The European Materials Conference

E-MRS 2004
FALL MEETING

European Materials Research Society
Fall Meeting

Warsaw University of Technology
Warsaw (Poland)

6th – 10th September, 2004

Conference Organisers:
Polish Materials Society
Warsaw University of Technology
Institute of Physics, Polish Academy of Sciences
High Pressure Research Center, Polish Academy of Sciences
European Materials Research Society, E-MRS

THE E-MRS FALL MEETING CONFERENCE CHAIRMEN:

K. Kurzydłowski,	Warsaw University of Technology
W. Łojkowski,	High Pressure Research Center, Polish Academy of Sciences
A. Mycielski,	Institute of Physics, Polish Academy of Sciences
P. Siffert,	European Materials Research Society, France

The European Materials Research Society

The European Materials Research Society (E-MRS) is a non profit scientific association founded in 1983 with its Headquarters in Strasbourg, France. The Society focuses its activity on creating synergy from the interactions between interdisciplinary, innovative fields of materials research. Great attention is given to 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 about the scientific and technological developments in their fields of interest, taking advantage of the society's links with other Materials Research Societies belonging to the International Union (IUMRS).

The 2004 Fall Meeting will include 9 symposia. The conference will also include an exhibition of products and services of interest to those participating in the event as well as training activities for young researchers or scientists wishing to extend their expertise to new fields.

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E-MRS European Co-ordination Group

H. Grimmeiss	E-MRS President
P. Siffert	E-MRS General Secretary
A. Slaoui	E-MRS Vice-President

Welcome

We are pleased to welcome delegates to the 2004 Fall Meeting of the European Materials Research Society, E-MRS, being held at Warsaw University of Technology.

This event is the third time E-MRS has held a Fall Meeting, in addition to the Annual Spring Meeting, held each May/June in Strasbourg, France. The 2003 Spring Meeting marked the twentieth anniversary of the Society which now holds the largest materials science conference in Europe. The inaugural E-MRS Fall Meeting in 2002 was held in three locations: Moscow, on Software Development for Process and Materials Design; Warsaw, Interfacial Effects and Novel Properties of Nanomaterials; and Zakopane, on Solid Solutions of the II-VI Compounds, Growth, Characterization and Applications.

The great success of the 2002 Meetings, both in scientific quality and organization, led to the E-MRS deciding to hold Fall Meetings in Warsaw. The organizers have followed the theme developed over the years by the Society to host a wide ranging multi-disciplinary conference to bring established scientists with a world reputation together to share experiences and state of the art knowledge. A very important philosophy of E-MRS is to facilitate scientific and social contacts between established researchers, young scientists and doctoral students. The 2004 Fall Meeting will endeavour to continue these themes and further enhance the contacts between scientists from Western and Eastern Europe, North America and Asia.

The 2004 Fall Meeting comprises nine parallel symposia and 2 Plenary Sessions which are being held in the morning on the first two days of the Conference 6th and 7th September.

The Conference Organizers and Committee hope that the E-MRS Fall Meeting meets your expectations, provides enlightenment in your subject area, enables you to make new contacts and, very importantly, proves to be a worthwhile and enjoyable experience from the scientific and social viewpoint.

Acknowledgements

THE E-MRS FALL MEETING 2004

is supported by:

kbn STATE COMMITTEE FOR SCIENTIFIC RESEARCH	Polish Ministry of Science and Information Technology
PTM POLSKIE TOWARZYSTWO MATERIAŁOZNAWCZE	The Polish Materials Society (PMS)
	Faculty of Materials Science, Warsaw University of Technology
IF PAN	Institute of Physics, Polish Academy of Sciences
unipress	High Pressure Research Center "UNIPRESS" Polish Academy of Sciences
	The European Commission Contract: No. G1MA-CT-2002-04055 Contract: No. ICA1-CT-2002-60028
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Local Arrangements

Hotel reservation and parcitipation in tourist programme can be arranged through the web site http://www.e-mrs.org/meetings/fall2004 by the Local Arrangements:

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Conference programme

PLENARY SESSIONS:

1. Monday, September 6, 9.00 - 12.30
2. Tuesday, September 7, 9.00 - 10.30

POSTER SESSIONS:

1. Monday, September 6, 19.00 - 21.00
2. Wednesday, September 8, 19.00 - 21.00

SYMPOSIUM A, Room 219:

NANOSTRUCTURED MATERIALS AND NANOTECHNOLOGIES FOR NEW CHEMICAL SENSORS AND ALTERNATIVE ENERGY DEVICES

SYMPOSIUM B, Room 213:

PROGRESS IN POLYMERIC MATERIALS FOR MEDICINE AND BIOLOGY

SYMPOSIUM C, Room 206:

SCIENCE AND TECHNOLOGY OF NITRIDES AND RELATED MATERIALS

SYMPOSIUM D, Room 226:

APPLICATIONS OF LINEAR AND AREA DETECTORS FOR X-RAY AND NEUTRON DIFFRACTION AND SPECTROSCOPY

SYMPOSIUM E, Room 144:

SUPERCONDUCTORS - NEW DEVELOPMENTS, NEW MATERIALS, NEW APPLICATIONS AND NANOSCALE INVESTIGATIONS

SYMPOSIUM F, Room 134:

WIDE BAND GAP II-VI SEMICONDUCTORS; GROWTH, CHARACTERIZATION AND APPLICATIONS

SYMPOSIUM G, Room 208:

FUNCTIONALISATION OF NANOPARTICLES

SYMPOSIUM H, Room 231:

COMPUTATIONAL MATERIALS SCIENCE

SYMPOSIUM I, Small Hall (Mała Aula):

METAL BASED NANOMATERIALS, THIN FILMS AND SURFACE STRUCTURES

Joint SYMPOSIUM G&I, Small Hall (Mała Aula):

organized by Symp G and I of EMRS Fall Meeting, the Network "Nanostructred materials" and Center of Excellence Prenabio.

Satellite events coordinated with the E-MRS Meeting:

▷ Funding and Investment Opportunities

in Poland and Central Europe - a European and International Perspective

Workshop, 5-6 September, Warsaw University of Technology

▷ Advanced Materials for Radiation Detectors and Sensors:

Wide-gap semiconductors and superconductors - NATO Advanced Research Workshop

Workshop, 8-10 September, Warsaw University of Technology

▷ Intergranular and interphase boundaries

- experimental techniques of investigation and computer simulation methods

Workshop, 1-4 September, Warsaw University of Technology, Faculty of Materials Science & Engineering

▷ Introduction to MS Modeling 3.0

Workshop, 6-7 September, ICM, Warsaw University of Technology

▷ Introduction to MedeA modeling

Workshop, 9 September, ICM, Warsaw University of Technology

Introduction

The E-MRS 2004 Fall Meeting will consist of the two Plenary Sessions, and 9 separate scientific symposia which will run concurrently.

The Opening Ceremony will take place on Monday 6th September at 8:45 am. To facilitate the exchange of ideas and information, especially between the experienced scientists, and between the researchers from different areas of interest - poster sessions, common for all the symposia, will be organized on Monday, September 6, 19.00-21.00 and Wednesday, September 8, 19.00-21.00.

The detailed timetable and abstracts for papers to be presented in each symposium will be found in the appropriate section.

The Polish Materials Society

The Polish Materials Society (PMS) was founded in 1995 with the aim of promoting and propagating materials sciences and engineering. Currently the PMS unites 160 specialists in materials engineering employed in various centres in Poland and Europe. The Society has two Sections: one established in Kraków and the other in Gdańsk. Under the patronage of the PMS President, an annual competition is organised for the best doctor's thesis in the field of materials engineering. The Society is a co-publisher of the scientific journal entitled Inżynieria Materiałowa (Materials Engineering) which publishes papers (subject to referee's reviews) in the Polish and English languages. The journal is devoted to materials problems, and is particularly concerned with metallic materials, various forms of plastics, ceramics and composites related to their application, and also promotes modern developments in surface engineering. During the last years, the PMS was the co-organiser of numerous conferences.

The Evolution of Warsaw University of Technology

At the end of the 19th century, Poland was partitioned by three invader powers: Russia, Prussia, and the Austro-Hungarian Empire. Warsaw was then the capital of the Kingdom of Poland which was a part of the Russia Empire.

At that time, efforts were made by Polish scientists to establish a technical university in Warsaw. In 1897 a special committee drafted a memorandum to the General Governor, Prince Alexander Imeretyński, justifying the need for an institution of higher technical education in the Kingdom of Poland. In January 1898, the Governor endorsed the initiative in his own memorandum submitted to Tzar Nicholas II. During the Tzar's visit to Warsaw, he was presented with one million gold roubles donated by members of Polish society, with the suggestion that the money should be used to found a technical university in Warsaw. Tzar Nicholas II expressed the official approval for the establishment of a technical university provided that the funds needed to build and furnish it, an additional 2.5 million roubles, would be collected by Polish society. The royal decree sanctioning the establishment of the Tzar Nicholas II Warsaw Polytechnical Institute was published in June 1898.

The ceremony to lay the foundation stone of the Institute's Main Building took place in August 1898. Thanks to the rapid rate of the construction work, classes began in the new building in the autumn of 1901 although the Physics and Electrical Engineering Building, Mechanics Building, and the Chemistry Building were still under construction.

During the First World War, when the Russian army was in the retreat, most of the movable property of the Polytechnical Institute (i.e., libraries, experimental and laboratory equipment, etc.) was taken to Russia.

In the interwar period, a few thousand engineers graduated from the Polytechnical Institute, renamed as the Warsaw University of Technology.

During the Second World War, the University of Technology buildings were largely destroyed, especially during the Warsaw Uprising of August 1944. The University Buildings were reconstructed and modernized to meet the then current needs in the immediate post-war period, 1945-48.

Exhibitors

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COST - the acronym for European COoperation in the field of Scientific and Technical Research - is the oldest and widest European intergovernmental network for cooperation in research. Established by the Ministerial Conference in November 1971, COST is presently used by the scientific communities of 35 European countries to cooperate in common research projects supported by national funds. The funds provided by COST - less than 1% of the total value of the projects - support the COST cooperation networks (COST Actions) through which, with only around €20 million per year, more than 30.000 European scientists are involved in research having a total value which exceeds €2 billion per year. This is the financial worth of the European added value which COST achieves. A “bottom up approach” (the initiative of launching a COST Action comes from the European scientists themselves), “à la carte participation” (only countries interested in the Action participate), “equality of access” (participation is open also to the scientific communities of countries not belonging to the European Union) and “flexible structure” (easy implementation and light management of the research initiatives) are the main characteristics of COST. As precursor of advanced multidisciplinary research COST has a very important role for the realisation of the European Research Area (ERA) anticipating and complementing the activities of the Framework Programmes, constituting a “bridge” towards the scientific communities of emerging countries, increasing the mobility of researchers across Europe and fostering the establishment of “Networks of Excellence” in many key scientific domains such as: Physics, Chemistry, Telecommunications and Information Science, Nanotechnologies, Meteorology, Environment, Medicine and Health, Forests, Agriculture and Social Sciences. It covers basic and more applied research and also addresses issues of pre-normative nature or of societal importance.

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Timetable of Events

Sunday 5th September

19:00 – 21:00 **Welcome reception, Main Hall**

Monday 6th September

08:45 – 09:00 **OPENING CEREMONY Small Hall (Mała Aula)**
Chairman: Professor H. Grimmeiss, President of E-MRS

PLENARY SESSION Small Hall (Mała Aula)

Chairman: Professor H. Grimmeiss, President of E-MRS

09:00 – 09:45 **Jose-Lorenzo Vallés-Brau**
Materials Research in The Sixth Framework Programme
Directorate-General for Research, Materials Unit
European Commission, Brussels, Belgium

09:45 – 10:30 **Erich Wimmer**
The growing importance of computations in materials science:
current capabilities and perspectives.
Materials Design s.a.r.l.

10:30 – 11:00 **Coffee Break** Main Hall (Duża Aula)

Chairman: Dr. Jose-Lorenzo Vallés-Brau, European Commission, Brussels

11:00 – 11:45 **Helmut Schmidt**
Chemical nanoparticle fabrication and processing -
from the basic to applications
INM-Institute for New Materials, Germany

11:45 – 12:30 **Richard W. Siegel, Robert W. Hunt**
Assembling Materials from Nanoscale Bulding Blocks
Rensselaer Nanotechnology Center, U.S.A.

12:30 – 14:00 **Lunch**

14:00 **INDIVIDUAL SYMPOSIA**
See plan of WUT for the location of each symposium

19:00 – 21:00 **POSTER SESSION Main Hall (Duża Aula)**

Tuesday 7th September

PLENARY SESSION Small Hall (Mała Aula)

Chairman: Professor Paul Siffert, General Secretary of E-MRS

09:00 – 09:45	**Tomasz Dietl** Wide band gap semiconductor as spintronic and ferromagnetic materials Institute of Physics, Polish Academy of Sciences, Warsaw
09:45 – 10:30	**Hugo Keller** Isotope effect in cuprate superconductors Physik-Institut der Universität Zürich
10:30 – 11:00	**Coffee Break** Main Hall (Duża Aula)
11:00	**INDIVIDUAL SYMPOSIA** See plan of WUT for the location of each symposium
20:00	**Dinner** – *tickets available at Registration Desk (price: 50 EUR)*

Wednesday 8th September

09:00 – 18:00	**INDIVIDUAL SYMPOSIA A-I** See plan of WUT for the location of each symposium
19:00 – 21:00	**POSTER SESSION** Main Hall (Duża Aula)

Thursday 9th *and* Friday 10th September

09:00 – 18:00	**INDIVIDUAL SYMPOSIA A-I** See plan of WUT for the location of each symposium

Coordinated satellite events

Wednesday 8th – Friday 10th, Room 134 and 144
09:00 – 18:00 **NATO Advanced Research Workshop**
see Programme of NATO ARW

Wednesday 1st – Saturday 4th, Faculty of Materials Science & Engineering
09:00 – 18:00 Workshop **"Intergranular and interphase boundaries - experimental techniques of investigation and computer simulation methods"**

Sunday 5th 14:00 – 16:45, Small Hall (Mała Aula)
Monday 6th 14:00 – 15:30, Small Hall (Mała Aula)
Special session **"Funding and Investment Opportunities in Poland and Central Europe - a European and International Perspective"**

Monday 6th 15:50 – 17:15, Small Hall (Mała Aula)
Tuesday 7th 11:00 – 12:30, Small Hall (Mała Aula)
Special workshop jointly organized by **Symp G and I** of EMRS Fall Meeting, the Network "Nanostructred materials" and Center of Excellence Prenabio
held at ICM, Warsaw University

Monday 6th – Tuesday 7th
10:00 – 16:00 Workshop **"Introduction to MS Modeling 3.0"**
held at ICM, Warsaw University

Thursday 9th
10:00 – 16:00 Workshop **"Introduction to MedeA modeling"**
held at ICM, Warsaw University

Book of Abstracts

Plenary session

Invited talks of Plenary session

Monday, September 6th

Opening address

Main Building, Small Hall (Mała aula)

08:45 - 09:00

Morning session

Main Building, Small Hall (Mała aula)

09:00 - 10:30

Materials Research in the Sixth Framework Programme

09:00 - 09:45
invited oral

Jose-Lorenzo Vallés-Brau[1)]

1) European Commission, Directorate-General for Research, Unit G3 "Materials", Brussels B-1049, Belgium

In 2000 the European Commission launched the idea of creating a European Research Area (ERA), where the scientific capacity in the Member States can be put to best use, where national and European policies can be implemented more coherently, where researchers and knowledge can circulate more freely, and which is also attractive to the best researchers from Third Countries. This strategy was then adopted by the European Council in Lisbon, with the ultimate goal to enable the European Union to become the most competitive and dynamic knowledge economy. The 6th Framework Programme (2002-06) has therefore been designed to have a higher integrating, structuring and strengthening effect on European Research, and to support industrial innovation. The third of the seven Thematic Priorities is devoted to "Nanotechnologies and Nanosciences, knowledge-based multifunctional materials and new production processes and devices". This priority, and in particular its component related to Materials, clearly represents an area where it is very promising to realise the ERA, as there is a need for multidisciplinary and multisectoral efforts. Under the 6th Framework
Programme there is a wider range of instruments to implement the Thematic Priorities. The two new instruments called Networks of Excellence and Integrated Projects have a high level of management autonomy and are expected to have the capacity to mobilise the critical mass of expertise needed to achieve ambitious objectives, and to have strong structuring and integrating effects. After introducing the main features of the 6th Framework Programme, and in particular of its Thematic Priority 3, the results of the First and Second Calls for proposals, which had deadlines in Spring 2003 and in Spring 2004, are commented. Finally, some information is provided on the preparations for the Third Call, and in particular with regard to the research areas which are likely to be open.

The growing importance of computations in materials science: current capabilities and perspectives

09:45 - 10:30
invited oral

Erich Wimmer[1)]

1) Materials Design, 44 avenue F.-A. Bartholdi, Le Mans 72000, France

Materials scientists are facing unprecedented challenges in a large number of areas including energy storage, microelectronics, display technologies, catalysis, and environmental degradation of structural materials. Advances in experimental methods, for example the use of synchrotron light sources and high-throughput synthesis produce massive amounts of data, which need to be interpreted. At the same time, new computational methods are being developed and the efficiency of computer hardware and software continues to increase rapidly. As a result, the importance of computational materials science is growing. Computations serve three major objectives: (i) they provide insight and allow the interpretation of experimental data, (ii) they offer guidance for new experimental efforts by computational pre-screening, and (iii) they allow the prediction of materials properties, which may be difficult or even impossible to measure directly. As illustrative cases, this lecture will focus on the areas of energy storage, notably hydrogen storage materials, the environmental degradation of structural materials, microelectronic materials, and catalysis. With the calculation of phonon dispersions, which has now become possible on a routine basis for large structures, temperature dependent thermodynamic functions can be evaluated systematically. Recent results, especially for metal-hydrogen systems reveal that the electronic total energy, even if calculated at a high level of accuracy, might be insufficient to make quantitative predictions of actually measurable properties such as formation and reaction enthalpies. A critical assessment will be provided of the current capabilities of predicting structural, thermomechanical, electronic, optical, and magnetic materials properties. A perspective on current and future scientific developments, their priorities and their impact on academic and industrial research strategies will conclude this contribution.

10:30 - 11:00

Coffee break

11:00 - 12:30

Morning session - continued

Main Building, Small Hall (Mała aula)

11:00 - 11:45
invited oral

Chemical nanoparticle fabrication and processing from the basics to application

Helmut Schmidt[1)]

1) Leibniz-Institut für Neue Materialien (INM), Im Stadtwald, Geb. 43 A, Saarbrücken 66123, Germany

Wet processing technologies have been developed for the synthesis of nanoparticles with tailored surfaces. The bottom-up as well as the top-down have been investigated. It could be shown that using this approach, dry powder handling could be avoided completely leading to a contamination-free and non-hazardous processing route. Nanoparticles with desired func-tional groupings were synthesized and various applications have been developed. Epoxy group functionalized nanoparticles have been used for the development of a star type poly-urethane nanocomposite showing extremely high abrasion resistance. Zirconia and tantalum oxide nanoparticles coated with polymerizable groupings have been used for the develop-ment of a new concept called photoinduced diffusion. By two-wave mixing or mask technol-ogy, an up-concentration of the high-reflective index nanoparticles has been obtained and light guidance foils for the display techniques have been developed. Other surface modified nanoparticles (ion oxide superparamagnetic particles) show a significant discrimination for the penetration of cell membranes. Tumor cells are penetrable and healthy cells not. Based on these results, Charité at Berlin developed a technology for tumor therapy. These few ex-amples show that nanoparticle technology for materials lead to highly interesting applica-tions. For the realisation, it was necessary to develop the complete line, starting with the ba-sics and ending up with the production technology.

11:45 - 12:30
invited oral

Assembling Materials From Nanoscale Building Blocks

Richard W. Siegel[1)]

1) Rensselaer Polytechnic Institute, Troy, NY, United States

The past decade has seen explosive growth worldwide in the synthesis and study of a wide range of nanostructured materials, the substance of nanotechnology. An overview of nanoscience and nanotechnology and their relationship to novel functional materials assembled from nanoscale building blocks will be presented within the framework of the U.S. National Nanotechnology Initiative and our Center for the Directed Assembly of Nanostructures at Rensselaer. Several examples from our recent research results will be presented including investigations of multifunctional nanocomposites that could find use in a variety of structural, electrical, and biomedical applications. Future opportunities and challenges in this exciting area will be discussed.

Lunch break

12:30 - 14:00

Tuesday, September 7th

Morning session

Main Building, Small Hall (Mała aula)

09:00 - 10:30

Wide band gap semiconductors as spintronic and ferromagnetic materials

09:00 - 09:45
invited oral

Tomasz Dietl[1,2]

1) Polish Academy of Sciences, Institute of Physics, al. Lotnikow 32/46, Warszawa 02-668, Poland

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In the recent years a considerable effort has been devoted to understand the nature of carrier-controlled ferromagnetism in tetrahedrally coordinated diluted magnetic semiconductors. In these materials conceptual difficulties of charge transfer insulators and strongly correlated disordered metals are combined with intricate properties of heavily doped semiconductors, such as Anderson-Mott localization and defect creation by self-compensation mechanisms. Nevertheless, I will argue that (Ga,Mn)As and related compounds have become the best understood ferromagnets. In particular, the theory built on Zener's model of ferromagnetism and the Kohn-Luttinger kp theory of semiconductors describes quantitatively the thermodynamic, micromagnetic, optical, and transport properties of these systems. Moreover, the understanding of these materials has provided a basis for the development of novel methods enabling magnetisation manipulation and switching. In the context of spintronics, however, especially promising are the group III nitrides and group II oxides. In these systems, the short bond length results in a strong hybridisation between valence band states and open d shells of transition metal impurities, which is predicted to enhance the Curie temperature of the hole-mediated ferromagnetism. While spontaneous magnetisation persisting above room temperature has been detected for a number of magnetically doped nitrides and oxides, we are still at the beginning of the road to understanding and controlling doping, defects, and magnetism of these systems. A review of pertinent experimental results will be presented together with models put forward for their interpretation. The work was partly supported by AMORE and FENIKS EC projects, by Humboldt Foundation, and carried out in collaboration with M. Sawicki, P. Kossacki, and T. Andrearczyk in Warsaw, as well as with groups of H. Ohno, J. Cibert, B. Gallagher, and A.H. MacDonald (a review: MRS Bulletin, October 2003, p. 714)

Unconventional isotope effects in cuprate superconductors

09:45 - 10:30
invited oral

Hugo Keller[1]

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A brief review on unconventional oxygen-isotope ($^{16}O/^{18}O$) effects (OIE) in cuprate high-temperature superconductors (HTS) is presented. First the doping dependence of the OIE on the superconducting transition temperature T_C in various HTS is discussed. For all cuprate HTS families the OIE exponent of T_C (α_O) shows a generic trend: In the underdoped regime α_O is large ($\alpha_O > 0.5$) and becomes small in the optimally doped and overdoped regime. Magnetization, magnetic torque, and muon-spin rotation OIE studies of the in-plane penetration depth $\lambda_{ab}(0)$ in doped $La_{2-x}Sr_xCuO_4$ and $Y_{1-x}Pr_xBa_2Cu_3O_{7-\delta}$ indicate a substantial oxygen-mass dependence of the quantity $\lambda_{ab}{}^{-2}(0)$, proportional to the superfluid density $\rho_s(0)$ which increases with reduced doping. Even at optimal doping, where the OIE on T_C is small, a pronounced OIE on $\lambda_{ab}(0)$ is present [1]. Note that an OIE on the penetration depth is not expected for a conventional phonon-mediated superconductor (for which the Migdal adiabatic approximation holds). The oxygen-isotope shifts of T_C and $\lambda_{ab}(0)$ exhibit a correlation that appears to be generic for various families of HTSC. Site-selective OIE investigations of $Y_{1-x}Pr_xBa_2Cu_3O_{7-\delta}$ clearly reveal that the planar oxygen atoms mainly contribute to the total OIE on T_C as well as on $\lambda_{ab}(0)$ at all doping levels. These unusual isotope effects strongly suggest that lattice effects play an essential role in the basic physics of cuprate HTS and have to be considered in any realistic theoretical model.

