Scarpa
tscarpa@units.it
- Università di Trieste
Trieste, Italy

Maja J. Šćepanović
maja@phy.bg.ac.yu
- Institute of Physics (IF)
Pregrevica 118, Belgrade 11080, Serbia

Martin Schaefer
info@schaefer-tec.com
- Schaefer Technologie GmbH
Morfelder Landstrasse 33, Langen 63225, Germany

Hanne Scheel
hanne.scheel@ww.uni-erlangen.de
- University of Erlangen-Nürnberg, Glass and Ceramics
Martenstr.5, Erlangen 91058, Germany

Thomas Scheibel
thomas.scheibel@uni-bayreuth.de
- Universität Bayreuth
Universitätsstr. 30, Bayreuth 95440, Germany

Alexey V. Scherbakov
scherbakov@mail.ioffe.ru
- A.F. Ioffe Physical-Technical Institute
Politekhnicheskaya 26, St-Petersburg 194021, Russian Federation

Ute Schmidt
ute.schmidt@witec.de
- WITec GmbH
Hoervelsingerweg 6, Ulm 89081, Germany

Ute Schmidt
info@witec.de
- WITec GmbH
Hoervelsingerweg 6, Ulm 89081, Germany

Dominique Schryvers
nick.schryvers@ua.ac.be
- University of Antwerp, EMAT
Groenenborgerlaan 171, Antwerp B-2020, Belgium

Ulrich Schubert
uschuber@mail.zserv.tuwien.ac.at
- Institute of Materials Chemistry, Vienna University of Technology (TU)
Veterinärplatz 1, Wien 1210, Austria

Roberto Scipioni
scipioni.roberto@nims.go.jp
- National Institute of Material Science (NIMS)
Tsukuba, Japan

Emmanuel Scolan
esn@csem.ch
- Centre Suisse d'Electronique et de Microtechnique (CSEM)
Jaquet-Droz 1, Neuchâtel 2002, Switzerland

Gaida Sedmale
gsedmale@ktf.rtu.lv
- Institute of Inorganic Chemistry, Riga Technical University
  Riga LV-2169, Latvia
- Riga Technical University
  Miera 34, Riga, Latvia

Jung Mo Seo
seo0918@kimm.re.kr
- School of Mechanical Engineering Pusan National University
  Busan 607-735, Korea, South
- Korea Institute of Machinery and Materials (KIMM)
  Daejeon 305-600, Korea, South

Kevin M. Shakesheff
kevin.shakesheff@nottingham.ac.uk
- University of Nottingham
  Nottingham, United Kingdom

Eugen M. Sheregii
sheregii@univ.rzeszow.pl
- University of Rzeszow, Institute of Physics
  Rejtana 16, Rzeszów 35-310, Poland

Yuzo Shigesato
yuzo@chem.aoyama.ac.jp
- Aoyama Gakuin University, Graduate School of Science and Engineering
  5-10-1 Fuchinobe, Sagamihara 229-8558, Japan

Shoso Shingubara
shingu@ipcku.kansai-u.ac.jp
- Kansai University
  Suita 3-3-35, Osaka 564-8680, Japan

Gagik Shmavonyan
gshmavon@yahoo.com
- State Engineering University of Armenia
  Yerevan 0002, Armenia

Lazar S. Shvindlerman
shvind@imm.rwth-aachen.de
- Russian Academy of Sciences, Institute of Solid State Physics
  Chernogolovka 142432, Russian Federation

Dariusz Siemiaszko
dsiemiaszko@wat.edu.pl
- Military University of Technology, Faculty of Advanced Technology and Chemistry
  Kaliskiego 2, Warszawa 00-908, Poland
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

Clara Silvestre
silvestre@ictp.cnr.it
- Istituto di Chimica e Tecnologia dei Polimeri (ICTP-CNR)
  via Campi Flegrei, 34, Napoli 80078, Italy