[1] R. Khasanov et al., Phys. Rev. Lett. 92, 057602-1 (2004).

Coffee break

10:30 - 11:00

Symposium A

Nanostructured materials and nanotechnologies for new chemical sensors and alternative energy devices

Introduction

This symposium will focus on the synthesis, processing, characterization, and modelling of nanostructured materials and their potential use as "nanoscale building blocks" for new electrochemical and catalytic properties; gas sensing mechanisms and energy management. Nanoscale structures can dramatically alter surface reaction rates and electrical transport, resulting in improvements in the electrochemical processes, gas sensing mechanisms and energy storage, conversion, and generation.

This symposium will focus on the structure-property relationship of nanomaterial surfaces. Especial emphasis will be devoted on the ability to design and control the structure of the nanocrystal surface and grain boundaries. Successful design of nanoscale materials,-nanoparticles, nanowires and nanotubes, and related alternative nanostructured materials- could lead to a wide range of novel devices and technologies useful and essential for the new generation of chemical sensor and alternative energy devices. This symposium aims also to discuss the most recent and relevant results pertaining to electrochemical and catalytic properties of nanomaterials, as well as their application to the chemical sensor and to alternative energy devices. Likewise, it will address the relations among synthesis, structures, and physics-chemical properties of nanoscale materials, studied using experiments and/or modelling. The focus will be on new phenomena observed in nanostructured materials when the characteristic length scales (such as grain size or layer thickness) approach nanometer dimensions.

Organisers

- Joan Ramon Morante, EME/CEMIC Dept. Electronics, University of Barcelona, Faculty of Physics
- G. Korotchenkov, Technical University of Moldova

Monday, September 6th

14:00 - 15:30

Afternoon session

Main Building, room 219

Quasi-one-dimensional nanostructures of semiconductor oxides for gas sensing

14:00 - 14:30
invited oral

GIORGIO SBERVEGLIERI[1)], **FAGLIA GUIDO**[1)], **CAMILLA BARATTO**[1)], **ELISABETTA COMINI**, **M ZHA**[2)], **ANDREA ZAPPETTINI**[2)]

1) INFM & UNIVERSITY OF BRESCIA (INFM), VIA VALOTTI 9, BRESCIA 25133, Italy

2) IMEM- CNR (IMEM), PARMA, Italy

Newly developed metal oxide nanobelts and nanorings are potential candidates for fabrication of nanoscale devices. Their extraordinary sensing properties have been recently shown for ultra sensitive gas and DNA detection The finite size of the metal oxide wires confines the electrons wave functions, leading to quantized energy levels and to a huge modification of the transport and optical properties of the material. The hugely enhanced surface/volume ratio augments the role of surface states in the sensor response.
Worldwide most recent research in the field of quasi one-dimensional inorganic structures for gas sensing and some promising results achieved at Sensor Lab in Brescia Italy in conductometric and visible photoluminescence quenching will be discussed.
Gas sensors based on the SnO2 and ZnO nanobelts, synthesized by thermal evaporation of oxide powders under controlled conditions, have been fabricated. Electrical characterization showed that these nanobelts were very sensitive to the surrounding atmosphere. The results show the experimental feasibility of fabricating nano-size sensors using the integrity of individual nanobelts.
The visible photoluminescence (PL) of tin oxide nanobelts is quenched by nitrogen dioxide at ppm level in a fast (time scale order of seconds) and reversible way. Besides the response seems highly selective towards humidity and other polluting species like CO and NH3. Adsorbed gaseous species that create surface states can quench PL by creating competitive non-radiative paths. PL change produced by the gaseous environment depends on: nanostructure size and shape, crystalline face exposed to the surrounding environment, surface oxygen vacancies and sample pre-treatment in oxidizing or reducing atmosphere. A comparison between conductometric and PL response suggests that the two response are ascribable to different adsorption processes.

Production of nanostructured gas sensor arrays and electrical characterization of deposited tin oxide nanoparticles in ambient gas atmosphere

14:30 - 14:45
oral

Tim P. Huelser[1,2)], **Hartmut Wiggers**[1)], **Axel Lorke**[2)]

1) University Duisburg-Essen; Institute of Combustion and Gas dynamic (IVG), Duisburg 47048, Germany

2) University Duisburg-Essen; Institute of Physics, Lotharstrasse 1, Duisburg 47048, Germany

In the past decade, nanostructured materials have increasingly played an important role in the area of gas sensing. Tin oxide SnO_2 is one of the most widely investigated sensor materials and is commonly used for environmental monitoring.
SnO_2 nanoparticles with small particle size distribution (σ <1.1), and diameters of 10nm, 15nm and 20nm have been deposited on platinum interdigital transducers with 2μm finger width and 2μm spacing. Impedance spectroscopy measurements in synthetic air, taken in the temperature range between 373 K and 573 K show a clear dependence of the measured impedance on the particle size. Three different contributions to the overall impedance have been resolved for 10nm particles and assigned to the contribution of bulk, intergranular contact (IC) and electrode contact (EC). Particles of larger diameters do not allow such a clear distinction. The experimental observations have been analyzed by fitting the measured data with equivalent circuit functions, where typical serial connections of R and parallel RCs are used for fitting. As expected for a semiconducting material, the resistance decreases with increasing temperature. Activation energies of the different charge carrier transport processes have been determined from Arrhenius plots. The calculated values are -499meV for IC, -126meV for EC and -27meV for bulk contribution. The measured data indicate that the gas sensing mechanism is dominated by the EC and that the IC is dependent on the particle size.
For detailed information on these correlations, short period sensor arrays have been produced. Interdigital

structures with a total width of 55μm and length of 100μm were written using electron beam lithography. The width of the contacts and their distances are varied between 100 nm and 1000 nm. Nanosized SnO_2 particles from a microwave reactor were mass separated within a particle mass spectrometer and consequently deposited on different interdigital structures.

OPTICAL SENSORS FOR BIOCHEMICAL MOLECULES BASED ON POROUS SILICON TECHNOLOGY

14:50 - 15:05
oral

Luca De Stefano[1)], **Luigi Moretti**[1)], **Ivo Rendina**[1)], **Paolo Arcari**[2)], **Annalisa Lamberti**[2)]

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2) Dipartimento di Biochimica e Biotecnologie Mediche, Università degli Studi di Napoli "Federico II" (DBBM), Napoli 80100, Italy

Porous silicon (PSi) can be used as smart transducer material in sensing application, and in particular in the detection of vapors, liquids and biochemical molecules. In fact, on exposure at chemical substances, several physical quantities, such as refractive index, photoluminescence, and electrical conductivity, change drastically. A key feature of a physical transducer, being sensitive to organic and biological molecules, either in vapor and liquid state, is a large surface area: PSi has a porous sponge-like structure with a specific area of the order of 200 - 500 m2cm-3, so that it can assure a very effective interaction with several adsorbates. Moreover, PSi is an available, low cost material, compatible with standard IC processes, so that it could usefully be employed in the realization of smart sensors and microsystems. In particular, in the last years, a lot of experimental work has been reported concerning its use as optical sensors in chemical and biological sensing. PSi monolayers were used as trial substrates in order to attach synthetic oligonucleotides for biosensing purposes. The critical issue in DNA recognition is the chemistry of the probe-oligonucleotides immobilization on the PSi surface, from which seems to depend on the stable and affordable sensor operation. Many of the results carried out to day, derived from the standard DNA immobilization chemistry exploited on silicon-oxide rich substrates (such as glass), involve the silanization of the oxidized PSi surface. A promising recently proposed alternative is that exploiting the reaction of acids molecules with the hydrogen-terminated porous silicon surface in order to obtain a more stable organic layer covalently attached to the PSi surface through Si-C bonds. In this work, we present new results about sensing of bio-chemical substances based on the functionalization of the hydrogen-terminated porous silicon surface by means of Si-C bonds.

An ammonia sensor based on porous SiC

15:10 - 15:25
oral

Eamon J. Connolly[1)], **Bjorn Timmer**[2)], **Mai Hoa T. Pham**[1)], **Jan Groneweg**[1)], **Lina Sarro**[1)], **Wouter Olthuis**[2)], **Paddy French**[1)]

1) University of Technology Delft, Rotterdamseweg 137, DELFT 2628 AL, Netherlands

2) University of Twente, Faculty of Science and Technology, Low Temperature Division and MESA+ Research Institute, Postbus 217, Enschede 7500 AE, Netherlands

Porous SiC has been found to be extremely sensitive to the presence of ammonia (NH3) gas. We report the fabrication and preliminary characterisation of NH3 sensors based on porous SiC and Al electrodes. The idea of the SiC is that it is a very durable material and that it should be good for sensors in harsh environments. Until now the only NH3 sensors using SiC have been FET based, and the SiC was not porous. The SiC was deposited by PECVD on standard p-type single-crystal Si and was made porous by electrochemical etching in 73% HF and anodisation current-densities of 1-50mA/cm2. Because the etch-rate of Al in 73% HF is very low, we can use Al electrodes instead of Au. This also facilitates our sensor fabrication, as Al is more cleanroom friendly than Au. Preliminary data is given for our devices response to NH3 in the range 0-10ppm NH3 in dry N2 carrier gas.

Coffee break

15:30 - 15:50

TPD analysis of the CO2 detection mechanisms using LaOCl sensing material

15:30 - 15:45
oral

Andreu Marsal[1], **F. Bimbela**[2], **C. Téllez**[2], **J. Coronas**[2], **A. Cornet**[1], **Joan R. Morante**[1]

1) Electronics Department, University of Barcelona, C/ Martí i Franqu?s, Barcelona 08028, Spain

2) Dpt. of Chemical & Environmental Engineering, Faculty of Science, University of Zaragoza, Zaragoza 50018, Spain

LaOCl has recently been proposed as an alternative material to perform a resistive solid state based CO2 gas sensor. After the main sensing characteristics of LaOCl material have been tested, the sensing mechanisms which describe the interaction with CO2 need to be sorted.
In this topic, TPD -thermal programmed desorption- measurements introduce meaningful information about available types of adsorption sites as well as the way in which key species are chemisorbed onto the material surface.
In this work we will present TPD experiments performed on two different LaOCl samples obtained through different synthesis routes.
From previous studies, the role of hydrated carbonate-like species is known to be a key point in the sensing mechanisms, thus, the desorption peaks of CO2 and water are specially examined.
TPD experiments show two differentiated CO2 peaks, on one hand a low temperature peak likely due to the physisorption and, on the other, a higher temperature peak associated with an analogous H2O one that confirms the presence of above-mentioned carbonate-like hydrated species.
Morphological and structural characterisation of samples has been performed using several techniques like XRD, TEM and XPS. These studies highlighted important morphological differences between samples. In fact we named the samples according to the shape of their particles: stick-shaped and quasi-spherical.
Results will be discussed and related with the morphology and structure of each sample and, finally, sensing mechanisms will be proposed.

15:50 - 17:20

Afternoon session - continued

Main Building, room 219

16:30 - 16:45
oral

CRYSTALLITE SIZE EFFECT ON THE CONDUCTIVITY OF THE NANOCRYSTALLINE CERAMIC SnO2 AND In2O3

Roman B. Vasiliev[1], **Marina N. Rumyantseva**[2], **Sergey G. Dorofeev**[2], **Yulia M. Potashnikova**[1], **Ludmila I. Ryabova**[2], **Alexander M. Gaskov**[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

Nanocrystalline metal oxides are used for the creation of materials applied in gas sensors, electrochemical devices, solar cells, optoelectronic transducers. These materials are usually electronic and in some cases ionic or mixed electronic-ionic conductors. The relation between the conductivity components varies with the hydratation degree variation and depends on the crystallite size. The latter factor is of great importance for the ceramics with nanometer scaled grain size. The present work is aimed to establish the correlation between the mean crystallite size and the ionic and electronic contributions to the conductivity for nanocrystalline In_2O_3 and SnO_2 with crystallite size in range of 3-40 nm. Samples of nanocrystalline In_2O_3 and SnO_2 were synthesised by precipitation of α-stannic acid and indium hydroxide gel. Powders of hydrated oxides were calcined in air at 300, 500, 700, and 1000^{o}C during 24 hours to obtain nanocrystalline samples with different crystallite size. Impedance spectroscopy and static current-voltage measurements were applied to investigate charge transport. Grain size increase results in reduction of ionic (proton) conductivity at the room temperature. On the contrary electron conductivity reduces as the crystallite size varies from 40 to 20 nm. The following reduction of the grain size down to 3 nm does not affect the electron conductivity value that may be associated with complete depletion of grains. Activation energy of the electron conductivity is practically independent on grain size and equals to 500-600 meV. That is significantly higher than ionisation energy of the oxygen vacancy of 130 meV. This argument indicates the existence of the barrier conductivity mechanism.
This work was done under a partial financial support of RFBR Grant N 03-03-32586 and Grant of President of Russian Federation N MK-1710.2003.03.

Transition metals (Co, Cu) as additives on hydrothermally treated TiO_2 for gas sensing

16:50 - 17:05
oral

Ana M. Ruiz[1)], **Albert Cornet**[2)], **Kengo Shimanoe**[3)], **Joan R. Morante**[2)], **Noboru Yamazoe**[3)]

1) Centre Nacional de Microelectrónica (CNM) - CSIC, Barcelona 08193, Spain

2) Electronics Department, University of Barcelona, C/ Martí i Franqu?s, Barcelona 08028, Spain

3) Kyushu University, Faculty of Engineering, Department of Materials Science and Engineering, Fukuoka 812-8581, Japan

Semiconducting metal oxide materials, such as TiO_2, SnO_2, In_2O_3 etc, play an important, steadily increasing role in almost all fields of electronics. Especially their application to gas sensors demand nanosize control strongly. In this case, nanoscale pure titanium dioxide with pertinent solid-state properties can be obtained by adopting hydrothermal treatments for the nanoprocessing of materials. On the other hand, the incorporation of catalytic additive has been a widely practiced method for tailoring the gas sensing characteristics. Depending on the element, the material processing and the fabrication of the device, it is possible to produce sensors with suitability improved for gas sensing.
In this work, hydrothermally treated TiO_2 has been modified with different transition metals (Co, Cu). The nanoparticles were calcined at several temperatures and characterised. The hydrothermal treatment stabilized the TiO_2 suppressing the thermal induced grain growth and shifting up the temperature of the anatase-to-rutile phase transformation. Besides the control of size and phase, the hydrothermal process highlighted how to obtain highly stable colloidal suspensions of titanium dioxide. Electrical measurement showed a particular behavior (n- or p-type) depending on the calcination or the operating temperature. We will discuss in more detail these features, together with structural characterization of the nanopowders.

Characterization of the Surface Chemistry of Iron Oxide Nanoparticles in the Transmission Electron Microscope

17:10 - 17:25
oral

Jacek Jasiński[1,4)], **Kent E. Pinkerton**[2)], **Ian M. Kennedy**[3)], **Valerie J. Leppert**[4)]

1) Lawrence Berkeley National Laboratory, National Center for Electron Microscopy (LBNL), Berkeley, United States

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4) University of California at Merced, School of Engineering, Merced, CA 95344, United States

In recent years, iron and other metal oxides have attracted substantial attention as promising inexpensive sensing materials. Iron oxide-based gas and humidity sensors have already been reported. The sensitivity of thick-film iron oxide sensors is rather low; however, it can be significantly improved by various doping schemes and by reducing film thickness. The enhancement is even greater when a nano-sized material is used due to increase in the metal oxide surface area, where the gas sensing takes place. Various methods have been used to produce nano-sized iron oxide powders, including chemical co-precipitation, sol-gel processes, pulsed laser evaporation, sputtering and spray pyrolysis. Here, in this work, we studied iron oxide nanoparticles prepared by a combustion method, with particle sizes varying in the range of 10-40 nm. Electron energy loss spectroscopy (EELS) in the transmission electron microscope was used to study the oxidation state of iron ions in these nanoparticles, with experiments performed in a nano-probe mode (with a probe size of 1.4 nm), allowing for very high spatial resolution. The studies showed that, depending on the formation conditions, a decrease in the oxidation state of iron could occur at the nanoparticle surface. This was indicated by changes in both the iron L_{23}- and the oxygen K-edges. These highly spatially resolved measurements showed broadening and a red energy-shift of both L_3 and L_2 iron lines at the surface of the particles. This was accompanied by a significant reduction of L_3:L_2-intensity, suggesting that there are mostly Fe^{2+} ions at the surface. A reduction in the pre-edge of oxygen K-edge also confirmed these results. This study shows that the surface oxidation state of iron oxide nanoparticles synthesized through combustion routes is highly dependent on formation conditions, and that EELS is an important research tool for investigating the surface-specific chemistry of nano-sized gas-sensing materials.

Poster Session 1

19:00 - 21:00

Electronic structure of the subnanometer diameter MoS2 single wall nanotubes

poster A-01

Anna Zimina[1)], **S. Eisebitt**[1)], **M. Freiwald**[1)], **S. Cramm**[2)], **W. Eberhardt**[1)]

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The synthesis of the subnanometer-diameter MoS_2 single wall nanotubes (NTs) was reported recently (Remskar et al., Science, 292, 479 (2001)). The structure reported are (3,3) tubes which in turn form bundles containing iodine. With a resulting diameter of 0.96 nm, the individual tubes are extremely compact with bond angles significantly deviating from bulk MoS_2. So far, the bonding and electronic structure in these NTs is not understood theoretically.
We investigate the electronic structure of the MoS_2-I_x NTs synthesized by M. Remskar, D. Mihailovic et al.. Nanotubes were studied in comparison to crystalline bulk material by combining soft x-ray absorption and soft x-ray fluorescence spectroscopy at the sulfur $2p_{3/2}$ resonance. We observe a significant modification of the density both unoccupied and occupied electronic states in the NTs.
To understand changes in the electronic structure of the MoS_2-I_x we simulate the resulting spectra for simple model clusters. The calculations are carried out with the StoBe code, based on a solution of the Kohn-Sham density functional theory equations. From our model calculations, we conclude that the redistribution of the electron density in the tubes compared to the bulk is mainly due to the S-Mo-S bond distortion.

Influence of Defect on Green Electroluminescence from Silicon Nanoparticles

poster A-02

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Silicon (Si) nanoparticles is one of promising materials for application to flat panel display such as light emitting diodes (LED) and electroluminescence (EL) because it emits visible light at room temperature. Previously, we obtained red luminescence with long lifetime and high brightness from the Si nanoparticles based EL device under relatively low operating voltage. In this paper, we report a correlation between defects and luminescent property from the EL device composed of Si nanoparticles which emits green light.
The Si nanoparticles were formed in a silicon dioxide (SiO_2) layer by co-sputtering of Si/SiO_2 targets and subsequently annealing at high temperature. The Si nanoparticles, then, were appeared on the sample surface by treating in hydrofluoric (HF) acid solution. The size of Si nanoparticles, which appeared on the surface, was tuned by the thermal oxidation treatment to vary the luminescent color. And the oxidized Si nanoparticles used as luminous layer of EL device.
The EL device using oxidized Si nanoparticles exhibited green luminescence with a peak of 560 nm by the reduction of particle size due to oxidation onto the surface. The luminance of green luminescence was increased with increasing the density of P_{ce}-center (radiative recombination center) on the Si nanoparticle surface because the P_b-center (non-radiative recombination center) was terminated with oxygen atoms.

Thin films of pure and Pt or Ru doped Al_2O_3 as catalytic membranes for selective semiconductor gas sensors

poster A-03

Andrey Ryzhikov[1,2)], **Michel Labeau**[2)], **Alexander M. Gaskov**[1)]

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Semiconductor gas sensor stability and selectivity can be improved by using catalytic filtering membranes to avoid interference of various gas molecules. The deposition of dielectric thin films doped with catalytic metals directly on the surface of semiconductor sensing element allows to increase the selectivity without considerable decrease of the sensitivity and increase of the response time.

The films were obtained by aerosol pyrolysis method. The filtering membranes of pure and Pt or Ru doped Al_2O_3 with various thickness (6-160 nm) were deposited on the surface of SnO_2(Pd) films. Phase composition and microstructure of the films were studied by X-ray diffraction, Atomic Force Microscopy, Transmission Electron Microscopy and Electron Probe MicroAnalysis.
Sensors properties of SnO_2(Pd)/Al_2O_3 and SnO_2(Pd)/Al_2O_3(Me) structures (Me = Pt, Ru) were studied under H_2, CH_4, C_3H_8 and CO-air gas mixtures in a temperature range 100-300C. The use of the membranes increases the response time of the sensors. All membranes reduce significantly the sensitivity to CO in the temperature range and increase the sensitivity to CH_4 and C_3H_8 at 200C. Ru-doped membranes significantly reduce the sensitivity to H_2. Sensitivity and response time considerably depend on membrane thickness.

Structural and electrical characterisation of MOS gas sensors made on SiC substrates

Olga Casals[1)], **Beatriz Barcones**[1)], **Albert Romano-Rodriguez**[1)], **Christophe Serre**[1)], **Alejandro Perez-Rodriguez**[1)], **Joan R. Morante**[1)], **Philippe Godignon**[2)], **Josep Montserrat**[2)], **Jose Millan**[2)]

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poster A-04

SiC, due to its chemical and physical inertness and large band gap, is an interesting substrate for the fabrication of electronic devices that have to work at high temperature and in aggressive environments, working conditions of most of the gas sensors. However, the lower maturity of the SiC technology, as compared to the Si one, requires the development and improvement of the technological steps.
The working principle of these sensors is the decomposition of the gas in the gate and the diffusion of some of the resulting chemical species towards the oxide, which is increased for porous gates, and that gives rise to modification of the electrical characteristics of the devices.
MOS tunnel diodes and capacitors have been fabricated on SiC substrates for their implementation as gas sensors. The devices use a thin Pt/$TaSi_x$ catalytic gate, formed by sputtering, and an oxide, with thickness varying between 1 and 40 nm. The devices are mounted on alumina plates with a printed Pt heater.
The as-fabricated devices cannot be operated above 200^{o}C and show limited sensing properties. Annealing at 600-800^{o}C for 3 minutes in an RTP furnace allows the devices to be operated at temperatures in excess of 400^{o}C and gives rise to an improved sensitivity for CO and NO_2 gases, with a maximum gas sensitivity at around 250^{o}C for CO and 320^{o}C for NO_2. A further improvement in the sensitivity to CO can be obtained by treating the samples in alternate pulses of 1% propane and 1% oxygen in argon gas at 600^{o}C, which is believed to increase the porosity of the gate material. In addition, the device becomes sensitive to propane, but no longer senses the presence of NO_2.
The sensing behaviour of these SiC devices in the presence of different gases will be presented as a function of the technological steps employed in their fabrication and correlation with the structural and chemical properties of the layers will be discussed.

Structural characterisation of V2O5-TiO2 thin films deposited by RF sputtering from a Ti target with V insets

Ivano Alessandri[1)], **Elza Bontempi**[1)], **Elisabetta Comini**[2)], **Giorgio Sberveglieri**[2)], **Laura E. Depero**[1)]

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poster A-05

Titania-based thin films are widely investigated in several areas of material science because of their appealing functional properties. In addition to the more traditional studies in the field of the photocatalysis, a renewed attention has been recently devoted to the integration of titania thin films in gas sensing devices, due to their good chemical stability at high temperature as well as in harsh environments. The conductivity of titanium dioxide can be improved by the addition of dopants, that offer the possibility to tune the electrical response of the sensor devices.
The deposition process may dramatically change the structure and microstructure of the film and, as a consequence, its functional properties. Radio-Frequency (RF) magnetron sputtering is one of the most suitable techniques for the industrial scaling-up of the thin films deposition process. In order to vary the concentration of vanadium in the film, a deposition from a target with a variable number of metal insets has been performed.
The present work is focussed on the structural investigation of different series of vanadia -titania thin films, prepared by sputtering. Bidimensional micro X-Ray Diffraction (XRD^2) and Glancing Angle X-Ray

Diffraction (GIXRD) techniques have been used for a complete analysis of the structure and the microstructure. Moreover, microInfraRed and microRaman measurements allowed us to obtain a deep comprehension about the role played by the modifications of the local structure as a function both of the dopant content and of the thermal post-deposition treatments. The electrical response of these materials, as a function of the surrounding atmosphere, are discussed in correlation with the structural/microstructural analysis.

Nanocrystalline Cr2O3-TiO2 thin films by pulsed laser deposition

poster A-06

Tea Avarmaa[1)], **Taavi Jantson**[1)], **Hugo Mändar**[2)], **Teet Uustare**[1)], **Raivo Jaaniso**[1)]

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Gas sensors based on semiconductor materials enable a large range of practical applications because of their easy implementation and low cost. Advances in nano-engineering allow dramatically increase the response of these materials and their overall performance, mostly because of increasing the exposed surface volume. One of the successful metal oxide semiconductor materials is a mixture of Cr_2O_3 and TiO_2, used in sensors in the form of pellets or thick films. In the present work, pulsed laser deposition (PLD) technique has been used for the growth of (1-x)Cr_2O_3-xTiO_2 (x=5-20wt%) materials with the aim to find the feasibility and optimal conditions for the growth of nanostructured (ultra)thin films. Target materials were prepared by sintering the fine mixture of TiO_2 and Cr_2O_3 at 1300C for 5h. The films were deposited by KrF excimer laser on Si [100] substrates in partial oxygen atmosphere, and were characterized by XRD, RHEED, and AFM. The substrate temperature (400 - 700 C), oxygen pressure (1.10^{-3} - 5.10^{-2} mbar) and laser energy density (1.5 - 4.5 J/cm^2) were varied for optimising the growth conditions. Structural analysis showed that the crystallisation of the films started at oxygen pressures at or above 10^{-2} mbar. At highest gas pressure (5.10^{-2} mbar) the crystalline structure began to reveal above the temperatures 450 C for x=20% and 500 C for x=5%. Relatively fast change towards crystalline phase occurred at around 550 C as indicated both by surface roughness analysis and by structural data. Smallest crystallite sizes (<10 nm) were obtained at 550 C, whereas the amount of amorphous phase was estimated to be around 20%. Bigger proportion of crystalline phase was obtained, if lower laser energy density and larger number of laser pulses were used during the growth.
[ABSTRACT TRUNCATED TO 2000 LETTERS]

Infrared radiation effects in TiO2 nanostructured films

poster A-07

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Attention is being paid to TiO2 oxide in either rutile or anatase phases for various applications such as its use in low-cost photovoltaic devices, the photodegradation of pollutants in air and the photoelectrochemical production of hydrogen. One of the principal attraction of this oxide is its tendency to aggregate in mesosocopic textured nanocrystallytes in films adhered to suitable substrates. We present results of the influence of infrared radiation on metal-TiO2-metal devices where the metal electrodes are composed of conducting ITO-based glass substrates. An 10-30 microns oxide film is obtained by deposition of TiO2 from a colloidal suspension followed by heating at high temperature which ensures sinterization of grains. The morphology of the film has been studied by AFM analysis and results in an array of 30 nm grains weakly separated, with resistance 100 Ohm per cm2. *-Under solar light illumination these devices show an open-circuit voltage of few millivolts. In the dark the device turns to be unbiased exhibiting strong sensitivity dc voltages induced by the infrared radiation. The principal characteristics of this response i.e its dependence on the infrared ac amplitude and frequency and oscillatory behaviour and polarity reversibility, suggest the existence of a Josephson effect. At infrared wavelengths the dielectric constant of bulk oxide is negative, suggesting that grains may have metallic character, so that we can explain the results as being due to pair tunneling between high Tc TiO2 grains.

Structural charaterization and gas sensing applications of mesoporous active filters

poster A-08

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Recently, the suitability of mesoporous materials, mainly those based on SiO_2, to be used as filters for solid state gas sensors has been reported. Basic properties of mesoporous based filters are low fluidic resistance as well as high active surface, higher than $100 m^2/g$.
In this work, mesoporous materials have been loaded with different catalytic metals. The presence of nanoclusters of these metallic elements allow to transform molecules flowing through the mesoporous filter.
Morphological, structural and functional characterization of mesoporous loaded materials are presented and analyzed. Data corresponding to their application as active filters of SnO_2 based gas sensors measuring combustion gases are also presented.

Sensing properties of surface-modified SnO2 nano-particles additivated with noble metal clusters obtained by chemical synthesis

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poster A-09

Catalytic additives are widely employed to improve the sensing characteristics of oxide-based solid-state gas sensors. The most frequently used additives are noble metals such as Pt, Pd and Au. In thick film techniques, several wet methods to introduce the additives in the sensing oxide matrix have been proposed, most of which are based in two basic procedures: a) impregnation of the oxide with a salt solution of the additive followed by a heat treatment; and b) introduction of a salt of the additive during the synthesis of the oxide.In both cases the additive is introduced as a molecular species ($PtCl_6{}^{-2}$, $PdCl_2$, etc.), which undergoes a chemical change to its final form, presumably metallic clusters, during a pyrolitic process. However, the final chemical states associated to the additives and its localization in the oxide matrix are issues still under debate.
In this work an alternative approach to the introduction of the catalyst is presented; based in the incorporation of previously synthesized metallic nanoparticles in the formulation of the SnO_2 screen-printing paste. Two different methods of nanoparticles incorporation were used. In the first, the as-prepared metallic clusters, suspended in a stabilizing media, were directly incorporated in the screen-printing mix. In this case physical adsorption of the metal clusters to the oxide surface is expected. Alternatively the SnO_2 powders were funtionalized by means of a suitable monomolecular coupling layer, which captures the metal clusters by ligand coordination. The metal clusters-coordinated oxides were then used in the preparation of the screen-printing paste.The sensitive pastes thus obtained were screen-printed onto 96% alumina substrates.
The gas sensing properties of the sensors were studied and the influence of the nano-particles size, concentration and synthesis method in the response of the sensors are discussed.

Semiconductor thin film sensor based on γ-Fe_2O_3 for CH_4 detection

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poster A-10

Generally, thin film sensors based on semiconductor oxides (In_2O_3, SnO_2, Fe_2O_3) are characterised by improved performance when detecting gases of acceptor nature (NO_x, O_3) and C_2H_5OH. Sensitivity of thin films to reducing gases is extremely low. In order to improve the characteristics of thin films to flammable gases, oxide layers are commonly been doped with noble metals. It is essentially, that gas-sensitive features of Fe_2O_3 are strongly determined by its structural features like phase composition, dispersity, defectiveness, morphology etc. γ-Fe_2O_3 is used as an individual layer and as a component of a multi-layer structure of ceramic sensors for detection of flammable gases. In the present work we report a study of gas-sensitive behaviour of γ-Fe_2O_3 thin films deposited on Si-substrate. The sensitive layers were formed from the stabilised sol of Fe_2O_3 prepared by the sol-gel rout. The sol was deposited onto micromachined Si-substrates of new design. Structure of the material was studied by XRD, HR-TEM, DTA/TG, FT-IR and Mössbauer spectroscopy. The applied conditions of Fe_2O_3 synthesis allow to obtain thin-film γ-Fe_2O_3, which is metastable at r.t. As it follows from the DTA/TG data, thus prepared γ-Fe_2O_3 remains stable up to 485 C. TEM characterisation gives spherical particles of size as high as 3-9 nm. Non-uniformity of the grain size distribution provides good quality of the films and close contact between grains. Thin film sensor, based on highly dispersive γ-Fe_2O_3, is characterised by high sensitivity to CH_4. Suitable sensitivity of the sensor to 100 ppm of CH_4 is reached at 350-425 C. Besides, the dynamic response profiles are well reproducible under repeated exposition of CH_4. Optimal operating temperature, at which the sample shows maximum response, fastest dynamics and linear response vs. concentration dependence, is found to be 425 C. This work was supported by the GASMOH project (2000-10041).

New technology of metal-oxide thin film preparation for chemical sensor application

poster A-11

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Grain size reduction in metal oxide films is one of the key factors to enhance the gas sensing properties of semiconductor layers. One of the basic ideas to create metal-oxide films with small grain size is to use a special regime of thin film deposition by the dc magnetron, ion-beam or r.f. sputtering of pure metal or metal oxide targets. The regime includes the thin film deposition with one or several interruptions of target sputtering. In this case "extra" interfaces are introduced into a thin film body. During the interruption of the sputtering process, an equilibrium surface is formed due to the free surface bond saturation by the atoms from residual atmosphere and/or the structural relaxation of the interface.
Among metal oxide semiconductors, tungsten oxide is a promising material for gas sensing. Therefore, we have checked the idea reported above by preparing WO_3 thin films using r.f. sputtering. The WO_3 films were reactively sputtered onto silicon wafers at an argon/oxygen flow ratio of 50/50, r.f. power of 200 W and a total pressure of 5 mtorr. This gave an average deposition rate up to 2.12 nm per min. The thickness was controlled by ellipsometry and stylus profilomentry and was calculated from AES profiles as well. Three types of films were prepared, i.e. using continual deposition, one and two interrupted depositions with a total deposition time of 40, 40.5 and 41 min, respectively. The interruption time was set to 30 s. It was found that the thickness of the WO_3 films decreased with the number of interruptions. The features of surface structures of these films have been investigated by XRD, AFM and TEM. The gas sensing properties of WO_3 thin films as a function of the number of interruptions have been studied as well. All these results will be presented and discussed in detail.

Influence of structural features of Fe_2O_3-In_2O_3 thin films on their gas-sensitive behaviour

poster A-12

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Gas-sensitive features of Fe_2O_3-based materials are essentially influenced by structural features of Fe_2O_3 and its concentration in oxide composite. Doping SnO_2 and In_2O_3 with Fe^{3+} ions results in increase of the layer resistance and decrease of sensitivity of the corresponding sensors to the most of gases. When Fe_2O_3 content reaches 50 mol % or more, gas-sensitive behaviour of the materials becomes hardly predictable. However, there are definite links between the functional characteristics of such materials and their structural features. In this work we reported the established correlations. The films were formed from colloid solutions of co-precipitated hydroxides of Fe and In. The sol-gel technique allows obtaining the oxide composites with required structure. Two types of samples were obtained: Fe_2O_3-In_2O_3 (9:1) prepared by using Fe^{3+} inorganic salt (sample I), and via less common Fe^{2+} precursor (sample II). The structure of the composites was characterised by XRD, TEM/ED and Mössbauer spectroscopy. The sample I remains X-ray amorphous up to 300 C; it consists of isometric particles of 2-6 nm. According to the XRD and ED data, the particles consist of solid solution of In^{3+} in α-Fe_2O_3 lattice. In contrast, sample II consists of grains, which differ in shape and size. Thus, along with fine particles, the grains with well-defined textures and growth anisotropy are present. ED examination of the sample II revealed highly dispersive α-Fe_2O_3 and γ-Fe_2O_3 phases. Thin films of Fe_2O_3-In_2O_3 (9:1) composites of the same chemical composition with homogeneous (sample I) and heterogeneous (sample II) structures differ essentially by gas-sensitive behaviour. The sample I are practically insensitive to NO_2 (0.5 ppm), CO (50 ppm) and C_2H_5OH (50 ppm). In contrast, the sample II demonstrates much greater response to the indicated gases. This work was supported by the projects GASMOH (2000-10041) and INTAS (2000-0066).

STRUCTURAL AND SPECTROSCOPIC CHARACTERIZATION OF A HIERARCHICAL MATERIAL MADE OF MCM41 AND CdS NANOPARTICLES

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poster A-13

The construction of materials presenting complex hierarchical structures is a particularly interesting challenge for the materials chemistry. Recently, hierarchical structure performed by assemblage of oxides [1], metals [2] or semiconductor nanoparticles [3], and mesoporous materials (MCM41 and MCM48) have been produced. These structures are highly ordered and show tuneable chemical, physical and mechanical properties, varying opportunely the chemical nature of guest-host species. These hierarchical structures could have applications in catalysis, separation processes, supports, highly efficient adsorbents, molecular hosting processes and sensors.
We report the synthesis and characterization of mesoporous silica (MCM41) containing CdS nanoparticles. MCM41 was synthesised using CTAB micelles as template; its structure was determined by X-ray diffraction (XRD); the CdS nanoparticles were synthesised using a water in oil microemulsion as reaction media.
The heptane containing CdS-amine capped nanoparticles was added to MCM41; CdS nanoparticles spontaneously localized inside MCM41 pores giving the CdS-MCM41 material.
The obtained hierarchical material was characterised using IR, UV-Vis, ATR, fluorescence spectroscopies and XRD and Small Angle Neutron Scattering (SANS) techniques. The spectroscopic investigation gave the size, polidispersity, surface and morphological properties of nanoparticles. SANS and XRD investigation gave structural information such as mesoporous structure, pore size and nanoparticles localization.

[1] Dharmesh Kumar, S. Bera, A.K. Tripathi, G.K. Dey, N.M. Gupta "Uranium oxide nanoparticles dispersed inside the mesopores of MCM-48: synthesis and characterization" Microporous and Mesoporous Materials 66 (2003) 157-167.
[2] Jin-Seung Jung, Won-Sik Chae, Robert A. McIntyre, Candace T. Seip, John B. Wiley, an
[ABSTRACT TRUNCATED TO 2000 LETTERS]

Rigorous analysis of the contribution of surface states to the conductivity of semiconductor thin layers

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poster A-14

III-V interfaces and thin layers are largely applied to gas-phase detection, e.g. H_2, NO_2 and O_3. The key role in the sensing mechanism of these structures plays the near-surface region of sub-micrometer size, which is strongly affected by the electronic surface states. The charge captured at these states largely modifies the height of interface potential barriers and often pins the surface Fermi level [1]. However, conventional theoretical approaches of the electronic properties of semiconductor gas sensors assume usually an unrealistically low density of the surface states in the band gap and thus lack of their contribution to the mechanism of thin layer conductivity.
In this work we performed a rigorous theoretical analysis of the conductivity of thin n- and p-type GaAs and InP layers as a function of the surface state density N_{SS} and the surface fixed charge Q_{FC} taking both positive and negative values. Such a charge represents both physically adsorbed ionic species and, on the other hand, the surface doping applied in order to control the gas sensitivity of the layer. The band bending induced by Q_{FC} changed from accumulation to inversion. In the calculations, a U-shaped continuous surface state distribution in the energy gap was assumed in accordance with the Disorder Induced Gap State model [2]. The layer thickness was changed in the sub-micrometer range down to the values approaching the depletion region width. In addition, the in-depth profiles of the potential barrier and carrier density were calculated and the Debye length for different doping was determined. For the numerical analysis we used a computer program for self-consistent simulations of the electronic phenomena in semiconductors.
As a result, the influence of surface states and doping on ion-sensitivity of III-V thin layers in terms of their conductivity was determined.

1. B.Adamowicz, et al. Thin Solid Films 436 (2003) 101
2. H.Hasegawa, H.Ohno, J.Vac.Sci.Technol.B4 (1986) 1130
[ABSTRACT TRUNCATED TO 2000 LETTERS]

EFECT OF SELENIUM TREATMENT ON PHOTOLUMINESCENCE PROPERTIES OF POROUS SILICON

Renata Jarimavičiute-Žvalioniene[1)], **Rolandas Tomaiónas**[2)], **Gintare Statkute**[2)], **Viktoras Grigaliunas**[3)], **Sigitas Tamulevičius**[3)], **Mindaugas Andrulevičius**[3)] poster A-15

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Recently, porous silicon (PS), as a promising material for visible light emission by photoluminescence (PL) attracted attention due to possible photonic applications in different devices like LED, waveguide, field emitter, optical memory etc. Theoretical assumption basis on quantum explanation of the visible light luminescence, but the details of the mechanism are still not completely understood. In other hand, from the practical viewpoint, stability and lifetime of photoluminescence is very important factor. Stability and lifetime of PS photoluminescence can be significantly improved in the way of application of the efficient surface passivation method. Recently different chalcogenide (selenium or sulfur) treatments received attention as an alternative heteroepitaxy-compatible Si surface passivation method. In present study PS surface selenium treatment has been performed in order to improve stability and lifetime of PS photoluminescence.
PS layers were prepared at room temperature by electrochemical etching in HF:H2O:C2H5OH solution at working current of the etching process from 50 to 800 mA and the anodization voltage from 1 to 29 V. The back side of the sample was illuminated with a 50 W halogen lamp. Selenium treatment was performed by silicon immersion into the selenious acid aqueos solution.
PL properties of initial and selenium treated PS structures were investigated in the visible and near-infrared spectral region. Silicon surface structural changes after selenium treatment were investigated by XPS. The influence of surface structural and composition changes on PL properties was defined.

Fabrication of Silicon Oxide Microneedles from Macroporous Silicon

poster A-16 **Angel Rodriguez**[1)], **David Molinero**[1)], **Enrique Valera**[1)], **Trifon Trifonov**[2)], **Luis F. Marsal**[2)], **Josep Pallares**[1)], **Ramón Alcubilla**[1)]

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This work presents a novel technique for Silicon dioxide microneedles fabrication. Microneedles are hollow microcapillaries with tip diameters in the range of micrometers allowing the fabrication of micro-syringes. These structures are interesting in medical and biological applications, such as DNA injection, antibody manipulation and delivery, or cell manipulation. For the fabrication of the needles, first, macropore formation in n-type silicon is performed by photoassisted electrochemical etching (ECE) in low concentration hydrofluoric acid. Using lithographical patterns the distance between pores can be defined. The microneedles morphology depends on the anodization conditions such as current density, etching time, HF concentration, temperature, bias as well as on substrate properties: doping density and orientation. Afterwards, the etched macropores were oxidized and then the microcapillaries were released using backside TMAH etching. The silicon oxide at the tip of microcapillaries is etched in buffered hydrofluoric acid. The resulting needles can be tailored to the desired shape, for instance to improve mechanical resistance. Microneedles can be fabricated by this method with diameters ranging from less than 1μm to several tens of microns. In this work microneedles arrays were fabricated with pore diameters in the range of 2-5μm, with lengths from 30-140μm and 70nm thick. Microneedles inner diameter can be further adjusted by controlling the thickness of SiO_2 on the walls. In this way inner diameters in the submicron range can be obtained.

New materials based on nanostructured Prussian blue for development of hydrogen peroxide sensors for biomedical applications.

poster A-17 **E. Puganova**[1,3)], **M. Vagin**[1)], **A. Karyakin**[1)], **Pankaj Vadgama**[2)]

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Monitoring of low levels of hydrogen peroxide is of great importance for modern medicine, environmental control and various branches of industry. In particular, H_2O_2 is the most valuable marker for oxidative stress.
We reported the specially deposited Prussian Blue (PB) to be the most advantageous hydrogen peroxide transducer allowing its low-potential detection down to 10^{-7} M in flow-injection mode [1]. However, in certain cases including medicine and environmental control, the detection of lower H_2O_2 levels is required. We report on the possibility for nano-structuring of Prussian Blue by its electrochemical deposition through liquid crystalline templates, which is noticed from AFM images of the resulting surfaces.
Analytical performance of the resulting Prussian Blue based nano-electrode arrays have been studied in course of hydrogen peroxide detection in FIA mode. They demonstrate a sub-ppb detection limit (1×10^{-8} M) and a linear calibration range starting exactly from the detection limit and extending over six orders of magnitude of H_2O_2 concentrations (1×10^{-8} - 1×10^{-2} M), which are the most advantageous analytical performances in hydrogen peroxide electroanalysis.
The developed sensors were applied for clinical research in pulmanology. Hydrogen peroxide was detected in patients condensates of breathing air.