Ana-Bogdana Simionescu
simionescubogdana@yahoo.com
- University of Oviedo, Dept. of Geology
  Calle Jesus Arias de Velasco, Oviedo 33005, Spain
- Petru Poni Institute of Macromolecular Chemistry of the Romanian Academy
  Aleea Grigore Ghica Voda 41A, Iasi, Romania

Terje Sjöström
omxts@bristol.ac.uk
- University of Bristol
  Tyndall Avenue, Bristol BS8 1TL, United Kingdom

Valeriy V. Skorokhod
dir@ipms.kiev.ua
- Institute for Problems of Materials Science, National Academy of Sciences of Ukraine
  Krzizanovsky, Kyiv 38(044), Ukraine

Zbigniew Skorupka
zk.skorupka@ilot.edu.pl
- Instytut Lotnictwa (ILOT)
  Al. Krakowska 110/114, Warszawa 02-256, Poland

Mikael Skrifvars
mikael.skrifvars@hb.se
- University College Boras (UCB)
  Allegatan 1, Boras 50190, Sweden

Aneta Slodczyk
slodczyk@glvt-cnrs.fr
- LADIR-CNRS (LADIR)
  2 rue Henry Dunant, Thiais 94320, France

Krisjanis Smits
smits@cfi.lu.lv
- Institute of Solid State Physics, University of Latvia
  8 Kengaraga, Riga LV-1063, Latvia

Stephen Soehnlen
stephen.soehnlen@springer.at
- Springer Publishing Vienna
  Wien 1201, Austria

Nikoletta G. Sofikiti
niksof@chemistry.uoc.gr
- University of Crete, Chemistry Department
  Voutes P.O Box 2208, Heraklion 71003, Greece

Vladimir V. Sokolovskiy
vsokolovsky84@mail.ru
- Chelyabinsk State University (ChelSU)
  Br. Kashirinykh Str, 129, Chelyabinsk 454021, Russian Federation

Károly Somogyi
karoly.somogyi@microvacuum.com
- MicroVacuum
  Kerékgyarto u. 10, Budapest H-1147, Hungary

Ratnasingham Sooryakumar
soory@mps.ohio-state.edu
- The Ohio State University, Department of Physics (OSU)
  191 W. Woodruff Ave, Columbus 43210, United States

Iis Sopyan
sopyan@iiu.edu.my
- International Islamic University Malaysia (IIUM)
  PO Box 10, Kuala Lumpur 50728, Malaysia

Jihane Souhabi
jihane.souhabi@univ-metz.fr
- Université Paul Verlaine, Laboratoire de Physique des Milieux Denses (LPMD)
  1 Bd. Arago, Metz 57000, France

Matthieu Soulis
matthieu.soulis@isen.iemn.univ-lille1.fr
- Institute for Electronics and Nanotechnology
  Lille 60069, France

Agnieszka Sozańska
poland@renishaw.com
- Renishaw Plc
  Szyszkowa 34, Warsaw 02-285, Poland

Jonathan E. Spanier
spanier@drexel.edu
- Drexel University
  3141 Chestnut St, Philadelphia 19104, United States

Ralph Spolenak
spolenak@mat.ethz.ch
- ETH Zurich
  Wolfgang-Pauli-Str. 10, Zurich 8093, Switzerland

Dieter Sporn
sporn@isc.fraunhofer.de
- Fraunhofer ISC (ISC)
  Neunerplatz 2, Würzburg 97082, Germany

Barbara Staniewicz-Brudnik
bbrudnik@ios.krakow.pl
- Institute of Metal Cutting
  Wrocławska 37A, Kraków 30-011, Poland

Mikhail D. Starostenkov
genphys@mail.ru
- Altai State Technical University (ASTU)
  Lenin st.46, Barnaul 656038, Russian Federation

Jean-Louis Stehlé
jeanlouis.stehle@sopra-sa.com
- SOPRA SA
  26 Pierre Joigneaux, Bois-Colombes 92270, France