Acknowledgements: The financial support through NATO Linkage SA (PST.CLG.978764) 6607/FP is greatly acknowledged.
References:
1. A.A. Karyakin (review). Electroanalysis, 13(2001) 813.

Homogeneous Precipitation of Lu-Based Nanocrystalline Phosphors

Eugeniusz Zych[1)], **Joanna Trojan-Piegza**[1)], **Leszek Kepinski**[2)]
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poster A-18

Simultaneous Topography and RECognition Mapping with PicoTREC - a new technology to map ligand-receptor interactions, study biological processes, or probe nanometer-scale molecular binding sites on a variety of surfaces

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poster A-19

AFM/SPM (Atomic Force Microscopy/Scanning Probe Microscopy) can be used to image active protein molecules or living cells in a non-destructive manner. In addition, a variety of molecules can be attached to AFM cantilevers, making them chemically selective sensors for studying individual molecular interactions. PicoTRECTM is a new Topography and RECognition imaging solution that requires no fluorescence, radioactivity, enzyme-linked detection schemes or other extraneous labels. It combines real-time detection of molecular recognition events and single-molecule sensitivity with the imaging capability of AFM/SPM. PicoTREC allows a researcher to quickly determine where specific, single molecule binding interactions occur on a sample, and resolves them from surface topography information. For example, when a drug or antibody are attached to an AFM/SPM tip, the forces involved in binding events with target molecules are detected and resolved by PicoTREC. The technique is being used to detect binding forces between antibodies and antigens, ligands and receptors, chemical bonds, and charge-charge interactions.
Consequently, entire maps of individual binding sites can quickly and easily be obtained across a variety surfaces. PicoTREC will be demonstrated on the avidin-biotin system with tip-bound ligands and antibodies, and on "adhesion-mapping" on single ferritin molecules and living cells.

Phase Evolution Induced by Polypyrrole in Iron Oxide - Polypyrrole Nanocomposite

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poster A-20

Nanocomposite of polypyrrole and iron oxide were prepared using simultaneous gelation and polymerization processes. Varied amounts of pyrrole were added to a solution containing an Fe(III) salt as precursor and 2-metoxy ethanol as solvent. The particles were found to be nanocrystalline. However, the composites exhibited mixed phase, belonging to both the corrundum α-Fe_2O_3 (nonmagnetic) and the cubic phase, Fe_3O_4, which is ferromagnetic. The presence of both the phases is clearly seen from the XRD studies. Electrical conductivity study of powders showed a slight variation in conductivity for lower concentration of pyrrole, with a sudden increase in conductivity at 15 percent of pyrrole concentration, that could be explained on the basis of percolation theory which predicts that at a certain amount of concentration of conducting polymer a full conducting path is formed for the flow of current. The properties of nanocomposites formed by combining conducting polymers and oxides nanoparticles are strongly dependent on concentration of polymer and have brought out more fields of applications such as smart windows, toners in photocopying, conductive paints, drug delivery, rechargeable batteries. These nanocomposites in the pellet form were used for humidity and gas sensors.

Tuesday, September 7th

14:00 - 15:30

Afternoon session

Main Building, room 219

Large Area Growth of Carbon Nanotubes and their Applications

14:00 - 14:30
invited oral

S. Ravi P. Silva[1)]

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Large Area Growth of Carbon Nanotubes and their Applications

S. Ravi P. Silva
Nano-Electronics Centre, Advanced Technology Institute, University of Surrey, Guildford GU2 7XH, United Kingdom.
The dawn of the Nanotechnology revolution that is taking place currently, was boosted by the identification of carbon nanotubes and the theoretical work associated with its properties in the early 1990's. In the area of carbon nanotubes (CNT) this offers great potential for scientist and engineers alike to come up with novel phenomena and highly functional devices. Novel phenomena previously only observed at very low temperatures are now possible with 1D nano-wires, even at room temperature. Yet, currently the nanostructures used to examine these properties are grown at high temperatures in order to produce materials with a well-defined crystal lattice structure.

In this paper, we will review the current state of the art in CNT growth and show methods for the growth of high quality nanostructures at low temperatures, even on substrates held at room temperature. This has significant impact in the production of these nanomaterials, and has opened a whole new set of device concepts as well as processing techniques and applications.

This talk will examine the process steps taken in lowering the substrate growth temperature of carbon nanotubes and nanofibres from the usual 700-1100 °C, right down to room temperature. We show how the energy is coupled to the nickel catalyst via a chemical vapour deposition (CVD) plasma process [1]. CVD growth offers high precision growth, with controlled positioning, diameter and height of nanostructures. We also introduce a novel laser annealing processes, which produces a high quality catalyst all processed with room temperature held substrates [2].

We will also introduce the use of the CVD growth process to create nanostructured Ni pillars, again on room temperature held substrates over large areas. The process adopted i
[ABSTRACT TRUNCATED TO 2000 LETTERS]

Synthesis of nanoscaled TiO_2 particles of tubular shape or supported on carbon fibers

14:50 - 15:05
oral

Laurence REINERT[1)], **Philippe RODRIGUEZ**[1)], **Marc COMET**[1)], **Hervé FUZELLIER**[1)]

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Titanium dioxide is widely used as a photocatalyst, mostly in its pulverulent form. The use of powders presents the advantage of a great surface contact between the catalyst and reactants; however, it generates other problems : catalyst recovering, particles agglomeration...
We present two different syntheses routes leading to TiO_2 nanoscaled particles, arranged in a tubular shape or supported on carbon fibers. Particles were obtained either by impregnation of a carbon substrate in a precursor solution or by chemical vapor deposition of the precursor on the substrate, both followed by heating treatments.
The immersion of carbon fibers (rough felt - Mitsubishi, surface area 10 $m^2\ g^{-1}$) in a 0.09 mol L^{-1} $TiCl_4$ solution in n-hexane led to the formation of a 200 nm titanium oxichloride layer covering nearly the whole surface of the fibers. Its conversion into TiO_2 was achieved after hydrolysis (air - H_2O, 400C, 15 hours). The surface area of the resulting material was considerably increased and reached 700 $m^2\ g^{-1}$. A complete oxidation of the carbon fibers occurred after calcination under air at 600C for 4 hours. The surface area of obtained TiO_2 tubes was 15 $m^2\ g^{-1}$. X-ray diffraction analyses showed the presence of a mixture of both rutile and anatase varieties (ca. 90 wt. % of anatase).
The second synthesis route consists in the deposition of $TiCl_4$ on the fibers by CVD. When $TiCl_4$ was directly vaporized on the carbon fibers (Ar, 350C), a non adherent TiO_2 layer composed of nanoscaled particles (200 nm) was formed. The adhesion of the layer was reached by first covering the fibers by a $POCl_3$ layer (Ar, 350C) or by activation (H_2O - air, 350C) prior to the deposition of $TiCl_4$. After conversion (air, 400C), nanoscaled adherent TiO_2 particles (100 nm) covering the whole surface of the fibers were observed. Samples were characterized by SEM, EDS and XRD. They will find their main applications as photocatalysts or gas sensors.
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[ABSTRACT TRUNCATED TO 2000 LETTERS]

Growth and Performance of nano-grained tin oxide films with a narrow size distribution using electron beam evaporation

15:10 - 15:25
oral

Simon Ahlers[1), **Gerhard Müller**

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Film morphology is one of the key design parameters for metal oxide gas sensors. With micromachined low-power substrates getting increasingly important, compatible deposition techniques must be investigated more thoroughly. In this paper we present results from experiments using electron beam evaporation with metallic tin as a source material and a subsequent thermal oxidation step. We examined how the grain size of evaporated tin oxide layers can be varied from several 100nm down to about 10nm by varying the thickness of the evaporated layer. Layers thinner than 80nm result in tin oxide layers with unconnected grains, necessitating the addition of a second tin-oxide layer to provide electrical conduction. The finest-grained layers showed the expected increase in sensitivity. In order to be able to reproduce the versatility of thick film sensors with evaporated films, the addition of Au, Pt and Pd to these nano-grained layers by depositing sandwich-structured layers was investigated.

Coffee break

15:30 - 15:50

Nanostructured metal oxides synthesized by hard template method for gas sensing applications

15:30 - 15:45
oral

Emma Rossinyol[1), **Francesca Peiró**[1), **A. Cornet**[1), **Joan R. Morante**[1), **B. Tian**[2), **D. Zhao**[2)

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Semiconductor gas sensors offer good advantages with respect to other gas sensor devices due to their simple implementation, low cost and good reliability for real-time control systems. As the adsorption is a surface effect, one of the most important parameter to tailor the sensitivity of the sensor material is the surface area. In order to increase the surface area, mesoporous oxides have been synthesized.
Nanostructured mesoporous materials have been widely studied in the development of catalytic systems, due to their large, controllable pore size and high surface are. The pore structure, such as pore size and channel conductivity can be designed for practical application, and a variety of synthetic pathways has been proposed for the development on these nanostructures. There are two main synthetic pathways for the preparation of mesoporous oxides: soft and hard template. For the preparation of ordered nanostructure

arrays, a hard template has some advantages when compared with a soft template, especially in its specific topological stability, veracity, predictability and controllability. We have used SBA-15 and KIT-6 as a template for the synthesis of different semiconductor oxides: CeO_2 , WO_3 and carbon. $Ce(NO_3)_3.6H_2O$, Phosphotungstic acid and sucrose have been used as a precursors. The solution with the precursors and the silica template has been stirred and dried at room temperature. After calcination, the silica has been removed using an acidic etching.

Crystalline mesoporous oxides have been synthesized, with a particle size about 5 nm and high surface area. Low angle XRD spectra show a high order mesoporous structure, in good agreement with the structure of the template used. TEM reveals that the silica host has been completely removed, therefore, the nanowires constitute a self-supported superlattice. The introduction of some catalytic additives inside the nanostructures has been also accounted for.

15:50 - 17:20

Afternoon session - continued

Main Building, room 219

16:30 - 16:45
oral

About the dependence of the frequency response of the nanostructure based on SnO2 [U+0096] Si from the different gases and their concentration

Vasyl V. Ilchenko[1], **Valery P. Chehun, Alexander I. Kravchenko, Volodymyr M. Telega, Alexander M. Gaskov**[2]

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Is shown, that the shift of the second derivative of the current - voltage characteristic of the testing signal frequency dependes on the sort of gas and the concentration of gas in an atmosphere.
A feature of the measuring technique was that at the measurement of current - voltage characteristics on the DC is padding the alternating voltage by the amplitude less than 0,1 V at the frequency range 100 - 1500 kHz was applied. The technique of research allowed to measure not only current - voltage characteristic on DC, but also second derivate of the current- voltage characteristics. So we can use the hardware differentiation of the non-linear current- voltage characteristics for the obtain additional possibilities for the gas sensors creation. In our work the results of the researches of the sensitivity and selectivity of the heterostructure formed by contact of the nanocrystal dioxide (SnO2) and silicon (Si) are presented. The response of the given structure was observed as the change of the second derivative of the current-voltage characteristic. Air, pairs ethyl alcohol and ammonia were used as researched gases.
Results of the researches have shown that with change of parameters of the environment in which the structure is placed the frequency of response is maximal. Besides it has been established that the response of the structure has resonant character. In other words there are frequencies on which the amplitude of the second derivative have the maximum volume and this frequnces are different for different gases. The research of the influence of the different concentration of the gas environment (ammonia) illustrates that the response of the structure changes of the amplitude of the second derivative. Thus, it is possible to speak about selectivity and sensitivity of researched structure to the researched gases to be shown as change of frequency and amplitude of the resonant response at the tamperature equal 300 K.

16:50 - 17:05
oral

Chemical sensors based on polymer composites

Stanislaw Frackowiak[1], **Marek Kozłowski**[1]

1) Wrocław University of Technology, Wybrzeże Wyspiańskiego, Wrocław 50-370, Poland

Developing sensors derived from electrically conductive polymer composites has been attempted. The matrices used were: HDPE, PS, PP and HDPE/PP blend.
The filler was carbon black of particle size 10 to 110 nanometers.
Electrical conductivity, mechanical strength, Vicat softening temperature and melt rheology were investigated.
The lowest percolation threshold was achieved at 2 wt% of carbon black, which resulted in electrical resistance of 10exp7 [Ohm*m]. Along with the filler volume the Vicat softening temperature increased at every polymer matrix for a few centigrades. At the highest filler content Young modulus of composites was even four times higher, whereas elongation at break decreased substantially if compare to the net polymers. Melt viscosity increased with

carbon black content, making composites hardly processable at high filler loadings.

Accurate determination of stability, thickness and dielectric constants of metal island films used for surface plasmon resonance biosensors

17:10 - 17:25
oral

T.W.H. Oates[1)], **M.M.M. Bilek**[2)], **D.R. McKenzie**[2)]

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2) University of Sydney, Sydney 2006, Australia

Discontinuous noble metal island films are utilised as biosensors by monitoring changes in their surface plasmon resonance, which are highly sensitive to adsorbed molecules. The reproducible production of such films is therefore of great interest. We present results of in-situ spectroscopic ellipsometric (SE) monitoring of metal island film growth by pulsed filtered cathodic vacuum arc (PFCVA). Utilising optical features in the silicon oxide substrate the film thickness is accurately determined to within 0.1 nm. Accurate knowledge of the film thickness provides the necessary information to unambiguously determine the film optical constants. The use of a highly reproducible pulsed plasma source allows us to determine the material mass deposition rate, and consequently the void content of the film. The percolation threshold of the island films is determined by from the film optical constants, and compared with the vakue determined by in-situ conductivity measurements and te predictions of percolation theory.

Instability in noble metal islands, especially in the period immediately following deposition by PFCVA, complicates the production of films of stable and reproducible area coverage for use as biosensors. In-situ film resistivity measurements reveal changes in the conductivity of PFCVA deposited silver island films for periods in excess of one hour. In-situ SE reveals morphological changes in the films for a period less than 4 minutes, corresponding to an increase in film thickness. We propose that an increase in silver island height during this period, caused by particle mobility and surface energy minimization, is responsible for the short term morphological changes. Conductivity changes for periods greater than 4 minutes are attributed to slow cooling of the film combined with the negative temperature coefficient of resistance of metal islands films.

Wednesday, September 8th

Morning session

09:00 - 10:30

Main Building, room 219

Doping effects in nanocrystalline tin dioxide

09:00 - 09:30
invited oral

Alexander M. Gaskov[1)]

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Doping effects in nanocrystalline tin dioxide
A.M. Gaskov

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Doped tin dioxide has found many technological applications such as optical electronic devices, catalysts, gas sensors, batteries and electrodes for aluminum production. The influence of doping with various impurities on the composition, microstructure, electrical and functional properties of nanocrystalline SnO2 is discussed. The materials have been prepared in the form of powders, ceramics, and thin films by chemical precipitation from solutions and aerosol pyrolysis of organometallic compounds. The structure of materials was examined by Transmission Electron Microscopy and X-ray Diffraction techniques. The impurities stabilize the microstructure of nanocrystalline tin dioxide. The reducing of average size of SnO2 crystallites in the doped materials can be caused by impurity segregation on the surface of SnO2 crystallites. To analyze the effect of impurities on charge carriers transport in nanocrystalline SnO2 the conductivity of materials was studied in the low-temperature range 77 K $<$ T $<$ 300 K. The impurities change the electrical resistance of SnO2 due to formation of donor or acceptor level in SnO2 band gap. The grain boundaries make also a contribution to the electrical resistance growth due to formation of barriers at the p-CuO/n-SnO2 or p-PdO/n-SnO2 boundaries. The doping effects on the interaction of nanocrystalline SnO2 with a gas phase were investigated by Mössbauer, Auger electron, and X-ray photoelectron spectroscopy and in situ by Raman spectroscopy and XANES coupled with conductivity measurements. It was demonstrated that the impurities are involved in specific chemical interactions with the gas molecules.

09:30 - 09:45
oral

FORMATION, STRUCTURE AND PROPERTIES OF THE NANOCOMPOSITES OF THIN AND IRON OXIDES

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Development of gas sensors on the basis of couple of nanocrystalline oxides of 1-2 metals creates opportunities for producing on their basis advanced materials, which meet modern requirements and have improved parameters. In such systems SnO2 attracts the most attention as main gas sensitive ma-terial. As inverter may be used oxides of metals, d-elements of chrome, molybdenum, tungsten, iron etc.
Formation of films of individual tin and iron oxides and their mixtures is carried out by oxidation pyrolysis of tin tetraethyl and pentacarbonil or iron ethylate from gas phase in the range of temperature from 110 to 500 0C. Concretion of films had been carried out on plates from monocrystalline silicone, NaCl crystals and on glassceramic substrates. Using RHEED, TEM, AFM, AES and Mössbauer spect-roscopy methods we probe the structure and composition of the films. It had been revealed that tin and iron oxide films, formed under 3000C and 150 0C were amorphous. By increase of temperature formation of polycrystalline phase in their composition take place. In case of iron film it had been observed that by inc-rease of temperature of film formation roughness of their surfaces had been reduced. In this case, the size of amorphous globules enlarges. They become larger in size, but more flat. Research of tin oxide films had been showed that temperature of their formation influences on their primary orientation and roughness. It had been established that roughness of amorphous films lower than polycrystalline ones. Research of phase composition of tin and iron oxides mixture films showed that all of them may be amor-phous and (or) crystal, depending on concentration temperature, and do not contain any other mix-tures, not peculiar for individual oxides. In this work electric properties of the formed films had been also stu-died.
This work was supported by INTAS, grant 2000-0066.

09:50 - 10:05
oral

Synthesis of nanoscaled oxides and metals with various shapes : powder, tubes or plates.

Laurence REINERT[1)], **Marc COMET**[1)], **Hervé FUZELLIER**[1)]

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Metallic oxides are widely used as catalysts because of their high surface area and low particle size. The most common method of synthesis to obtain such materials is the sol-gel technique. We describe the synthesis of nanoscaled high surface area aluminum and alumina materials of various shapes by adsorption of a precursor solution on various substrates, followed by controlled calcinations.
The adsorption of a 0.3 mol L^{-1} aluminum hydride solution in diethyl ether on fibrous carbonaceous substrate (cellulose fibers, carbon fibers or felts), followed by a calcination (Ar, 250C) led to the thermolysis of the hydride and the formation of metallic particles (300 nm, s.a. : 30 - 90 m^2 g^{-1}) on the surface of the fibers. Aluminum microtubes composed of similar sizes particles and of equivalent surface areas were obtained by oxidation of the substrate at 600C. By heating treatments at higher temperatures, both γ and α alumina phases respectively crystallized. Microtubes are formed of agglomerated particles, the surface area of the α phase obtained at 1600C is about 40 m^2 g^{-1}.
Lamellar aluminas (s.a. 80 to 250 m^2 g^{-1}) of extremely low apparent density (15 g dm^{-3}) were synthesized by immersion of exfoliated or exfoliated-recompressed graphite (Papyex) in 1 mol L^{-1} aluminum trichloride solutions in diethylether. In a first step, after a partial calcination (exfoliated graphite) or a pseudo-exfoliation (Papyex), a carbon / aluminum oxichloride composite was obtained. Its subsequent calcination (O_2, 1200C) led to the crystallization of α - alumina sheets with nanometric thicknesses (ca. 10 nm). After dispersion in water, these latter were divided into nanometric pulverulent fragments by the mechanical effect of ultra sounds.
Similar methods were used for the synthesis of other metallic particles (Co, Ag) and oxides (Co_3O_4, TiO_2, HfO_2, CeO_2...) that are reported as catalytic materials.

Non-homogeneous nanocrystalline oxide materials for gas sensor applications

10:10 - 10:25
oral

Marina N. Rumyantseva[1], **Alexander M. Gaskov**[1]

1) Chemistry Department, Moscow State University, Leninskie Gory, 1-3, Moscow 119992, Russian Federation

The heterogeneous nanometer-scaled oxide materials M1O-M2O (nanocomposites) has pronounced advantages for solid state gas sensor applications. The electronic properties of grain boundaries in two-phase systems are very sensitive to the atmosphere composition. The solid-gas interaction in such systems involves selective chemical reactions on the M1O-M2O grain boundaries. If M2 is a transition metal, the solid-gas interaction may change its oxidation state and distribution between the surface and lattice positions. The behaviour of SnO_2-M2O nanocomposites (M2O = Fe_2O_3, NiO, CuO, PdO, PtO_2, RuO_2) in relation with gas sensing phenomena has been analysed. The work includes the methods of SnO_2 thin and thick films elaboration, investigation of microstructure, surface state and electrical behaviour of nanocomposites in different atmospheres. The mechanism of solid-gas (CO, H_2, CH_4, C_2H_5OH, H_2S, NO_2) interaction is discussed on the basis of results of Mössbauer and Raman spectroscopy, AES, XPS, XAS and conductance measurements. The main information was obtained by in situ techniques. Depending on the ionic radius and charge the M2 elements are variously distributed between the bulk and surface of nanometer-scaled SnO_2 grains. In air all regarded elements being distributed in SnO_2 matrix are in oxidised state. The common points for all nanocomposites studied are: (i) in nanocoposites the SnO_2 grain size is reduced, that can be caused by M2O segregation on SnO_2 grain surface leading to kinetic limitations of recrystallisation processes; (ii) M2O affect the SnO_2 electrical properties, however the mechanism of resistance growth may be different: the compensation effect or barrier formation at the grain joints. At the same time, M2O brings the special properties. They can be involved in specific chemical interactions with the particular gas.
This work was financially supported by INTAS 2000-0066 and RFBR 03-03-32586 grants.

Coffee break

10:30 - 11:00

Morning session - continued

Main Building, room 219

11:00 - 12:30

STUDY OF CHARGE ACCUMULATION AT SnO_2 (110) SURFACE

11:00 - 11:15
oral

Vyacheslav Golovanov[1], **Matti A. Maki-Jaskari**[2], **Tapio T. Rantala**[2]

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2) Tampere University of Technology, Tampere, Finland

Basic features of surplus electrons of order 10^{21} - 10^{22} cm^{-3} in bulk and at different (110) surfaces of tin dioxide are considered computationally, by using density functional theory. The additional charge is found to effect on surface energetics and surface relaxations considerably with respect to their charge neutral counterparts.