Anna Stęplewska
asteplewska@ps.pl
- Szczecin University of Technology, Institute of Chemical and Environment Engineering
  Szczecin 70-322, Poland

Manuela Stir
manuela.stir@empa.ch
- EMPA Materials Research and Technology (EMPA)
  Feuerwerkerstr. 39, Thun 3602, Switzerland

Dusanka Stojanovic
dusanka@phy.bg.ac.yu
- Institute of Physics (IF)
  Pregrevica 118, Belgrade 11080, Serbia

Tomasz Strachowski
tomasz@unipress.waw.pl
- Polish Academy of Sciences, Institute of High Pressure Physics (UNIPRESS)
  Sokolowska 29/37, Warszawa 01-142, Poland
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

Satoshi Suganuma
suganuma.s.aa@m.titech.ac.jp
- Materials and Structures Laboratory, Tokyo Institute of Technology
  4259 Nagatsuta, Midori-ku, Yokohama, Yokohama 226-8503, Japan

Efthymios C. Svoukis
kanenas33@hotmail.com
- University of Cyprus (UCY)
  Kallipoleos Avenue, Nicosia 1678, Cyprus

Anna Swiderska - Sroda
annas@unipress.waw.pl
- Polish Academy of Sciences, Institute of High Pressure Physics (UNIPRESS)
  Sokolowska 29/37, Warszawa 01-142, Poland

Dariusz Świerczyński
darek@chimie.u-strasbg.fr
- Institut de recherches sur la Catalyse et l'Environnement de Lyon (IRCELYON)
  2, avenue Albert Einstein, Villeurbanne 69626, France

Wojciech Swieszkowski
Wojciech.Swieszkowski@materials.pl
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

Renata G. Świrkowicz
renatas@if.pw.edu.pl
- Warsaw University of Technology, Faculty of Physics
  Koszykowa 75, Warszawa 00-662, Poland

Tetiana Sydorenko
tvsid@ukr.net
- Institute for Problems in Materias Science (IPMS)
  3, Krzhizhanivsky Str., Kiev 03680, Ukraine

Mikolaj Szafran
szafran@ch.pw.edu.pl
- Warsaw University of Technology, Faculty of Chemistry
  Koszykowa 75, Warszawa 00-662, Poland

Peter Szanto
peters@hu.inter.net
- Kurt J. Lesker
  Godolloi-utca 19/A, Budapest H1141, Hungary
- Kurt J. Lesker Company
  Hastings TN354NN, United Kingdom

Roman Szewczyk
szewczyk@mchtr.pw.edu.pl
- Warsaw University of Technology, Faculty of Mechatronics
  Św. Andrzeja Boboli 8, Warszawa 05-525, Poland

Wojciech Szuszkiewicz
szusz@ifpan.edu.pl
- Polish Academy of Sciences, Institute of Physics
  al. Lotników 32/46, Warszawa 02-668, Poland

Henryk Szymczak
szymh@ifpan.edu.pl
- Polish Academy of Sciences, Institute of Physics
  Warszawa 02-668, Poland

Wiesław Szymczyk
w.szymczyk@wme.wat.edu.pl
- Military University of Technology (WAT)
  Kaliskiego 2, Warszawa 00-908, Poland

Yoshiki Takagi
takagi@ntu.ac.jp
- Teikyo University of Science and Technology
  2525, Uenohara, Yamanashi 409-0193, Japan

Anna Taubenberger
anna.taubenberger@biotec.tu-dresden.de
- Biotechnology Center, University of Technology Dresden (TUD)
  Am Tatzberg 47-49, Dresden 01307, Germany

Thomas B. Tengen
thomas@vut.ac.za
- Vaal University of Technology (VUT)
  Johannesburg 1900, South Africa

Steve Tennison
steve.tennison@mastcarbon.co.uk
- MAST Carbon Technology Ltd (MAST)
  Henley Park, Guildford Surrey GU32AF, United Kingdom

Yuden Teraoka
yteraoka@spring8.or.jp
- Japan Atomic Energy Agency (JAEA)
  1-1-1 Kouto, Sayo-cho,Sayo-gun, Hyogo 679-5148, Japan

Andrea Terenzi
andrea.terenzi@mdpsrl.it
- MDP Materials Design and Processing Srl (MDP)
  Loc. Pentima Bassa, 21, Terni 05100, Italy

Chloe M. Thieuleux
thieuleux@cpe.fr
- Chimie, Catalyse, Polymère, Procédé, UMR CNRS CPE UCBL (CCPP)
  43 bd du 11 Nov. 1918, Villeurbanne 69616, France

Didier Tichit
didier.tichit@enscm.fr
- Institut Charles Gerhardt
  CC15, Place eugène Bataillon, Montpellier 34095, France

Hisaaki Tobushi
tobushi@aitech.ac.jp
- Aichi Institute of Technology (AIT)
  1247 Yachigusa, Takusa-cho, Toyota 470-0392, Japan

Jelena M. Todorović
jelenatodorovicksc@gmail.com
- Institute of Physics (IF)
  Pregrevica 118, Belgrade 11080, Serbia

Milica Todorovic
todorovic.milica@nims.go.jp
- National Institute for Materials Science (NIMS)
  1-2-1 Sengen, Tsukuba 305-0047, Japan

Lyudmil V. Todorov
lvt@dep.uminho.pt
- University of Minho (UM)
  Campus of Azurém, Guimarães 4800-058, Portugal

Ranna Tolouei
ranna.tolouei@gmail.com
- Ceramics department from Materials and Energy Research Center
  Tehran 15914, Iran

Jolanta Tomaszewska
jolanta.tomaszewska@utp.edu.pl
- University of Technology and Life Sciences, Faculty of Chemical Technology and Engineering (UTP)
  Seminaryjna 3, Bydgoszcz 85-326, Poland

Henryk Tomaszewski
tomasz_h@itme.edu.pl
- Institute of Electronic Materials Technology (ITME)
  Wólczyńska 133, Warszawa 01-919, Poland

Jan Toporski
info@witec.de
- WITec GmbH
  Hoervelsingerweg 6, Ulm 89081, Germany

Jelena Trajic
jelena@phy.bg.ac.yu
- Institute of Physics (IF)
  Pregrevica 118, Belgrade 11080, Serbia

Andrea Travan
andrea.travan@iol.it
- Università di Trieste
  Trieste, Italy

Vo-Van Truong
truong.vo-van@concordia.ca
- Concordia University, Department of Physics
  1455 de Maisonneuve West, Montreal H3G1M8, Canada

Nick Tucker
tuckern@crop.cri.nz
- The New Zealand Institute for Crop and Food Research Ltd (CFR)
  Private Bag 4704, Christchurch 8140, New Zealand
- Department of Physics and Astronomy, The MacDiarmid Institute for Advanced Materials and Nanotechnology, University of Canterbury, Christchurch, New Zealand
  Christchurch, New Zealand
- Dept. mechanical Engineering, University Canterbury (ME-UOC)
  Private Bag 4800, Christchurch 8140, New Zealand
- University of Southern Denmark (SDK)
  Niels Bohrs Allé 1, 5230 Odense M, Odense 5230, Denmark

Maciej Tuliński
maciej.tulinski@doctorate.put.poznan.pl
- Poznań Technical University
  pl. Marii Skłodowskiej-Curie 5, Poznań 60-965, Poland

Maria Tymieniecka
maria@comef.com.pl
- COMEF Aparatura Naukowo-Badawcza
  Rakowiecka 36/317A, Warsaw 02-532, Poland

Iryna V. Uvarova
uvarova@ipms.kiev.ua
- Institute for Problems of Materials Science, National Academy of Sciences of Ukraine
  Krzizanovsky, Kyiv 38(044), Ukraine