This is true especially in case of oxygen rich environments and surfaces, where oxygen can be adsorbed on-top of five-fold coordinated surface tin atoms. The highest occupied orbital of O^- corresponds to oxygen p-orbital oriented parallel to the surface normal and cause adsorbate to become spin polarized. Based on the evaluated total energy differences it is shown that its formation is favorable if there are initially surface oxygen vacancies, or alternatively, if there is initially surplus electrons present at the surface. It is shown that the adsorbed O^- can in principle decompose by transforming to negatively charged dioxygen species.

In cases of stoichiometric and slightly reduced surfaces the additional charge is accumulated increasingly at surface layers with a considerable amount of the surplus charge accumulated around Sn atoms. A pronounced charge accumulation around under-coordinated surface tin atoms is observed especially in the cases of oxygen deficient surfaces. Different charge accumulations are seen around five-fold coordinated surface Sn, four-fold coordinated surface Sn atom and around a single bridging oxygen vacancy. The Sn^{2+}

type of surface Sn atom has a relatively strong additional charge trapping character, without decline when slab thickness was increased.

11:20 - 11:35
oral

Simulation of the influence of particle size distribution and grain boundary resistance on the spectral response of 2D polycrystals.

ALEJANDRO MORATA[1), GUILHEM DEZANNEAU[1), ALBERTO TARANCÓN[1), FRANCESCA PEIRÓ[1), Joan R. Morante[1)

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Nanostructured ceramic materials exhibit a wide range of technological applications. Particularly, they have acquired increasing importance in so highly topical fields as fuel cells and gas sensors. Impedance spectroscopy technique has become an essential tool in the correlation or the micro and nanostructure characteristics of polycrystalline ceramic materials with their electrical properties.
In the analysis of the spectral response of a sample, it is used the so called "brick layer model", which assumes a simplified microstructure composed of cubic-shaped grains. J. Fleig [1] showed a disagreement between the ideal model and the results of simulations performed in samples with a random grain size distribution. In the present work, a systematic study of the influence of particle size distribution on the impedance arcs has been carried out. Spectral response of computer generated images representing polycrystal with various microstructure distributions have been simulated. The calculations consisted on the direct resolution of kirchoff equations in the nodes of a 2D square grid superposed on the simulated image of the polycrystal. The impedance associated to each node consists on a resistance and a capacitance connected in series, taking different values when located in a point of the bulk (R_{BULK} , C_{BULK}) or of the grain boundary (R_{GB}, C_{GB}). The validity of the brick layer model for the correct interpretation of impedance spectra is discussed as a function of grain size distribution and the R_{GB}/R_{BULK} ratio.

1. J. Fleig, Solid State Ionics 181-193 (2002) 150.

11:40 - 11:55
oral

HYDROTHERMAL SYNTHESIS OF NANOSTRUCTURED ZIRCONIA MATERIALS: PRESENT STATE AND FUTURE PROSPECTS

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2) CNRS Institute de science et de genies des materiaux et procedes (CNRS/IMP), Av. Felix Trombe, Odeillo Font-Romeu, France

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Hydrothermal procedures for the synthesis of zirconia-doped nanocrystalline powders (hydrothermal reactions and hydrothermal crystallization) show important advantages from the thermodynamic and kinetic point of view (larger domain stability of precipitated species, faster kinetics of crystallization) as well as from technological point of view (direct synthesis of crystalline materials in one-step process, low synthesis temperatures, better control of the crystallization and grain sizes with possibilities to obtain nanocrystalline materials, versatility, environmental friendly technology).
Establishment of the conditions for obtaining ZrO2 doped with different oxides is based on thermodynamic predictions. Kinetic modeling of the hydrothermal synthesis of zirconia nanopowders is presented.
Future progress is expected using in-situ hydrothermal synthesis of polymer surface modified nanopowders and hydrothermal/electrochemical thin films deposition to control the morphology and texture of the materials. The impact of these materials in development of fast ionic conducting materials and materials with controlled luminescent properties for SOFC and highly efficiency sensors is discussed.

12:00 - 12:15
oral

Reverse Micelle synthesis of Zirconia nanopowders

Harpreet Singh[1), Olivia A. Graeve

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Pure zirconia nanoparticles were obtained using a Reverse Micelle (RM) synthesis technique. The objective of this study was to obtain the smallest possible ZrO_2 nanoparticles with minimum possible agglomeration. In this investigation, XRD results show that ZrO_2 nanoparticles are in the range of 5 - 20 nm. As synthesized powders were cubic/tetragonal and were relatively X-ray amorphous. It was also found that a metastable tetragonal phase exists at temperature of < 600C. The metastable tetragonal ZrO2 transformed to monoclinic phase after 360 hours. This shows that even the particles < 20 nm are metastable which is in contrast to some earlier studies. For further insight, TEM analysis of the particles will be conducted. The size of the nanoparticles was influenced by the amount of water and the synthesis conditions such as temperature. RM technique can be further utilized to produce partially stabilized zirconia and fully stabilized zirconia by co-precipitation of the stabilizing species. ZrO_2 nanoparticles have immense potential as solid electrolytes in fuel cells, oxygen sensors, etc.

Lunch break

12:30 - 14:00

Afternoon session

Main Building, room 219

14:00 - 15:30

Designed Self-Doped Titanium Oxide Thin Films for Efficient Visible-Light Photocatalysis

14:00 - 14:30
invited oral

Albert Figueras[1)]

1) Institut de Ciencia de Materials (ICMAB) - CSIC (ICMAB), Campus de la UAB, Barcelona 080193, Spain

The ecological elimination of pollutants is an issue of increasing concern in today's society. Many researchers have proved that semiconducting TiO2 is an excellent photocatalyst that permits the degradation and finally the mineralization of stable organic pollutants such as detergents, dyes and pesticides in water. However,
it requires ultraviolet (UV) radiation whose energy exceeds the bandgap of 3.2 eV
(λ 380 nm) of the anatase crystalline phase, hence practically ruling out the use of sunlight as an energy source for photodegradation. Another aspect of the problem is the manufacturing of the material: usually, aqueous suspensions and powders are used. However, less activity has been focused on the use of thin films for the decomposition of organic compounds. Filtration, necessary when aqueous suspensions are used, would in this case be avoided.

The talk will focus on thin films with strong oxygen sub-stoichiometry presenting enhanced photocatalytic properties in the visible range, which make them ideal candidates for low-cost photodegradation applications. One example on nonylphenol photodegradation using visible light will also be provided.

Nanostructural HRTEM, HREELS and HAADF characterization of the La2Mo2O9 ion conductor

14:30 - 14:45
oral

Jordi Arbiol[1,3)], **ALBERTO TARANCÓN**[1)], **GUILHEM DEZANNEAU**[1)], **ALEJANDRO MORATA**[1)], **FRANCESCA PEIRÓ**[1)], **Joan R. Morante**[1)], **Rolf Erni**[2)], **Nigel D. Browning**[2,4)]

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4) Lawrence Berkeley National Laboratory, National Center for Electron Microscopy (LBNL), Berkeley, United States

In the recent years, solid ionic and mixed ionic-electronic conductors (MIECs) have attracted much attention due to their applicability in solid oxide fuel cells (SOFCs) as electrolyte and electrode materials, respectively. Recently, $La_2Mo_2O_9$ has been presented as a promising electrolyte material for SOFCs, and recent results from our group confirmed that such compound fulfill some of the requirements for SOFCs applications such as a high ion conduction and a wide oxygen partial pressure range of pure ionic conduction. Nevertheless, the mechanism of oxygen conduction in $La_2Mo_2O_9$ is still not understood, in particular some questions remain about the strong decrease of conductivity from the cubic high-temperature (HT) phase to the monoclinic low-temperature (LT) phase. In the present work, we report a detailed structural and compositional characterization of the $La_2Mo_2O_9$ LT phase. The nanocompositional and nanostructural features of the LT-$La_2Mo_2O_9$ superstructure are put into evidence by means of HRTEM, HREELS, HREFTEM and HAADF.

14:50 - 15:05
oral

First solar cells based on CdTe nanoparticles/MEH-PPV composites

Sandeep Kumar[1), **Thomas Nann**[1)]

1) Materials forschungcentrum (FMF), Stephen Meier str. 21, Freiburg 79104, Germany

Market expansion in the use of conventional inorganic solar cells remains limited due to high costs imposed by fabrication procedures involving elevated temperatures, high vacuum and numerous lithographic steps and discrete processing due to glass carriers.
Organic solar cells having one of the components as conducting polymers can serve as a cost effective alternative to conventional inorganic solar cells because of the processing advantages of polymers. These polymers can be solution processed and their good mechanical properties opens the possibility to design it in flexible shape and sizes. Solar cells based on CdSe nanoparticles and conducting polymers were realised and a maximum efficiency of 1.7% was obtained. The performance of such a solar cell can be improved further by extending partly the nanoparticle absorption in the IR region by using CdTe nanoparticles. The onset of absorption of of CdSe in bulk is 720 nm while that of CdTe is 820 nm. This shift of 100 nm in wavelength for CdTe can improve the absorption of of sunlight by 20% relative to CdSe. Furthermore the electron mobility of CdTe is higher compared to CdSe and hence can be looked as a better material to be used in polymer solar cells.
In this report we present for the first time a solar cell based on CdTe nanopartricle/ MEH- PPV composites. Being a new system a systematic approach was carried out from synthesising nanoparticles to building solar cells. A new organometallic route was developed for synthesis of CdTe nanorods. Cyclic voltammetry measurements were carried to determine the HOMO and LUMO levels of the nanoparticles and MEH-PPV to see if they meet the proper energy level alignment for a possible charge transfer. Evidence for charge transfer was further confirmed by PL quenching. Once the evidence for charge transfer was confirmed solar cells were build using spin coating on ITO substrate and an efficiency of 0.05% was obtained for first cells under AM 1.5 conditions.

15:10 - 15:25
oral

Novel Approach of Multicrystalline Silicon Texturing for Large Area Commercial Solar Cell of Low Cost and High Efficiency

Suresh Kumar Dhungel[1)], **Kyunghae Kim**[1)], **Jinsoo Yoo**[1)], **Hwang Sunwoo**[1)], **Bojan Karunagaran**[1)], **Devanesan Mangalaraj**[1)], **Junsin Yi**[1)]

1) School of Information and Communication Engineering, Sungkyunkwan University, 300 Chunchun-dong, Jangan-gu, Suwon 440746, Korea, South

Multicrystalline silicon wafers were textured in an alkaline bath, basically using NaOH and in acidic bath, using mainly HF, HNO_3 , De-ionized water, Na_2 PO_4 and H_3PO_4 in different composition ratio and treatment time. Comparison of average reflectance of the treated samples for the range of 400 nm to 1100 nm wavelength of light showed low reflectance value ($<$ 5 %) for the acid textured sample in the optimized condition. The solar cells were thus fabricated with the samples following the main steps such as Phosphorus doping for emitter layer formation, PECVD Silicon Nitride deposition for anti-reflection coating and front surface passivation , Screen Printing metallization, RTP co-firing and Laser edge isolation and confirmed 14 % conversion efficiency from the best textured samples. This isotropic acid texturing approach can be instrumental to replace conventional alkaline texturing approach for the mass production of low cost and efficient solar cell with the multicrystalline silicon as the starting material.

15:50 - 17:20

Afternoon session - continued

Main Building, room 219

Conducting polymers based nanocomposites for lithium batteries and sensor arrays.

16:30 - 16:45 oral

<u>Oleg Posudievsky</u>[1)]

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

Nanostructured materials have already become a subject of active researches in solid state chemistry and physics. Special attention is devoted to hybrid nanocomposites based on conducting conjugated polymers due to unique combination of physical and chemical properties this class of organic materials possesses.
Various methods for preparation of guest-host nanocomposites based on conducting polymers (polyaniline, polypyrrole, polythiophenes, etc.) and transition metal oxides (vanadium, molybdenum, manganese) are considered. Structural and spectroscopic data provide evidence for polymer insertion inside the interlayer galleries of inorganic nanoparticles. Mechanism of polymer intercalation is presented. Structure-property relationships are analyzed. Charge-discharge characteristics of the nanocomposites are discussed.
Conducting polymer sensor array with a set of sensitive polyaniline and polypyrrole films doped with different dopants is described. The array consists of polymeric sensors based on the interdigitated gold electrode systems on the glassceramic substrate. The thin polyaniline or polypyrrole films were electrochemically deposited on gold electrodes using addressable polymerization of each element of array with various doping agents and conditions of electrodeposition. Employment of different heteropolyacids as dopants together with a set of simple doping acids provides a wide range of sensitivities for individual sensor elements. The effect of the polymer nature on the sensor response is discussed. Principal Component Analysis performed over sensor array data was used to separate samples of different organic vapors (10 species of different nature) by their images.

Application of net shape technology to the development of solid oxide fuel cells

16:50 - 17:05 oral

<u>Piotr Jasinski</u>[1,2)], **Vladimir Petrovsky**[2)], **Toshio Suzuki**[2)], **Tatiana Petrovsky**[2)], **Harlan U. Anderson**[2)]

1) Gdansk University of Technology (PG), Narutowicza 11/12, Gdańsk 80 952, Poland

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Solid oxide fuel cells (SOFCs) are concerned to be the most efficient future energy source. At the current development stage several problems must still be solved to increase the performance and stability of SOFC and decrease its price. In particular:
1.cost effective ways of thin film electrolyte processing should be developed,
2.interfacial reactions, which occur between the electrodes and electrolyte due to high-temperature processing, should be avoided,
3.catalytic activity of electrodes should be increased.
This paper presents an alternative and cost effective method, which may offer solution to described problems. The method called net shape technology is a low sintering temperature process technique which employs a combination of colloidal suspension and polymer precursor techniques. Using proposed technology both dense and porous films having the thickness from 1 to 10 [U+F06D]m can be prepared. Therefore this technology can be used to the preparation of dense electrolyte films on either cathode or anode support, as well as porous electrodes on dense electrolyte. The net shape technology can be used to preparation of anode or cathode support. In this case, instead of colloidal suspension technique, conventional sintering of powder with pore former is performed. Obtained in this way ceramic skeleton is backfilled with polymer precursor. In the paper examples of application of net shape technology to the development of electrolytes, anodes and cathodes have been presented.

Studies of magnetoresistance of manganite-lanthanum perovskites

17:10 - 17:25 oral

<u>Igor Zhikharev</u>[1,2)], **Valentin P. Pashchenko**[1)], **Aleksey V. Pashchenko**[1)], **Aleksandr A. Shemiakov**[1)], **Vasilij K. Prokopenko**[1)], **Anna Silcheva**[2)]

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High-temperature X-ray analysis and magnetoresistance method allow us to reveal the anomalous behaviour of crystalline-lattice parameter of La_0,6A_0,2Mn_1,2O_3[U+F0A1]$_{delta}$ (A^{2+}: Ca^{2+}, Sr^{2+}, Pb^{2+}) near the temperatures of transitions - T_c, T_m (colossal magnetoresistance), and T_p. The sample consists of a single phase. The La_0,6A_0,2Mn_1,2O_3[U+F0A1]$_{delta}$ (A^{2+}: Sr^{2+}, Pb^{2+}) - structure is rhombohedral (R3c)

and includes the plane clusters of gamma-Mn_2O_3 or Mn_3O_4 types [1]. The clusters are dissolved in the matrix structure, when the temperature is increased and the matrix structure is transformed into the cubic one at the temperatures within the range 1070-1100 K (Pm3m). Structure La_0,6Ca_0,2Mn_1,2O_3[U+F0A1]$_{delta}$ is cubic (Pm3m), but also consist the plane clusters of gamma-Mn_2O_3 or Mn_3O_4 types [2].
The linear relationship is determined between the width of NMR spectrum from octahedral manganese ions taking place in a high-frequency electronic exchange and the tolerance factor calculated for defect structure accounting the infringement of a co-ordination number, giving rise to distortions of polyhedrons owing to anionic vacancies.
The broad asymmetric NMR spectra suggest that there is a high-frequency electron exchange between Mn3+ and Mn4+ and that the environment of Mn^{3+}, Mn^{4+} and La^{3+} is nonequivalent because of the vacancies and clusters and different valence of the ions.
Probably, the origin of the structural anomaly is Mn^{2+}+Mn^{4+}[U+F0AE]2Mn^{3+} transformation or transition of Mn^{3+} ions from low-spin state into high-spin one.

15:50 - 16:30

Coffee break

19:00 - 21:00

Poster Session 2

Acoustic and Adsorbtion Properties of Nanostructured Carbon Material

poster A-21

Viatcheslav V. Barkaline[1)], **Alexandre S. Pautino**[1)], **Alexander S. Chashinski**[1)]
1) Belarussian National Technical University (BNTU), F. Skariny, 65, Minsk 220027, Belarus

Carbon nanostructured material (C-nano) was studied theoretically as an sensitive material for surface acoustic wave (SAW) based chemical sensors based on $LiNbO_3$ single-crystalls and Si/SiO_2/ZnO structures. The influence of O_2 and H_2 adsorbtion by C-nano layer on fundamental SAW mode velocity was examined. SAW phase velocity culculation in multilayer SAW structures was based on the method of effective material constants depending on temperature, deformations and electric field. C-nano layer was represented by ordered composite material consisting of equidirectional carbon nanotubes embedded to the amorphous carbon matrix. The material parameters of C-nano layer were determined by effective elastic medium method. Single- and two-wall nanotubes of (10,10), (12,6) and (16,0) chiralities with close diameters and equal lengths where investigated with various orientations with respect to SAW waveguide crystallographic orientations and various distances between nanotubes axices.Elastic moduli and adsorbtion characteristics of nanotubes where estimated by molecular dynamics calculations based on MM3 force field. The dependences of the energies of adsorbtion of O_2 and H_2 on single nanotubes with various chiralities and nanotube bundles from the position of adsorbate molecules was studied. The adsorbtion minima are influenced radically by the presence of carbon "hat" at the nanotube ends and very slightly by the nanotube length. Adsorbtion energy for tube bundle exceedes that on graphite claster for all gases studied. The difference between adsorbtion properties of single and multi-wall tubes seems to be very essential. The adsorbtion capacity and thermodesorbtion spectra of various C-nano composites with respect to O_2 and H_2 was estimated.The data presented have shown prospects of usage of nanostructured carbon materials for SAW chemical sensors on the basis of $LiNbO_3$ and Si/SiO_2/ZnO structures.
[ABSTRACT TRUNCATED TO 2000 LETTERS]

Characterization of the nanofibers from different PAN concentrations for sensor application

poster A-22

Ana Neilde R. da Silva[1,3)], **Demétrius S. Gomes**[1)], **Luis T. Freire Mendes**[3)], **Rogerio Furlan**[2)], **Nilton I. Morimoto**[1)], **Idalia Ramos**[2)]
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ELECTROCHEMICAL CHARACTERIZATION OF 'HERRINGBONE' CARBON NANOFIBRES, PREPARED BY CVD METHOD

ZULFIQUR ALI[1)], ANDREW DEAN[1)], STELA M. PRUNEANU[1)], CHRIS MALINS[1)], ABDELHAKIM BOUGHRIET[1)], DAN LUPU[2)], ALEXANDRU R. BIRIS[3)], LILIANA OLENIC[4)] poster A-23

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Since the discovery of carbon nanotubes (CNT) in 1991 by Iijima /1/ considerable effort has been made in demonstrating the unique properties of these materials. Carbon nanotubes display excellent chemical stability and a range of electrical conductivity /2,3/. They can be metallic or semiconducting, depending on tube diameter and chirality. Carbon nanotube surfaces show enhanced electron transfer rates when used as electrode in electrochemical reactions.
The interaction and electron exchange between redox-enzymes and nanocarbon has also attracted increasing attention. Typically, the enzymes are complicated and large molecules, with redox centers deeply inlaid within their structure. Hence it is difficult for enzymes to directly exchange electrons with the smooth surface of the electrode. Mediator molecules have previously been used to impose electron contact between redox enzymes and electrode surface.
In this paper we present a study of the electrochemical properties of herringbone carbon nanofibres in the presence of a redox system, potassium ferrocyanide. Carbon nanofibres, with diameter of approximately 250 nm, were prepared by a chemical vapour decomposition method (CVD), using ethylene as the carbon source. The purification process involved hydrochloric acid reflux, cycles of washing and finally filtration. We have used potassium ferrocyanide as a mediator in the construction of a glucose oxidase biosensor. The characteristics of this biosensor have been studied by amperometry, cyclic voltammetry and impedance spectroscopy.

References

1. S.Iijima, Nature, 1991(354)56
2. E.W.Wong, P.E.Sheehan, C.M.Lieber, Science 1997(277)1971
3. B.I.Yakobson, R.E.Smalley, Am.Sci. 1997(85)324

SYNTHESIS OF NANOSIZED POWDERS Nd-DOPED YAG BY COPRECIPITATION AND MICROEMULSION METHODS

Eugenio F. Caponetti[1)], Delia Chillura Martino[1)], Lucia Pedone[1)], Maria Luisa Saladino[1)] poster A-24

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Doped yttrium aluminum garnet (YAG, $Y_3Al_5O_{12}$) materials are studied for their peculiar luminescence properties.
In order to explore the properties of one of these materials in the nanometric range, Nd:YAG (Nd:$Y_3Al_5O_{12}$) nanoparticles have been produced by using two synthesis procedures, coprecipitation and microemulsion methods.
In the former, the Nd-YAG nanoparticles formation is performed by co-precipitation of two hydroxides, $Al(OH)_3$ e $Y(OH)_3$, in an aqueous solution containing Nd^{+2} ions. The thermal treatment at 900 C of the mixed hydroxide nanoparticles, allows obtaining the final product.
In the latter, the co-precipitation happens inside the aqueous core of the reverse micelle that constituted the water/CTAB/butanol/n-heptane microemulsion. The thermal treatment at 900 C of the microemulsion containing the mixed hydroxide allows to eliminate surfactant and oil and to obtain the doped mixed oxide.
The obtained materials, of stoichiometric composition $Nd_{0.15}Y_{2.85}Al_5O_{12}$, i.e. 5% in Nd atoms, was characterised using XRD, SEM, TEM and luminescence techniques. Characterization results will be discussed.

Fabrication and electrical properties of Eu^{3+}:$BaTiO_3$ nanoceramics for SOFC

poster A-25

Dariusz Hreniak[1)], **Wiesław Stręk**[1)], **Jacek Chmielowiec**[2)], **Grzegorz Paściak**[2)], **Robert Pązik**[1)], **Stanisław Gierlotka**[3)], **Witold Lojkowski**[3)]

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It is well known that perovskite-type oxides can be used both as electrolytes as electrodes or oxygen separation membranes for SOFC (Solid Oxide Fuel Cell). Recently, the dependence of the size of crystallites on the electric properties of oxide materials was found. It has been reported that mechanism of electron conductivity is governed by the grain sizes of ceramic [1].
In this work the new method of fabrication of nanoceramics by the hot-pressing under high pressure of sol-gel derived Eu^{3+}:$BaTiO_3$ nanocrystalline powders is reported. The preliminary studies of conductivity of fabricated nanoceramics are presented. The energy of activation from alternating current measurements was determined. The influence of size of crystallites on the conductive properties of Eu^{3+}:$BaTiO_3$ was investigated. The possibility of application of perovskite-type nanoceramics doped with rare-earth ions in the fuel cells systems is discussed.

[1] N. Setter, R. Waser, Acta mater. 2000, 48, 151.

ELECTRIC PROPERTIES of Ag3SbS3 and Tl3SbS3 THIN FILMS PREPARED BY PULSE LASER DEPOSITION

poster A-26

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Ag3SbS3 and Tl3SbS3 are seemed to be very attractive for many technical applications due its high electro-optical effect, significant double-beam refraction and transparency in the wave length 0.6-14 mm. The possibility of optical recording information on Ag3SbS3 and Tl3SbS3 thin films was stated earlier. The effect of laser-evaporator pulse recurrence frequency (n) and substrate temperature (TS) on structure of deposited films has been studied. Transmission electron microscopy (TEM), scanning electron microscopy electron microscopy (SEM) and electron diffraction examination were used to study the structure and phase state of the films. The SEM image of the film is shown in Fig. 1. Nevertheless, the electric properties of the compounds (bulk materials and thin films) are poorly investigated. The abstract reports first data of electric characteristics of thin films deposited on KCl wafers by pulse laser deposition technique under following conditions: the substrate temperature was 300 K, time of deposition was varied from 5 to 17 minutes, and thickness of the film did not exceed 0.8 mm. The current - voltage measurements carried out at the room temperature were shown power-behaved dependence similar to that of the current limited by space charge region in typical barrier structures. The so-called electric field-induced aging was also studied. It was found that the experimental current is sufficiently changed (the power-like mode of charge carriers transport is replaced by the velocity saturation mode of the carriers transfer). These data made it possible to perform numerical simulation of the results obtained and construct an energy band diagram of the structures.

Ionic Conductivity of 4%mol, 9.5%mol Yttria doped Zirconia Nanomaterials and (YSZ)0.98-(Al2O3)0.02 Nanocomposites

poster A-27

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Ionic conductivity of nanophases of 4% and 9.5 yttria doped zirconia YSZ were studied using impedance spectroscopy technique. In this study our aim is to find optimal conditions for any improvement of ionic conductivity at low temperature. Experimental results show that ionic conductivity of nanosized YSZ with 4% mol is higher than for single crystal YSZ with 9.5% mol and this for the most part of temperature domain studied (300-500C). For nanocomposite with 2 % mol Al2O3, we found that an light increase of ionic conductivity even at low temperatures. This work has shown that conductivity in these materials depends not only on concentration in alumina but also of microstructure. Comparing with N9, the nanocomposite NC2 with 2 % mol Al2O3 gives the highest conductivity in grain and not in grain boundary.

Transparent Conducting Oxides as Ohmic Contacts for GaSb-based Thermophotovoltaic Cells

Krystyna Golaszewska[1)], **Eliana Kaminska**[1)], **Emil Kowalczyk**[1)], **Renata Kruszka**[1)], **Radoslaw Lukasiewicz**[1)], **Ewa E. Papis**[1)], **Anna Piotrowska**[1)], **Tadeusz T. Piotrowski**[1)], **Pawel Skoczylas**[1)], **Adam Barcz**[1,2)], **R. Jakieła**[3)]

poster A-28

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Of the available materials for thermophotovoltaic cells, quaternary compounds of the GaSb family have the advantage of optimal band gap and excellent minority carrier transport in InGaAsSb/GaSb TPV diodes. To take full advantage of these devices high quality transparent ohmic contacts are required. At present the front contact metallization relies on the use of photolitographically patterned thin film metallic structures that introduce a shadowing loss. The use of transparent conducting oxides (TCOs) could potentially eliminate this loss. However, TCOs may introduce other losses due to electrical resistance.
The most successful oxide to date for such application has been indium tin oxide, which has seen widespread use in thin photovoltaic cells. However, no results have been reported on its use over wider spectral range. Moreover, recent studies of other oxides of the same family, such as $GaInO_3$ and CdO indicate that other material systems may offer better transparency in mid-infrared range.
In this work comparative studies of transparent ohmic contacts to GaSb-based materials have been performed. Thin conducting films of ITO, SnO_2, CdO, and ZnO have been deposited by reactive magnetron sputtering. (100) GaSb wafers and LPE-grown InGaAsSb and AlGaAsSb epilayers were used as substrates. The influence of parameters of deposition on electrical and optical properties of TCO films was assessed by measurements of resistivity and photospectrometry. Electrical properties of TCO/semiconductor contacts were extracted from I-V and contact resistivity measurements. Contact microstructure was analysed using XRD, SIMS, SEM, and AFM.
We show that highly transparent (T>90% in the spectral range up to 2.4 μm) TCO films have been produced enabling fabrication of ohmic contacts with the specific resistance about 10^{-4} Ωcm^2 to GaSb-based semiconducting materials.
Work supported by the grant from the State Committee for Scientific Research 3 T11B 009 026.

Fabrication of Crystalline and Multicrystalline Black Silicon Solar Cells

Jinsu Yoo[1)], **Kyunghae Kim**[1)], **Bojan Karunagaran**[1)], **Suresh Kumar Dhungel**[1)], **Manoharan Gowtham**[1)], **Sunwoo Hwang**[1)], **Devanesan Mangalaraj**[1)], **Junsin Yi**[1)]

poster A-29

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This paper deals with the investigation on formation of microstructures on silicon surface using reactive ion etching (RIE) in a multi-hollow cathode system. This reactor consists of a Pyrex tube defining the vacuum chamber, with the outer metal cylindrical electrode (grounded) acting as a counter electrode for the aluminum plate electrodes assembly which is in electrical contact with silicon wafers. The plate electrodes have a diameter of 150 mm each. These electrodes are electrically and structurally connected by metal supports, close to their outer rim, with a separation space of 25 mm between each of them. The Pyrex tube has an inner diameter of 190 mm. RF power applied to the electrodes creates an electrical field on their surfaces and causes an excitation of reactive gases in the space between them, preferably between the silicon wafers. This produces a high level of ionization of the gas and dense plasma therein due to the repelling movement of the entrapped electrons between the powered electrodes; and this is called the hollow cathode effect. . In this work, optogalvanic (OG) signal is used to analysis the variation of plasma conductivity caused by the absorption of radiation at a certain spectral transition of the plasma medium. The OG effect technique was developed for the purposes of laser spectroscopy and has been used to diagnose plasma parameters such as, the ionization rate, atomic density and translational temperature of the plasma. The multi-hollow cathode plasma system used in the present work generated plasma ion density up to 2×10^{12}cm^{-3} . Plasma texturing has been shown to produce black silicon surfaces with almost zero reflectance. The silicon surface was covered with columnar microstructures each having diameter ranging from 50 to 100 nm and depth of about 500 nm. Solar cells with efficiencies 11.7% and 10.2% were fabricated using black c-Si and black mc-Si wafers respectively by making use of industrial mass production line system.

Growth Mechanism of InAs/GaAs and GaP/GaAs Strained Layered Superlattices by Atomic Layer Epitaxy

poster A-30

Masashi Ozeki[1)], **Tomohiro Haraguchi, Takeshi Takeuchi, Kouji Maeda, Kenji Yoshino**[1)]
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Atomic layer epitaxy (ALE) has received considerable attention as a novel approach to crystal growth in nanotechnology. A central idea in ALE is a self-limiting mechanism that automatically stops the layer growth at a certain atomic layers and therefore allows complete control of the layer thickness with single atomic layer accuracy.
In homoepitaxies, ALE proved a great success. However, many difficulties appeared in some heteroepitaxies where the self-limiting was easily broken. Even the growthof a simple heterosturucture of eaptaxial layer A on epitaxial layer B requres three types of ALEs; ALE for epitaxial layer B on epitaxial layer B (homoepitaxy), ALE for epitaxial layer A on epitaxial layer B (heteroeptaxy), and ALE for epitaxial layer A on epitaxial layer A (homoepitaxy).
We have investigated the self-limiting mechanism in the ALEs of InAs/GaAs and GaP/GaAs heteroeptxies and strained layered superlattices. Superlattices were grown on GaAs(001) and InP(001) by "Pulsed-Jet-Epitaxy" with trimethylgallium, trimethylindium, trisdimethylaminoarsine, and phosphine as source materials. We report that the strain between epitaxial layer and the substrate, an atomic level surface morphology, and an interface electric neutrality had great effects on the self-limiting mechanism in heteroepitaxy.

Formation of intermetalic bonds in the Pd-Cu system for MIS sensor application

poster A-31

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Formation of Pd-Cu structures in the process of MIS sensors fabrication ensures a high quality of devices if the corresponding electronic states in Pd-Cu system lead to large number of free active bonds on the electrode surface. In the present work the role of Pd surface doping with copper and related mechanisms of adsorption, desorption and bulk dissolution of hydrogen were considered. The theoretical modeling of Pd-Cu alloy was performed using density functional theory combined with coherent potential approximation. The total energy and the partial density of states (PDOS) for Pd_xCu_{1-x} alloy were analyzed for the Cu atomic fraction varied in the range of 0 - 100 at%.

The results show that the most radical changes in the electron structure of alloy take place when the Cu content is less than 50 at%. In this case p-states of Cu are mainly responsible for the reconstruction of intermetallic bonds in Pd-Cu system that leads to activation of catalytic processes in the system and formation of stable Pd-Cu compounds. The reorganization of a surface caused by formation of surface Cu_XPd composite may be applied for enhancement of Pd surface catalytic activity as to dissociative adsorption of H_2 with the following dissolution of atomic hydrogen in the bulk.

The obtained results allow us to explain the observed copper induced slowing down of Pd surface aging and degradation in MIS structures and predict behavior of sensor surfaces formed by this compound. The reconstruction of the surface layers that was observed experimentally [1] is explained on the basis of obtained results.

[1] V. Litovchenko, T. Gorbanyuk, A. Efremov and A. Evtukh, Sensors and Actuators (1999) 74, 233-236.

Application of Rapid Thermal Processing for Large Area High Efficiency Solar Cell Fabrication in Industrial Scale

Kyunghae Kim[1], **Suresh Kumar Dhungel**[1], **Bojan Karunagaran**[1], **Jinsu Yoo**[1], **Kaustuv Chakrabarty**[1], **Hwang Sunwoo**[1], **Devanesan Mangalaraj**[1], **Yi Junsin**[1]

poster A-32

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We carried out thorough investigation of the co-firing profiles of the screen printed single and multicrystalline silicon wafer surfaces (front and back) in Rapid Thermal Processing (RTP) furnace for the formation of metal contact. The firing profiles and the performance parameters of the cells were analysed for wafers of different sheet resistances such as 20, 30, 40, 60 and 80 ohm per square. The Phosphorous doping for the generation of emitter layers of different sheet resistances was done by high temperature diffusion using POCL3.The sheet resistance was measured using four point probe device and metal thickness on the front and back surfaces after co-firing were obtained by using a- step measurement technique. On the best textured and silicon nitride deposited surface a conversion efficiency of 17 % and 14 % could be ensured in the single crystalline and multicrystalline silicon solar cells respectively, fabricated by using our optimized co-firing approach after front and back metal printing. This approach could be used for industrial production of low cost and high efficiency silicon solar cells of large area.

Implantation Damage in implanted poly-Si investigated by Nanocalorimetry technique

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poster A-33

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The heat released during the annealing of ion-implanted polycrystalline Si (p-Si) is investigated for the first time by nanocalorimetry technique. This later operates on similar principles as Differential Scanning Calorimetry (DSC), but achieves heating rates up to 10^6 K/s, which allows measuring small amount of heat with high sensitivity. Thus, one can measure in situ the heat released by near-surface processes such as damage annealing in Si implanted at low energy.
30 keV Si^- implantations have been performed at fluences ranging from 6.10^{11} to 8.10^{14} at/cm^2, and the heat released as a function of temperature during scans between 30 and 450C are presented. It was shown that the heat released has the same shape in all cases, indicating that kinetics of ion implantation defects annealing is independent of fluence. It is also shown that the heat release starts to saturate around a fluence 10^{14} at/cm^2 while for similar fluences, the damage in mono-crystalline Si is far from being saturated, according to channelling measurements. This would imply that further lattice disorder does not occur at the expense of more stored energy. The effect of changing of the heating rate, fluence rate and time evolution on the released heat is also discussed.

NANOCOMPOSITE PHOTONIC SENSORS: FIRST APPROACH BY THE NANOPHOS INITIATIVE

Giannis Manasis[1], **Anna Tsigara**[1], **George Anyfantis**[1], **N Madamopoulos**[1], **George Mousdis**[1], **Katerina Gatsouli**[1], **Stergios Pispas**[1], **Nikos Vainos**[1], **Alessio Perrone**[2], **R. Datta**[3], **Jerzy Ciosek**[4], **Krystyna Golaszewska**[4], **Eliana Kaminska**[4], **Renata Kruszka**[4], **Anna Piotrowska**[4], **Stelios Couris**[5]

poster A-34

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Complex materials structures based on metal oxide and metal composites have been proposed for novel photonic sensors. Materials involved include: SiOx
SnO_x, InO_x , ITO, TiO_x, ZnO_x, WO_x and metals such as Pt, Pd, Cu, Ag etc. They have been grown on glass and metal substrates by magnetron sputtering techniques. Special designs include optical structures

that can be affected by exposure to simple oxidizing and reducing gas chemical agents as well as to external physical parameters. Zinc and tin oxide structures have been shown to offer significant temperature response and further studies are underway to induce enhanced chemical sensitivity.

In a alternative approach, hybrid materials composed of polymer or sol-gel derived silica matrices containing cobalt chloride nanocrystals are fabricated and evaluated as hybrid humidity sensors. The composite films were produced by either spin coating or casting the initial polymer/$CoCl_2$ or $Si(EtO)_4/CoCl_2$ solutions on glass substrates. $CoCl_2$ nanocrystallites are formed within the films due to polymer or silica cobalt chloride interactions. At various degrees of humidity the formation of such molecular complexes affects severely the surface morphology due to changes of the molecular volume which results in significant and controlled diffractive and scattering effects. The variation of the complex refractive index may also affect the process, however, playing a secondary role, in contrast to the well known colorimetric effects.

Work supported by the grant from the European Comission NANOPHOS (contract IST-2001-39112).

Application of Laser Edge Isolation for the Solar cell fabrication with Spin-On - Doped Emitter Layer on Multicrystalline Silicon Substrate

poster A-35

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We applied Spin- On - Doping (SOD) method to form emitter layer on the p-type multicrystalline silicon wafers. A stable and consistent sheet resistance of 40 ohms per square was obtained in all the doped wafers. Solar cells were fabricated with those wafers using the main steps such as PECVD silicon nitride deposition for antireflection coating and front surface passivation, screen printing metallization on front and back surfaces, co-firing in rapid thermal processing furnace and finally the edge isolation by using Nd-YAG laser. SEM (EBIC) and ASR were used to examine the p-n junction profile of the wafers. Solar cells with at least 13 % conversion efficiency could be fabricated as the end product by this method.

Synthesis and Characterization of Cyclohexene Polymer Thin Films by PECVD Method

poster A-36

I.-S. Bae[1,2)], **C.K. Jung**[1,2)], **Y.S. Park**[2)], **B. Hong**[2)], **D.-H. Shin**[2)], **J.-G. Kim**[2)], **J.-H. Boo**[1,2)]

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Polymer-like cyclohexene thin films have been deposited on glass, silicon and copper substrates at below 100 °C for analysis of their various properties by plasma enhanced chemical vapor deposition (PECVD) method. Cyclohexene monomer was utilized as organic precursor, and hydrogen and Ar were used as bubbler and carrier gases, respectively. In order to compare the influence of the electrical and the optical properties of the plasma polymerized organic thin films with deposition conditions such as RF power and deposition temperature. The as-grown plasma polymerized thin films were analyzed by FT-IR, UV-Visible spectroscopy and ellipsometry as well as I-V and C-V curves. As the plasma power was increased, the refractive index of thin films increased and transmittance decreased by ellipsometry and UV-Visible measurement, respectively. The minimum dielectric constant and the best leakage current were 3.0 and 7×10^{-12} A/cm^2, respectively. The corrosion protective abilities of polymerized cyclohexene films were also examined by AC impedance measurements in 3.5 wt.% NaCl solution. We found that the corrosion protection efficiency (PK), which is one of the important factors for corrosion protection in the interlayer dielectrics of microelectronic devices application, was increased up to 90 % with increasing RF power. AFM and SEM showed that the polymer films with smooth surface and sharp interface could be grown under various deposition conditions. The contact angles also increase with increasing RF power. We also carried out in situ plasma diagnostics by optical emission spectroscopy (OES) for understanding the initial growth behavior of organic polymerized thin films.

An Arc Plasma Route to Magnetic Nanoparticles for biomedical applications

poster A-37

Michał Bystrzejewski[1], **Hubert Lange**[1], **Andrzej Huczko**[1]
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Arc plasma synthesis of carbon-encapsulated FeNdB nanocrystallites is reported. The influence of pressure and anode composition on the morphology, structure and magnetic parameters of encapsulates was studied. The products were analyzed using different techniques: SEM, HR TEM, XRD, and magnetic measurements. A possibility to use synthesized nanostructures for biomedical applications was also disscussed.
Acknowledgment: The work was supported by the Committee for Scientific Research (KBN) through the Department of Chemistry, Warsaw University, under Grant No. 4 T08D 021 23

Electron and hole spectra in complicated opened cylindrical nanoheterosystem at the presence of outer magnetic field

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poster A-38

The investigation of nanosystems and their utilization have been opened the range of new scientific problems. The particular interest is devoted to the specific properties of electrons, holes, excitons at the media interfaces. In the nanoheterosystems created on the base of quantum wires and systems of other dimensions there arise the unique physical properties due to which the latter are utilized for the creation of injector lasers, optical modulators and single-electron devices.
The theory of single cylindrical quantum wires is developed in details till now, but the influence of outer magnetic field at the physical properties of such systems is not studied rather well yet.
In this paper the influence of outer magnetic field into the electron and hole energy spectra in complicated cylindrical semiconductor nanoheterosystem consisting of the core (CdS) in the shell (HgS) embedded into the massive medium (CdS) is under study. Herein the electrons and holes can be in the bound quasistacionary states with the finite lifetimes. At the fixed thickness of the potential barrier there is the number of levels of size quantization due to the probability of penetration through the barrier is bigger for the higher energy levels.
The closed nanosystem CdS/HgS with the finite and infinite potential barriers is studied at the presence of the magnetic field too. The electron and hole wave functions are obtained as the solutions of stationary Schrodinger equation. The analytical expression for the S-matrix is derived within the effective mass approximation. The dependences of electron and hole energy spectra on the magnitude of the magnetic field and geometrical sizes of nanosystem are calculated. The exciton lifetimes are evaluated too. It is shown that the electron energy is bigger, the smaller is the radius of quantum wire. Herein the magnetic field holds the electron near the quantum wire axis.

Phonon spectra in quantum dots, quantum wires and nanosystems created of them

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poster A-39

Phonon spectra in single quantum dots and quantum wires have been studied for a long time in the framework of different models. Recently the theory of phonon spectra in multishell quantum dots (QD's) and quantum wires (QW's) have been established within the dielectric continuum (DC) model. The latter provides the ability to study the interaction between phonons and different quasiparticles (electrons, holes, excitons) not only in closed but in opened nanosystems too. The intensive experimental research in the creation of complicated nanosystems, the so called, spatial "architecture complexes" consisting of QD's, QW's and quantum wells stimulate the development of the theory of phonon spectra in such systems.
In the proposed paper the theory of the phonon spectrum and polarizational field is established for the complicated nanoheterosystem consisting of cylindrical QD surrounded by two cylindrical quantum antidots (QAD) located in cylindrical QW embedded into the massive media (MM). The nanosystem under study is described by the quasi 1D model.
The phonon spectra and polarization of the potential field are obtained within the DC model using the electrostatic boundary conditions. The quantization of the polarizational field is performed. It is established that the phonon spectra of the system contains two energies of confined phonons (equal to

the energies of longitudinal phonons of massive crystals analogue to QD and QAD); the energy of semi-confined phonons (equal to the energy of longitudinal phonons of surrounding media) and two types of interface phonons modes arising due to the side and main interfaces between cylindrical QD and cylindrical QW.
The dispersion law of interface phonons is calculated for the particular nanosystem. It weakly depends on the radius of QD and QW and the phonon energies are located between the smallest energy of transversal and the biggest energy of longitudinal phonons of the compositions of nanosystem.

Metallofullerenes and "magnetic soot" from arc evaporation of Nd/Fe/B/C composite.

poster A-40

Yulii S. Grushko[1], **Vitalii A. Trunov**[1], **Victor M. Lebedev**[1], **Taisia M. Pershikova**[1], **Svetlana G. Kolesnik**[1], **Vasilii T. Lebedev**[1]

1) St.Petersburg Nuclear Physics Institute RAS (PNPI), Orlova Roshcha, Gatchina 188300, Russian Federation

Pulse electric arc evaporation of graphite rods heavy doped with Nd_2O_3/Fe/B mixture or $Nd_2Fe_{14}B(C)$ alloys is used to prepare nanostructured carbon-based magnetic materials and metallofullerenes. Chemical treatment of "magnetic soot" is used to evaluate perfectness of encapsulation of metal particles in carbon shells. Composition, structure and morphology of the material are studied by Rutherford backscattering spectrometry and concurrent nuclear reactions analysis of 2 MeV deuterons and by thermal neutron scattering. The results are discussed in comparison with earlier publications on Nd-Fe-B(C) and Sm-Co-C nanoparticulates. Metallofullerenes are separated from metallosoot by two-stage solvent extraction with o-xylene and dimethylformamide (DMFA) and analyzed by HPLC on Cosmosil BuckyPrep columns (Nacalai Tesque Inc.). Possible effect of presence of Boron and large amount of metals on yeild and composition of metallofullerene fraction is discussed.