Mykhailo Valakh
valakh@isp.kiev.ua
- Institute of Semiconductor Physics NAS Ukraine
  Kyiv, Ukraine

Luca Valentini
mic@unipg.it
- Civil and Environmental Engineering Department, University of Perugia
  Pentima Bassa, Terni 05100, Italy

Vicky Vamvakaki
vickyvam@chemistry.uoc.gr
- University of Crete, Chemistry Department
  Voutes P.O Box 2208, Heraklion 71003, Greece

Clemens Van Blitterswijk
c.a.vanblitterswijk@tnw.utwente.nl
- University of Twente, Faculty Science and Technology, department of Tissue Regeneration
  P.O. Box 217, Enschede 7500AE, Netherlands

Els Van der Burght
els.vanderburght@UGent.be
- Ghent University, Centre for Materials Science and Engineering (UGENT-CMSE)
  Technologiepark-Zwijnaarde 907, Gent 9052, Belgium

Herre S. Van der Zant
h.s.j.vanderzant@tudelft.nl
- Delft University of Technology (TUDELFT)
  Julianalaan 67, Delft 2628BC, Netherlands

Estelle Vanhaecke
estelle.vanhaecke@chemeng.ntnu.no
- Norwegian University of Science and Technology (NTNU)
  Trondheim N-7491, Norway

Paul Van Loosdrecht
p.h.m.van.loosdrecht@rug.nl
- Zernike Institute for Advanced Materials
  Nijenborgh 4, Groningen 9747AG, Netherlands

Borislav Vasic
bvasic@phy.bg.ac.yu
- Institute of Physics (IF)
  Pregrevica 118, Belgrade 11080, Serbia

Alexander V. Vasiliev
a.vasiliev@inorg.chem.msu.ru
- Faculty of Materials Science, Moscow State University
  Lenin Hills, Moscow 119992, Russian Federation

Oleksandr V. Vdovychenko
ovdovychenko@yahoo.com
- Institute for Problems of Materials Science, National Academy of Sciences of Ukraine
  Krzizanovsky, Kyiv 38(044), Ukraine

Miklos Veres
vm@szfki.hu
- Hungarian Academy of Sciences, Research Institute for Solid State Physics and Optics (SZFKI)
  Konkoly Thege M. út 29-33, Budapest H-1121, Hungary

Laurent Veyre
veyre@cpe.fr
- Chimie, Catalyse, Polymère, Procédé, UMR CNRS CPE UCBL (CCPP)
  43 bd du 11 Nov. 1918, Villeurbanne 69616, France

Pauline Vitoux
vitoux@icmcb-bordeaux.cnrs.fr
- Institut de Chimie de la Matiere Condensée de Bordeaux, ICMCB - CNRS
  87 avenue du Dr Albert Schweitzer, Pessac 33608, France

John F. Wager
jfw@ece.orst.edu
- Oregon State University School of EECS
  4091 Kelley Engineering Center, Corvallis 97331-5501, United States

Anna Wajler
anna.wajler@itme.edu.pl
- Institute of Electronic Materials Technology (ITME)
  Warszawa 01919, Poland

Frank Walboomers
f.walboomers@dent.umcn.nl
- Radboud University Nijmegen Medical Centre (RUN-MC)
  po box 9101, Nijmegen 6500hb, Netherlands

Łukasz Wasilewski
piescirogi@tlen.pl
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

Bartlomiej J. Wasniewski
barva@poczta.onet.pl
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

Kinga Wawer
kiniac@o2.pl
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

Ludger Weisser
weisser@atomicforce.de
- ATOMIC FORCE GmbH
  Hauptstrasse 161, Mannheim 68-259, Germany

Amir Weizman
amirwa@bgu.ac.il
- Department of Materials Engineering, Ben Gurion University of the Negev
  Beer-Sheva 84105, Israel