FeBO3 nanoparticles

poster A-41

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Symposium B

Progress in Polymeric Materials for Medicine and Biology

Introduction

Polymers and polymer-containing hybrid materials are indispensable for production of a great variety of products used in medicine. Many drug delivery systems are based on polymers. Polymers and polymer-containing hybrid materials are used for fabrication of permanent or temporary wound coverings, implants and for scaffolds for tissue engineering. From polymers are made elements of biosensors and other analytical devices. Important reagents in medical diagnostics are of the macromolecular nature.

In recent years there are carried on intensive studies on development of nano- and microstructured materials (organic polymers and organic polymer - inorganic hybrids) that could be used as scaffolds for hard and soft tissue. Many projects have been initiated in an answer to the need of nano- and microparticulate drug delivery systems directing bioactive compounds not only to selected tissue, but even more precisely - to the required intercellular compartments. Intensive studies are carried on in the area of medical diagnostic with a hope that using polymeric submicro-detectors would allow designing extra-sensitive, fast and reliable diagnostic devices. In today's world in which fast transportation strongly increases possibilities of spreading contagious illnesses such diagnostic tools are in a great demand.

Progress in the field of polymeric materials for medicine is extremely rapid and thus, researchers would benefit from an opportunity for sharing results of their recent studies and visions on the future of polymeric materials for medical and medical applications.

Organisers

- Prof. S. Slomkowski, Center of Molecul and Macromolec. Studies, Lodz, Poland
- Prof. J. Rosiak - Institute of Appl. Radiation Chemistry, Tech. Univ., Lodz, Poland
- Prof. C. Tsvetanov, Institute of Polymers, Sofia, Bulgaria

Scientific Committee:

- Haruma Kawaguchi (Yokohama, Japan)
- Jan Lukaszczyk (Gliwice, Poland)
- Christian Pichot (Lyon, France)
- Nevena Manolova (Sofia, Bulgaria)

Monday, September 6th

14:00 - 15:30

Afternoon session

Main Building, room 213

14:00 - 14:45
invited oral

Advances in intelligent biomaterials for protein delivery, biological recognition and bioresponsive systems

Nicholas A. Peppas[1)]

1) University of Texas at Austin (UT Austin), University Code C0400, Austin, TX 78712, United States

Engineering biomaterials by controlling recognition and specificity is the first step in coordinating and duplicating complex biological and physiological processes. Design and synthesis of artificial molecular structures capable of specific molecular recognition of biological molecules leads to biomimetic materials. Biomimetic configurational imprinting and microimprinting techniques, which create stereo-specific three-dimensional binding cavities based on a biological compound of interest, produce these biomimetic materials for intelligent drug delivery, drug targeting, and tissue engineering devices.

We present new developments of particular interest to the field that include recognition of undesirable biologicals, nano-scale patterning and recognition of proteins, site specific interaction with tissues, etc. Macromolecular networks with precise chemical architecture are prepared that possess enhanced mechanical, thermal, and recognition properties compared to their biological counterparts.

We have been successful in synthesizing novel glucose-binding molecules based on non-covalent directed interactions formed via molecular imprinting techniques within aqueous media. Numerous polymer systems were identified. Of particular importance in our polymer design is the network morphology, which spatially varies in crosslinking density (microporous and macroporous regions). Emphasis has also been placed on fundamental studies regarding the specific recognition event needed to produce a spatially defined recognition site. By tailoring the polymer gel structure composition, effective recognition sites can be created in polymer gels.

We have used micropatterning techniques for the preparation of synthetic polymer films with highly specific molecular recognition capabilities. We present recent data on their use as recognitive protein delivery systems.
[ABSTRACT TRUNCATED TO 2000 LETTERS]

14:45 - 15:05
oral

Polymeric Nanoparticles for Targeted Administration of Therapeutic Proteins

Federica Chiellini[1)], **Vincenzina Caruso**[1)], **AnnaMaria Piras**[2)], **Tiziana Pizzi**[1)], **Roberto Solaro**[1)], **Bruno Fiorentino**[2)], **Emo Chiellini**[1)]

1) University of Pisa - Dept. Chemistry & Ind. Chemistry (UNIPI), Via Risorgimento, 35, Pisa 56126, Italy

2) Kedrion SpA (Kedrion), Loc. Ai Conti 5, Castelvecchio Pascoli (Lucca) 55020, Italy

In the last decades, the original uses of polymers in clinical medicine as essential components of permanent prosthetic devices are being replaced by the development of new strategies. Among the others, controlled drug delivery technology represents one of the most rapidly advancing areas of science in which polymer and pharmaceutical scientists are contributing to biomedical research field. The possibility of achieving time and space controlled release of drug is a main challenge that drives much of current innovation in biomaterials science. In particular, controlled release is strongly required for unconventional drugs such as proteins and oligopeptides. Moreover, if polymer surface modification is possible, a targeted delivery is achievable, resulting in enhancement of the therapeutic efficacy of the dosage forms and lowering the toxic effects. Particularly, the use of synthetic bioerodible polymers for the formulation of protein loaded nanospheres offers the advantage of a tailored design of release and bioerosion kinetics. In this respect, the present work aimed at reporting on a study for aimed at the formulation of nanoparticles loaded with a protein drug with catalytic activity. Copolymers of maleic anhydride with butyl vinyl ether converted into the corresponding amphihilic graft copolymer by hemiesterification with 2-methoxyethanol (VAM41) were prepared with molecular weight ranging from 300 to 30 kDa. Nanoparticles were prepared by mean of a proprietary method based on co-precipitation technique using a combination of the prepared synthetic polymers, human serum albumin, a steric stabilizer and trypsin as a model protein drug. A careful in vitro evaluation of synthetic polymers and nanoparticles cytotoxicity was carried out as well as investigation to assess the preservation of biological activity of trypsin loaded in nanoparticles.

Polycations based on polyasparthylhydrazide for gene therapy

15:05 - 15:25
oral

Gennara Cavallaro[1], **Manfred Ogris**[2], **Fabio S. Palumbo, Gaetano Giammona**
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2) Ludwig Maximilians Universitaet, Department of Pharmacy (LMU), Butenandtstr. 5-13, Munich 81377, Germany

Hydrophilic polycations can be potentially useful for systemic gene delivery since their ability to form polyplexes with nucleic acids. α, β-poly(asparthylhydrazide) (PAHy), a water soluble synthetic macromolecule, was functionalized by using EDCI chemistry with 3-(carboxypropyl)trimethyl-ammonium chloride (CPTA) obtaining PAHy-CPTA copolymers. The derivatization degree (DD% mol/mol) of polycationic derivatives were detected by 1H-NMR and their main physico-chemical properties by SEC analysis. Previous chemical reactivity studies of naked PAHy evidenced the influence of condition reactions on molecular weight and degree of derivatization (DD% mol/mol) of obtained polycations. The capability of four different PAHy-CPTA derivatives (DD % mol/mol ranging from 18 to 58 % mol/mol) to complex plasmid DNA coding for luciferase and to transfect tumor cells at different plasmid to polycation ratios were performed using as positive control PEI polyplexes. In vitro transfection results evidenced that PAHy-CPTA copolymers having 48 and 58 % mol/mol show a high efficiency of transfection at DNA/polycation weight ratios 4.

Coffee break

15:30 - 15:50

Afternoon session - continued

Main Building, room 213

15:50 - 17:20

New Components for Dental Filling Materials

15:50 - 16:20
invited oral

Norbert Moszner[1], **Frank Zeuner, Jörg Angermann, Simone Klapdohr, Urs Fischer**
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Tooth-shaded dental restorations are becoming more and more popular. In this context, new chemical components, such as monomers or fillers, enable the improvement of important properties. Starting with a description of the general composition of currently used filling composites and dental adhesives examples of new components with a great potential for application in these materials will be presented.
Today, restorative composites are light-curing hybrid materials consisting of a resin matrix, which is a mixture of various cross-linking dimethacrylates and inorganic fillers, such as milled glasses or highly dispersed silica. Cyclic monomers as new components are of interest for dental fillings. One example of such cyclic monomers are new vinylcyclopropyl acrylates, which show a low volume shrinkage. Furthermore, polycondensates of functionalised silanes, which enable the improvement of the biocompatibility of composites will be presented. Nano-sized fillers improving the abrasion resistance and radiopacity of restorative composites will also be mentioned.
Enamel-dentin adhesives are used to achieve a strong bond between a filling composite and dental hard tissues. The used self-etching enamel-dentin adhesives contain different monomer components. Particularly adhesive monomers, such as polymerizable phosphoric acids modify the enamel and dentin surface and mediate the formation of a strong bond to the composite. Cross-linking monomers are used in order to improve the polymerization reactivity of the adhesive. In self-etching adhesives water is preferred as solvent. Thus, especially in the case of one-bottle adhesives, the methacrylates undergo hydrolysis, which changes the chemical composition of the adhesive and also impairs its performance. In this respect new phosphonic acid acrylates and bis(acrylamide)s, which feature an enhanced hydrolytic stability, can be used to substitute commonly used methacrylates in self-etching enamel-dentin adhesives.

SHRINKAGE OF DENTAL POLYMERIC COMPOSITES

16:20 - 16:40
oral

Tomasz Boguszewski[1), **Malgorzata Lewandowska**[1), **Wojciech Swieszkowski**[1), **Krzysztof J. Kurzydlowski**[1)

1) Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland

Introduction
One of the main problems influencing longevity of dental restorations is shrinkage of the resin/ceramic composites during their polymerization precess. The resin shrinkage results in developing of high stresses between the composite and the wall of the tooth. When the stresses are too high the failure of the bonded interface occurs, with possible margin failure, secondary caries and need for re-restoration.
The aim of the study was to investigate an influence of ceramic contribution in the dental composite on its polymerization shrinkage. Moreover, the influence of resin shrinkage itself on the whole composite shrinkage was investigated.

Methods
In 3-D linear elastic finite element analyses, the process of shrinkage of dental resin/ceramic composites during their polymerization was simulated using Ansys ver. 5.4. The influence of the ceramic contribution and resin shrinkage on the shrinkage of the dental composites was investigated.
The composites were modeled as the bricks with different volumetric contribution (from 0% up to 70%) of ceramic aggregate. The aggregate was represented in the model by the balls with radii of 0.15 micrometers. Volumetric resin shrinkage of 3%, 9%, 12%, and 30% was applied to the composite brick via the thermal analogy.

Results & discussion
Quantitative estimates have been obtained of the reduction in the composite shrinkage with increase of volumetric contribution of the ceramic aggregate or decrease of shrinkage of the resin. It was also found that when the shrinkage of the composite resin is below 5% the influence of the aggregate contribution in the composite can be neglected. However, for the resin shrinkage of over a dozen percentages the contribution of the ceramic aggregate has a crucial influence on the shrinkage of the composite.
This study indicates that by proper changing of the aggregate contribution and resin shrinkage the lower shrinkage of the dental composite may be obtained.

Evaluation of fatigue behaviour of elastomeric biomedical polymers

16:40 - 17:00
oral

Miroslawa El Fray[1)

1) Technical University of Szczecin, Polymer Institute, Pulaskiego 10, Szczecin 70322, Poland

Polymeric materials are utilised in the manufacture of a high number of load-bearing structural components. Since many loads are cyclic in nature, the deformation under cyclic loads (fatigue) is of particular interest. Especially creep properties of elastomers are of great importance when materials are expected to remain structurally stable within long duration loading. Generally, two experimental strategies can be applied: one is fracture mechanical investigations of fatigue crack growth behaviour; the other is hysteresis measurements conducted for the evaluation of fatigue behaviour using engineering parameters, i. e. deformation, dynamic modulus, stored and lost energies, and damping. This second method is particularly valuable for evaluation of structural changes of soft materials under cycling loading. Hysteresis loops are induced by the viscoelastic material behaviour and the slope of the hysteresis loop is affected by the cyclic degradation. During the fatigue experiments the hysteresis loop is digitalized by a computer and from the slope of the hysteresis loop the stress, strain, stiffness and energy related parameters are determined.

Evaluation of fatigue behaviour of novel and the reference elastomeric biomaterials will be presented. Novel poly(aliphatic/aromatic-ester)s (PED) containing poly(butylene terephthalate) (PBT) hard segments and dimer fatty acid (DFA) soft segment are soft, rubbery thermoplastic elastomeric materials. The dynamic creep was investigated by monitoring the position of the hysteresis loop. Especially, the change of the strain-related material properties as a function of the hard/soft segments concentration will be presented. The fatigue properties (dynamic creep) were also investigated under simulated physiological conditions (simulated body fluid, SBF), and the influence of the testing temperature and environment will also be discussed.

Mechanical characteristics of polymeric support as an important factor in osteoblast culture in vitro

17:00 - 17:20
oral

Wojciech R. Fabianowski[1), **Malgorzata Lewandowska-Szumiel**[2), **Beata Polak**[1)

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,

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Polymeric implant for bone regeneration in order to be useful has to fulfill several conditions: biocompatibility, mechanical properties similar with real bone, suitable rate of degradation subjected to rate of bone reconstruction with harmless degradation byproducts, proper porosity, etc. There is a distinct difficulty in finding only one right material completing these tasks. That is why researches are directed into composite materials with additionally surface modification in order to make it more attractive for cells. A principle condition of growth, proliferation and differentiation of osteoblast is their adherence and suitable interactions with support.
In our preliminary research we were observing growth of osteoblasts on solid support modified with alternating polymeric polyelectrolyte films. One solid polystyrene PS support was coated with poly(acrylic acid) A film, next one with A and bentonite B film, next with A/B/A and continuously next one with A/B/A/B and so on. Each support with top layer from A or B had roughly the same wettability measured by contact angle CA of water or DMEM drops. But the osteoblast cells growing on PS support coated with alternating A and B layers were somehow "recognizing" how thick this polyelectrolyte film is. We suggest, that surface properties - surface elasticity and fluidity play more important role in the cells growth than surface wettability measured by CA values. The influence of mechanical properties on cells growth is widely discussed. In purpose to clarify this point we have decided to make the following experiments:
Deposition of multilayer system prepared from A/B layers.
Surface wettability (CA)
Surface properties with AFM: topography.
Surface properties with AFM: friction mode.
Biological tests - morphological observations, cell proliferation (crystal violet staining), XTT viability assay
Obtained results are discussed.

[ABSTRACT TRUNCATED TO 2000 LETTERS]

Poster session 1

19:00 - 21:00

In-situ preparation and characterization of novel polyester/TiO2 nanostructured composites

poster B-01

Miroslawa El Fray[1], **Aldo R. Boccaccini**[2]

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2) Imperial College London, Department of Materials, London, United Kingdom

Nanocomposites comprising biocompatible polymer matrices and inorganic nanoparticle fillers represent a new group of biomaterials for tissue engineering scaffolds and biomedical implants and devices. It has been demonstrated that addition of ceramic nanoparticles to polymer matrices greatly influences mechanical, physical and biological properties. The key to good performance is to achieve good homogeneity of the nanoparticle dispersion and uniform microstructure. Thus, these systems require controlled formulation methods (melt/solution processing, improved mixing). Much of the research to date has focused on homopolymer/nanofiller composites, while block or multiblock copolymers/nanofillers have not been yet extensively studied. Multiblock poly(aliphatic/aromatic-ester)s (PEDT) represent novel and interesting biocompatible materials offering the processability of thermoplastics combined with the good elasticity of rubber (thermoplastic elastomers, TPE). It is expected that incorporation of biocompatible ceramic phases (e.g. TiO2 nanoparticles) may be effective in increasing bioactivity as well as cell adhesion and growth for use of the composites in tissue engineering and other biomedical applications.

In this contribution, an original approach to prepare nanocomposites using in-situ polycondensation of PETD copolymer in presence of TiO2 nanoparticles will be presented. The thermoplastic elastomer/TiO2 nanostructured composites exhibited tensile strengths 100% higher compared to that of neat polymer samples, while the elongation at breaking point increased by 300% with addition of titania nanoparticles. The preliminary results of the cell culture investigation indicate that both concentration of ceramic nanoparticles as well as the nanotopography of the composite surface affect cell proliferation. Further studies regarding the optimization of elastomer/TiO2 nanostructured composites in terms of mechanical and biological properties will be discussed.

Carbon and polymeric composites modified by nano-hydroxyapatite

poster B-02

Barbara Szaraniec[1)], **Patrycja Rosół**[2)], **Jan Chłopek**[2)]

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2) AGH University of Science and Technology (AGH), al. Mickiewicza 30, Kraków 30-059, Poland

The attempts to develop a bioactive material with physical and chemical properties similar to a natural bone remains still an unsolved problem. Current research work concentrates mainly on composite materials. The first possibility is to improve the mechanical properties of bioactive material like e. g. hydroxyapatite, especially its strength and fracture toughness. Unnecessary the results of the investigations deal with reinforcements in the form of plates, dispersions, whiskers or fibres are not quite satisfactory. It is much better to introduce bioactive phase in volume or onto the surface of material with appropriate mechanical properties in which it will play a role of active centres favouring the formation of natural HAP, i.e. the bone tissue. Such materials with good mechanical and chemical properties, successfully applied in medicine are polysulphone and carbon-carbon composites. Addition of hydroxyapatite to these materials has beneficial effects on their biological behavior and assimilates them to natural bone. The present work analyzes the effects on the mechanical and biological properties of carbon and polymeric composites modified by hydroxyapatite, both natural (of nano-particles) and synthetic (of mikro-particles).
The results show that the carbon-HAP composites have the mechanical properties similar to carbon-carbon composites, while addition of HAP to polysulphone cause advantageous growth of Young modulus and limitation of creep and disadvantageous fall of tensile strength.
Tests performed in SBF for carbon-HAP and polysulphone-HAP composites prove that the process of hydroxyapatite's build up becomes the most intensive in the case of a composite modified with use of nano-particles originating from natural hydroxyapatite and containing the carbonaceous phase.

SPECTROSCOPIC CHARACTERIZATION OF POLYACID MODIFIED RESIN COMPOSITES (PMRC)

poster B-03

Renata Babiarz-Zdyb[1)], **Ewa Talik**[1)], **Andrzej Hacura**[1)], **Arkadiusz Dziedzic**[2)]

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2) Śląska Akademia Medyczna (Śl.A.M.), Warszawska 14, Katowice 40-006, Poland

Polyacid Modified Resin Composites, so-called Compomers, are very prospective materials for direct filling in restorative dentistry. They are composed from polymer matrix, reinforced with fluoro-alumino-silicate glass particles. Commercial compomers taken into consideration during the study were: Compoglass F (Ivoclar-Vivadent), Dyract AP (DeTrey Dentsply), Hytac (3M-ESPE), Glasiosite (VOCO), Freedom (SDI) and Luxat (DMG). Polymerization time of disc-shaped, light-cured specimens was 40 s according to manufacturer's recommendations. These six samples of light-cured dental compomers were examined using photoelectron spectroscopy, Fourier transform infrared spectroscopy and Raman scattering.
The XPS permits qualitative and quantitative analysis of all elements in the periodic table (except H and He) and has the advantage of showing the binding energy of emitted photoelectrons, depending on the chemical environment in which the element occurs. The major elements composing all measured polymers are: C, O, N, Al, Si, P and F. Others trace elements were indicated: Na, Ca was present in polymer C, H and L, Ba in C and G polymer, Sr in D polymer, Fe in polymer F, Zn in polymer F and H and S in polymer G and H. The ratios: Al/Si ranged from 0.04 (polymer G1) to 0.84 (polymer C); F/Si ranged 0.03 (polymer G1) to 1.84 (polymer C). The relative value of F/Al and F/Si ratio were found to vary from low (0.7 for Freedom) to high (5.15 for Hytac) and from 0.03 (Glasiosite) to 1.84 (Compoglass F), respectively.
Infrared and Raman spectroscopy proved particularly suitable for evaluating the molecular structure and crystallinity of PMRC polymers and structural changes in time (especially related to liberation of fluorine). In this study we present a set of micro-FTIR and micro-Raman spectra with group frequency interpretation and relative qualitative analysis. This long lasting research is in early stages of development and only preliminary results will be presented.

SOME ASPECTS CONCERNING DRUG RELEASE FROM A POLYMERIC MATRIX BASED ON POLYMETHYLMETHACRYLATE AND ITS COPOLYMERS

poster B-04

Nita Loredana Elena[1)], **Popescu Mihaela Carmen**[1)], **Chiriac P. Aurica**[1)], **Vasile Cornelia**[1)]

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During the past two decades, significant advances have been made in the area of controlled release of bioactive substances so that now several well-known controlled release products are commercially available for the delivery of a variety of compounds useful in pharmaceutical, agricultural and veterinary domanis [1-3] It is well known the use of polymers as carrying matrix of bioactive substances with application in biomedical field. In our previous studies [4-6] were presented our results concerning possibilities of polymer matrices obtainment in order of coupling bioactive substances.
The aim of this work is to couple the codeine onto polymeric structures obtained through polymerization and respectively copolymerization of methyl methacrylate (MMA) itself or with 2,3-epoxypropyl methacylate (GMA).
Copolymers are regarded as preactivated polymers owing to the presence of the functional groups susceptible to undergo reactions with amines, carboxylic, anhydrides and hydroxyl groups as well to perform supplementary physical linkages.

The drug release profiles have been established using UV spectra. The rate of drug release is lower higher is content of functional groups in polymer matrix.