Horst Weller
weller@chemie.uni-hamburg.de
- University of Hamburg, Institute of Physical Chemistry
  Grindelallee 117, Hamburg 20146, Germany

Horst Weller
weller@chemie.uni-hamburg.de
- University of Hamburg, Institute of Physical Chemistry
  Grindelallee 117, Hamburg 20146, Germany

Bernard Wenger
bernard.wenger@csem.ch
- Centre Suisse d'Electronique et de Microtechnique (CSEM)
  Jaquet-Droz 1, Neuchâtel 2002, Switzerland

Matthew S. White
matthew_white@nrel.gov
- National Renewable Energy Laboratory (NREL)
  1617 Cole Blvd, Golden, CO 80401, United States
- University of Colorado
  Boulder, CO 80309, United States

Lawrence C. Whitmore
whitmore@ustem.tuwien.ac.at
- University Service Centre for Transmission Electron Microscopy (USTEM)
  Wiedner Hauptstraße 8-10/138, Wien 1040, Austria

Ken Williams
ken.williams@renishaw.com
- Renishaw plc (SPD)
  Old Town, Bristol BS375UP, United Kingdom

Ken Williams
tracey.stokes@renishaw.com
- Renishaw Plc
Old Town Wotton under Bridge, Gloucestershire GL127DW, United Kingdom

Kent J. Williams
zordoh@phy.bg.ac.yu
- Renishaw (KPJ)
Finchley road 123, London 1180, United Kingdom

Mark Wilson
mark.wilson@chem.ox.ac.uk
- Oxford University, Physical and Theoretical Chemistry Laboratory
South Parks Road, Oxford OX1 3QZ, United Kingdom

Richard J. Winfield
richard.winfield@tyndall.ie
- University College Cork, Tyndall National Institute (TYNDALL)
Lee Maltings, Prospect Row, Cork, Ireland

Holger Winter
monika.lelonek@marcotech.de
- HiNanoAnalytics Network
Heisenbergstasse 11, Münster 48149, Germany

Paweł Wiśniewski
pawelwi@ch.pw.edu.pl
- Warsaw University of Technology, Faculty of Chemistry
Noakowskiego 3, Warszawa 00-664, Poland

Grzegorz Wojas
emrs.exhibit@gmail.com
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
Wołoska 141, Warszawa 02-507, Poland

Hon Fai Wong
07900999r@polyu.edu.hk
- Department of Applied Physics and Materials Research Centre,The Hong Kong Polytechnic University
Hung Hom, Kowloon, Hong Kong 00-852, China

Piotr Woźniak
pwozniak@ib.amwaw.edu.pl
- Medical University of Warsaw, Department of Biophysics and Human Physiology
Chałubińskiego 5, Warszawa 02-004, Poland

Jan Wróbel
jwrobel@if.pw.edu.pl
- Warsaw University of Technology, Faculty of Physics
Koszykowa 75, Warszawa 00-662, Poland

Rafał Wróblewski
rwroblewski@inmat.pw.edu.pl
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
Wołoska 141, Warszawa 02-507, Poland

Jeremy P. Wu
j.wu@irl.cri.nz
- Industrial Research Limited (IRL)
69 Gracefield Road, Wellington 5040, New Zealand

Andreas Wurm
andreas.wurm@uni-rostock.de
- University of Rostock, Inst. of Physics, Polymerphysics
Rostock 18051, Germany

Andrzej Wysmolek
Andrzej.Wysmolek@fuw.edu.pl
- University of Warsaw, Institute of Experimental Physics (IFDUW)
Hoża 69, Warsaw 00-681, Poland

Yaroslav I. Yakimov
yar_yakimov@mail.ru
- Siberian Federal University (SFU)
Krasnoyarskii rabochii 95, Krasnoyarsk 660095, Russian Federation

Boris I. Yakobson
biy@rice.edu
- Rice University
6100 Main St., Houston, TX 77005, United States

Daizo Yamaguchi
hp_yamaguchi@newkast.or.jp
- Kanagawa Academy of Science and Technology (KAST)
3-2-1 Sakado, Takatsu-ku, Kawasaki 213-0012, Japan

Yang Yang
yangyang@mpi-halle.de
- Max Planck Institute of Microstructure Physics (MPI)
Weinberg 2, Halle 06120, Germany

Yingbang Yao
yaoyingbang@126.com
- Department of Applied Physics, The Hong Kong Polytechnic University, Hung Hom, Kowloon
Hong Kong 00852, Hong Kong

Nazdaneh Yarahmadi
nazdaneh@sp.se
- SP Technical Research Institute of Sweden (SP)
Brinellgatan 4, Boras 50115, Sweden

Yin Ye
yeyinthu@gmail.com
- The Hong Kong Polytechnic University (HK, PolyU)
  Hung Hom, Hong Kong, Hong Kong

Onur Yilmaz
onuryilma@gmail.com
- Ege University, Leather Engineering Department
  Ege University Campus, İzmir 35100, Turkey

Chul Yoon
xefe26@kut.ac.kr
- Korea University of Technology and Education
  Cheonan 330-708, Korea, South

Andrew P. York
ayork@matthey.com
- Johnson Matthey Technology Centre
  Blount's Court, Reading RG49NH, United Kingdom

Gleb Yurkov
iourkov@rambler.ru
- Kurnakov Institute of General and Inorganic Chemistry RAS (IGIC)
  Leninsky prospect, 31, Moscow 119991, Russian Federation

Dietrich RT Zahn
zahn@physik.tu-chemnitz.de
- Technische Universitdt Chemnitz, Institut fur Physik
  Chemnitz D-09107, Germany

Mikołaj Zając
m.zajac@prevac.pl
- Prevac sp. z o.o.
  Raciborska 61, Rogów 44-362, Poland

Mikołaj Zając
m.zajac@prevac.pl
- PREVAC sp. z o.o. (PREVAC)
  Raciborska 61, Rogów 44-326, Poland

Ilmars Zalite
ilmars@nki.lv
- Institute of Inorganic Chemistry, Riga Technical University
  Riga LV-2169, Latvia

Eugenio Zapata-Solvas
ezapata@us.es
- Universidad de Sevilla (USE)
  Sevilla 41012, Spain

Teresa Zaremba
teresa.zaremba@polsl.pl
- Silesian University of Technology, Department of Inorganic Chemistry and Technology
  ul. Krzywoustego 6, Gliwice 44-100, Poland

Ewelina A. Zawadzak
ewelina205@wp.pl
- Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
  Wołoska 141, Warszawa 02-507, Poland

Anita Zeidler
az207@bath.ac.uk
- University of Bath, Department of Physics
  Claverton Down, Bath BA27AY, United Kingdom

Weiqing Zheng
zheng@fhi-berlin.mpg.de
- Fritz-Haber-Institute of Max-Planck-Gesellschaft
  Faradayweg 4-6, Berlin D-14195, Germany

John Zhuang
jzhuang@chemcat.com
- Chemcat Technology
  9034 Winnetka Ave, Northridge 91324, United States

Mark S. Zhukovskiy
zhukovsky@list.ru
- Altai State Technical University (ASTU)
  Lenin st.46, Barnaul 656038, Russian Federation

Janis Zicans
zicans@ktf.rtu.lv
- Riga Technical University (RTU)
  Azenes St. 14/24, Riga LV-1048, Latvia

Cordt Zollfrank
cordt.zollfrank@ww.uni-erlangen.de
- University of Erlangen-Nürnberg, Glass and Ceramics
  Martenstr.5, Erlangen 91058, Germany

Konrad Zubko
kzubko@wat.edu.pl
- Military University of Technology (WAT)
  Kaliskiego 2, Warszawa 00-908, Poland

Index