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[ABSTRACT TRUNCATED TO 2000 LETTERS]

Hybrid siloxane-polyaminoamides for the absorption of heparin from blood

Daniele Cauzzi[1], **Alessandro Stercoli**[1], **Giovanni Predieri**[1], **Stefano Mucciarelli**[2] poster B-05
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Heparin is an anticoagulant which is widely used during blood-dialysis. To now, there is not a commercial device able to "filter" heparin from blood after or during the medical treatment. Heparin can give, on life-long treatements, several health problems. In the literature, as far as we know, the only practically applied method is a plasmapheresis system that uses polylysine cationic polymers [von Segesser L. K. et al., Perfusion, (2000) 15, 453]. Other polymers that have shown heparin binding properties are PAAs (polyamidoamines), which are widely reported in the literature [Ferruti P. et al., Macromolecular Rapid Communications (2002), 23, 332]. PAAs are prepared from bis-acrylamides and primary or secondary amines or diamines; every NH group can react with one acryl group by a 1,4 Michael reaction. We prepared siloxane-modified hybrid PAAs by introducing $(EtO)_3Si(CH_2)_3NH_2$ (APTES) or $(EtO)_2MeSi(CH_2)_3NH_2$ (MAPDES) in the polymerization reaction of diacrylpiperazine (DAP) and N-N-dimethyl-1,6-hexanediamine (C6). The batch solution was then sol-gel processed by addition of a catalyst. The "organic" and "inorganic" polymerizations occur in a one-pot reaction using ethanol and water as solvents. At the end of the reaction a gel is obtained which, after drying, is unsoluble and can be used to effectively absorb heparin form blood. Modifying relative ratios of DAP, C6 and APTES or MAPDES, polymers with different properties can be obtained. These hybrid materials shown good activity in binding heparin as determined by UV spectrophotometry and on blood tests. A patent application has been submitted.

Human Plasma Proteins as a New Haemostatic Material. Biocompatibility Testing.

Leonardo Adamo Pajewski[4], **Raniero DAscoli**[1], **Maria Adelaide Continenza**[2], **Elena Gandolfo**[2], **Janusz M. Rosiak**[3], **Francesco Veglio**[4] poster B-06
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The present work is finalized to control the biocompatibility of an haemostatic sponge derived from human plasma proteins. The open cellular structure of the new haemostatic sponge is required to obtain a good performance as material absorbing body fluids and promote the coagulation. In addition of this haemostatic properties the material might be soft, insoluble in body fluids, hypoallergic, flexible and sterile. In order to improve the cohesion of protein chains and, consequently, mechanical behaviour of this sponges, when placed on injured tissues, a little amount of glutharaldehyde to the system was added. The final sponges were sterilised with a dose of 25 kGy of Co 60 [U+F067] radiation as suggested by hygienic requirements but, as known, both this treatments may result in a modification of protein structures and, especially aldehydes added to the system, are highly toxic. In order to verify the biocompatibility of the new final compound, an in vitro investigation was carried out using a fibroblast cell culture system. The results of this investigation show the complete biocompatibility of new protein sponges, nevertheless glutharaldehyde addition and Co60 [U+F067] sterilisation. Finally an in vivo coagulation test was performed. Also the results of such investigation show a good haemostatic behaviour of new biomaterial.

Mechanical Properties of Human Plasma Derived Haemostatic Sponges Undergoing Radiation

poster B-07

Leonardo Adamo Pajewski[3)], **Raniero DAscoli**[1)], **Katarzyna Filipczak**[2)], **Caterina Riccucci**[3)], **Janusz M. Rosiak**[2)], **Roberto Volpe**[3)]

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A haemostatic material is designed to arrest bleeding from injured blood vessels. In addition to its properties inherent the capacity to stop blood loss it must exhibit some additional characteristics such as sterility, biocompatibility and purposeful mechanical properties to allow handling and placing it on the blood vessels injury. Here one may appoint a great flexibility and capacity to undergo marked deformations in absence of material failure.
Generally proteins and plasma proteins particularly, are very soft structures and common sterilisation processing with heat treatments leads to their destruction. It is known that the ionising radiation interacts with protein structures inducing their degradation and, also, it is known that proteins can be reticulated with aldehydes which are not properly tissue friendly substances. For these reasons we have investigated the mechanical properties of new hemostatic material derived from human plasma in order to quantify the influence of sterilising dose of radiation (25 kGy) and aldehyde addition. The tests were carried out by means of compressive testing machine.
The results of this investigation, followed by biocompatibilty testing, show the opportunity of an aldehyde weak protein reticulation and the possibility to process material with Co60 radiation.

Lipids and products of lipid peroxidation at various biomaterials implantation (clinics and experiment)

poster B-08

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The lipids and lipid peroxidation products in blood serum were studied for rabbits and patients at transplantation of tendon bioimplants.
It was established that at earlier post-surgery period the lipid exchange for animals with autoplastics was characterized by decreasing of cholesterol (CS) contents and by the acute processes of lipids peroxidation which were pronounced for animals with alloplastics. It was revealed the decrease of very low density lipids (VLDL) content and increase of high density lipids (HDL) content as well. It gave evidence to development of acute phase processes.

At 14-21 days was noted the further rise of HDL content at the expense of LDL decrease in blood serum for rabbit with autoplastic that in the whole gave evidence to inflammatory process progressing. For animals with alloplastics the increase of VLDL at the expense of LDL was noted. These data of lipids variation bear evidence to active mobilization process of lipids and lipolysis due to the pronounced inflammatory process than for animals with autoplastic.
The 45th day of experiment was characterized for animals with autoplastic by normal indexes of CS and lower level of triglycerides (TG). Moreover the HDL and VLDL contents were more than normal limits, and in whole this has characterized the appearance of inflammatory process. For animals with alloplastics (at the same period) the decreasing the CS and TG contents relatively to normal were revealed. But in deference on animals with autoplastics lipoproteins content was characterized by increasing of LDL and this was evidence about aterogenic changes of vessels.
Thus the peculiarities of lipid content change in blood serum could be as evaluation criteria of inflammatory reaction character during post-surgery period at bioimplants application.

Modification of polymers by ultrasonic treatment in aqueous solution

Bozena Rokita[1), Renata Czechowska-Biskup[1), Piotr Ulanski[1), Janusz M. Rosiak[1) poster B-09

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Polymers remain the most versatile class of biomaterials, being extensively applied in medicine and biotechnology, as well as in the food and cosmetics industries. Polymers used as biomaterials should have chemical and physical characteristics appropriate for specific application. This can be achieved either during synthesis or by performing modifications.

In this work selected polymers were modified by ultrasound treatment in aqueous solutions. This technique allows carrying out the processes and obtaining products different than these in classical thermally initiated chemical reactions. Macromolecules in solution can undergo chemical transformations under the influence of ultrasound by at least three mechanisms: reactions of macromolecules with radicals generated during periodic compression of cavitation bubbles (i.e. minor gas bubbles created as a result of violation of continuity in liquid phase under ultrasound influence), pyrolysis in or at the boundary of cavitation bubbles (the implosive collapse of a bubble is an adiabatic process that leads to a rapid, momentary temperature increase), as well as mechanochemical effects (resulting from the shear forces generated around collapsing cavitation bubbles).

Selected water-soluble polymers were: poly(ethylene oxide), poly(ethylene glycol), poly(acrylic acid) and chitosan. Changes of weight-average molecular weights and molecular dimensions were determined by low-angle laser light-scattering and viscometry.

It was observed that ultrasound can act as an efficient tool for controlled degradation of polymers, but is also capable of inducing cross-linking processes. Controlled degradation induced by ultrasound is useful e.g. in producing low-molecular-weight chitosan, which is much more efficient in selected biomedical applications than the original, high-molecular-weight material.

This work has been financed by the State Committee for Scientific Research (grant No. 4 T09A 128 22).

Porous polymeric scaffolds for bone regeneration

Katarzyna Filipczak[2), Ireneusz Janik[2), Marek Kozicki[2), Piotr Ulanski[2), Janusz M. Rosiak[2), Leonardo Adamo Pajewski[3), Radosław M. Olkowski[1), Piotr Wozniak[1), Anna Chróścicka[1), Malgorzata Lewandowska-Szumiel[1) poster B-10

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One of the aims of tissue engineering is to provide means for self-regeneration of tissues which requires reconstruction due to pathology, trauma or surgery (eg.: tumor resection). Important examples of this approach are devices intended to support regeneration of bones. The design investigated in our project is based on the idea of porous biomaterials - scaffolds - that are strong enough to maintain the mechanical function of the bone segment and in parallel can act as a support for osteoblast proliferation. Depending on the application, degradable or non-degradable materials are desired.

In this work, a technique has been elaborated to synthesize highly porous polymeric scaffolds of controlled pore size, based on non-degradable poly(methyl methacrylate) - PMMA - and degradable poly(ϵ-caprolactone) - PCL.

It has been found that both kinds of products can be sterilized by ionizing radiation. In order to utilize this possibility in an efficient and controllable way, mechanisms of the underlying radiation-chemical processes have been studied in some detail, using the techniques of pulse radiolysis, laser light scattering, sol-gel analysis, spectrophotometry and viscometry. In case of PCL, irradiation causes an additional effect - cross-linking - that leads to an improvement of the mechanical properties of the scaffold.

In parallel to radiation-chemical studies, first steps towards the target application have been made. Porous, sterile scaffolds of PMMA and PCL were subjected to in vitro studies as supports for cell cultures. It was found that that the products exhibit no cytotoxicity towards fibroblasts and that the osteoblast cells can be efficiently cultured at the surface and in the pores of the scaffolds.

This work has been financed by The Polish State Committee for Scientific Research (grant No 05/PBZ-KBN-082/T08/2002/05) and International Atomic Energy Agency (POL/6/007 and 11513/RO).

COMPLICATIONS OF THE UNIPOLAR ENDOPROSTHESIS AT MALIGNANT TUMOURS OF THE KNEE JOINT BONES.

poster B-11

Yuri G. Yutovetc[1)]

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COMPLICATIONS OF THE UNIPOLAR ENDOPROSTHESIS AT MALIGNANT TUMOURS OF THE KNEE JOINT BONES.

V. A. Babosha, Y. Yutovetc, Abdel Kader Tajsir

Donetsk state medical university named after M. Gorky
Donetsk.
The purpose: improvement of quality of life of the patient by preservation of extremities and its function, the prevention and treatment of possible complications at malignant tumours of knee joint bones.
There 39 patients were operated on: with the osteogenic sarcoma - 12, chondrosarcoma - 3, parosseaal sarcoma - 2, synovial sarcoma - 2, osteoclastoma - 15 (including 7 malignant), cancer metastasis - 3.
By 32 patient the unipolar endoprosthesis were carried out: a distal femur - 15, proximal tibia - 17. In 7 cases the subchondral femur endoprosthesis was taken place.
In 10 cases relapse of a tumour, in 2 - a purulent arthritis, in 1 - necrosis of skin rags took place. Concerning complications it were performed amputation of extremities to 9 patients, at 2 cases - removal of tumour units. The purulent gonarthrosis was managed by the drainage and the intraosseal antibiotics introduction.
Two patients have died in 3 weeks after operation from pulmonary arteries tromboemoly. At persons of advanced age it follows to prolong the anticoagulant therapy about two weeks.

SYNTHESES AND PROPERTIES OF CELLULOSE PHOSPHATE

poster B-12

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Cellulose is most abundant natural, renewable, and biodegradable polymer in the world. Polysaccharides, like cellulose, are the polymer group with the longest and widest medical applications experience because of their unique properties: nontoxicity, water solubility or high swelling ability by simple chemical modification.
The large concern is introduced by cellulose phosphates, the physical-chemical properties which one are caused by an opportunity of applying in various fields of medicine.
In present study the synthesis by $H_3PO_4/P_2O_5/Bu_3PO_4/CCl_4$ method was optimized in terms of reaction parameters.
Cellulose samples (viscose) were swollen for 24 h in CCl_4 to assess the influence of swelling prior to chemical modification. The reaction parameters were investigated and products characterized. Parameters investigated were: reaction time, temperature, concentration of H_3PO_4, CCl_4, Bu_3PO_4 (TBP), P_2O_5. The products were characterized by the following methods: Kjeldhal method (phosphorous content), SEM, potentiometric titration, X-ray diffraction, IR. The molecular masses of obtained samples were determined

by static of light scattering.
On the establishment of received results were determined the optimal conditions of the of reception of the cellulose phosphate.

Absorbable surgical sutures on the base of cellulose phosphate

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poster B-13

The relevant problem at building surgical stuffs is the development of the degradable surgical sutures with adjustable terms of the resorption. Series of valuable properties of the cellulose phosphate: biocompatibility, degradation in tissues of an alive organism, and also variety of the physical forms, - enable the applying them as a surgical suture material.
The influence of the conditions of the phosphorylation in the system on the contents of the phosphate groups, explosive strain in a dry condition and in a knot, the lose of strength in vitro and in vivo of the viscose and the cotton fibers were studied. The studies in vivo have shown, that the explosive strain of a suture material on the basis of the cellulose phosphate with metabolic capacitance of 0,25 - 0,5 mmol/g is conserved practically invariable for 30 day. At 60-th day after an implantation the biodegradation of fibers is observed. The complete resorption takes place at 180-th day.

Effect of diisocyanate chemical structure on biocompatibility of segmented polyurethanes

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poster B-14

Chemical structure of diisocyanates, poliols and chain extenders affect biocompatibitity of obtained polyurethanes. Hard segments of polyurethanes for biomedical applications are based on both aromatic and aliphatic diisocyanates. The obtained materials have different physico-mechanical properties and their interactions with live tissue.
In this study, polyurethanes with different hard segment diisocyanates (MDI, HMDI) were obtained and their structure, physical properties and biocompatibility were studied. Scanning electron microscopy (SEM), differental scanning calorimetry (DSC), contact angle measurments were used for polyurethane properties characterization.

Project supported by The Polish State Committee for Scientific Reasearch PBZ - KBN-082/T08/2002

Effects of glass and polymer on the setting and mechanical properties of water - activated glass ionomer cements

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poster B-15

Glass-ionomer cements are currently used for various dental applications including luting, liners, bases and direct restorations. Adhesive property to the tooth, less toxic effect to dental pulp, as well as their continuous release of fluoride are the main advantages of glass ionomer cements.
They consist of a sodium calcium aluminosilicate glass powder and an aqueous solution of a polyalkenoic acid. The single compounds react as soon as they are mixed together.
The aim of the investigation conducted in the Institute of Glass and Ceramics was to prepare water activated glass ionomer cements for restoration of the teeth.
An aluminosilicate glasses, in which calcium has been substituted by strontium and barium, were prepared by melting. Steel quenched pieces of glass and water-cooled granular frit were produced. Glass were ground and sieved to prepare <45 mm powder. Particle size analysis of glass powder was made by using the laser analyzer.
The polyacid powder was obtained by freeze drying of aqueous solution of polymer and grinding. Then the polymer was added as dry powder to the glass and the reaction of setting was initiated by addition of water. Specimens of water-activated glass ionomer cements prepared from various glasses and acrylic polyacid have been tested for setting time and compressive strength.

It was concluded that the obtained glasses could be used to produce water-activated glass ionomer cements for use in dentistry.

Influence of radiation sterilization process on properties of poly(siloxaneurethanes) used as scaffolds for tissue engineering.

poster B-16

Izabella Legocka[1,2], Małgorzata Lempert[1], Stanisław Warchoł[1], Jarosław Sadło[1], Janusz Kozakiewicz[2], Jarosław Przybylski[2]

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The main objective of the presented study is to understand the influence of sterilization by the radiation method on chemical structure of segmented poly(siloxaneurethanes) (PSU) designed for medical scaffolds for tissue engineering.
Such polymers should meet the following basic requirements after sterilization:
- to allow for cells adherence to scaffold surface - this should be achieved through ensuring the optimal hydrophobic-hydrophilic surface balance,
- to allow for growth of new cells, no toxic substances should be produced.

The segmented polyurethanes investigated in this study contained hard segments (from aliphatic (IPDI) or aromatic (MDI) diisocyanates) and soft segments(from oligosiloxanediols.The films of samples were irradiated with a standard dose of 28 kGy using EB (from accelerator) or gamma - rays.
The following methods of investigations were applied: ESR, FTIR-ATR,DRS,DCA.
The ESR spectra showed no signals at 298K. However, signals of different intensity depending on chemical structure of the samples were observed for samples irradiated and investigated at 77K. These signals disappeared with increase in temperature. The same differences were observed in DRS spectra(range 200-600 nm), but no significant structural differences in FTIR-ATR spectra were found. This could result from recombination process of alkyl-type radicals created under irradiation.When the increased irradiating dose was applied (28 to 200 kGy) distinct structural changes were observed, in particular when the sample contained MDI (aromatic) hard segments.
For all irradiated samples increase in DCA (resulting in decrease in SFE)was found what may be explained by the recombination of radicals, presumably leading to crosslinking of the siloxane segments of PSU.
In order to improve the biocompatibility of the PSU surface and in the same time to trap the free radicals formed during sterilization, phenylalanine and anthranilic acid were used as modifiers of PSU surface [ABSTRACT TRUNCATED TO 2000 LETTERS]

Polyester particles obtained by dialysis - new material for cell cultures

poster B-17

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We developed a new method for obtaining biodegradable poly(L,L-lactide) and poly(L,L-lactide-co-glycolide) particles by dialysis, which consists in the change of a polymer solvent to water. During this process the particles are formed by polymer precipitation. We used poly(ethylene glycol)-b-polyglycidol-b-poly(L,L-lactide) block terpolymer as a stabilizer of the suspended matter.
Several polymer solvents such as THF, acetonitrile, 1,4-dioxane, DMSO and DMF were used. For poly(L,L-lactide-co-glycolide) used solvent does not affect neither shape nor size. In case of poly(L,L-lactide) we observed strong influence of the solvent on the particle shape and size.
The variations of process parameters lead to obtain a microporous particles, which can be applied as a biodegradable support for cell cultures.
By pressing and heating of polymer particles we have obtained a porous polymer samples, which can be used as a biodegradable support for cell culture. The influence of temperature, pressing condition on samples morphology are in progress.

Modulation of the properties of functional polysuccinate based temporary bone cement compositions with use of hydrophilic monomers

poster B-18

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Synthetic biodegradable aliphatic polyesters are widely used in biomedical applications because of their susceptibility to hydrolytic degradation [1]. In the last decade the intense investigation on the injectable, biodegradable bone cements based on poly(1,2-propylene fumarate) (PPF) was conducted [2,3]. Liquid composition of a polyester and a vinyl or methacrylic monomer can be cured in a site of application and provide temporary structural support to bone tissue. Similar idea was realized by us recently with use of poly(3-allyloxy-1,2-propylene succinate)4].
However, relatively high hydrophobicity of these materials slow down their hydrolytic degradation. In order to increase their susceptibility to hydrolytic degradation, a part of methyl methacrylate (MMA) comonomer was replaced by hydrophilic oligo(ethylene glycol) dimethacrylates (OEGDMA).
The influence of the composition of liquid resin (MMA:OEGDMA ratio) and of the length of the oxyethylene chains in dimethacrylates on curing process (setting time, peak temperature) as well as on selected properties of cured materials (hydrophilicity, hardness, compressive strength) was investigated. Both variables appeared to influence hydrophilicity of cured resins. Generally increasing hydrophilicity was accompanied with decreasing peak temperature, hardness, stiffness and compressive strength.

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Bioimplant effect on tendon tissue regeneration processes (clinics and experimental studies)

Lyudmila I. Donchenko[1)] poster B-19
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The peculiarities of degeneration and regeneration processes after autoplastics and alloplastics applications for tendon implantation for rabbits of Chinchilla breed were studied in comparison of clinical and experimental results.
The activity of studied processes was evaluated on the basis of morphological and biochemical investigations.
It was revealed on the base of experimental studies that acute at post-surgical period the degenerative-dystrophic processes are developed and moreover they were more expressed at using of the alloplastic implant as against the autoplastic one.
Since the 14-th day the regeneration processes are activated. The regeneration processes were more active for animals with autoplastic tendon in comparison with animals with alloplastics. The differences in the regeneration terms for animals with autoplastics and alloplastics are about 20-25 days.
For patients with alloplastics of tendon at the regenerate period the degenerate-dystrophic processes prevail and that in a number of cases results to complications.
Thus the obtained experimental and clinical results have the essential differences. And this fact is necessary to take into account at allotransplant applications in reconstructive surgeries.

Microstructure of alumina bone graft material

Zbigniew Jaegermann[1)], **Anna Ślósarczyk**[2)] poster B-20
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2) AGH University of Science and Technology, Department of Ceramics Technology (AGH), Kraków, Poland

Bone filling guiding regeneration of bone tissue and the subsequent restitution of bone function is one of the most important fields of application of ceramic materials in modern bone surgery. Whereas in the case of bioceramics used for manufacturing of structural elements for joint prosthesis, reliability and mechanical properties matter most, in the case of materials for bone regeneration the features that enable forming of good mineralized bone tissue, closely connected to the surface of implanted (grafted) material are the most important ones. Therefore the shape and texture as well as microstructure, chemical and phase composition, and surface properties of this kind of ceramic biomaterials are of singular importance. The present work evaluates alumina biomaterials of different microstructure and surface properties that were obtained from parent compositions of diversified raw materials. For this goal test samples of porous

and compact alumina were prepared. Comparative tests of the main properties were conducted, including the following: degree of consolidation, chemical and phase composition, identification of the type and layout of crystalline phases and mechanical properties of alumina materials. Chemical methods, X-ray and microscopic examinations were used.
Analysis of the results demonstrated differences in apparent density, compressive strength and microstructure of alumina materials obtained from diversified raw materials. These differences could affect the behavior of porous alumina grafts in the environment of living organism.
This research was supported by the State Committee of Scientific Research (grant No. 3 T08D 044 26)

SEM investigations of tooth/ filling bonding

poster
B-21

Joanna Siejka - Kulczyk[1], **Malgorzata Lewandowska**[1], **Marta Raczyńska**[2], **Elżbieta Jodkowska**[2], **Krzysztof J. Kurzydlowski**[1]

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SEM investigations have been conducted to determine the influence of the material on tissue/ material bonding.
Extracted, human teeth were used in this study. Resin - modified glass - ionomer cement and resin composites were tested as dental fillings. To reveal the structure of the tissue/ filling interface the teeth were cut parallel to the long axis.
Bonding quality was determined by direct SEM observation. Fluorine release was estimated by microanalysis with the use of X - ray energy spectrometry (EDS). The results show, that investigated materials have good bonding with enamel. Not fluorine release was observed.

Tuesday, September 7th

Morning session

11:00 - 12:30

Main Building, room 213

Degradation of polymeric systems aimed at temporary therapeutic applications : structure-related complications

11:00 - 11:45
invited oral

Michel Vert[1]

1) Research Centre for Artificial Biopolymers, UMR CNRS 5473, University of Montpellier 1, Faculty of Pharmacy, Montpellier, France

During the last 10 years, many novel polymeric compounds have been introduced in literature as degradable or biodegradable polymers. However studies generally stopped at the level of the synthesis. It is now well known that the degradation of polymer chains can be achieved via various processes, namely cell-mediated degradation and abiotic chemical or enzymatic degradation. Considering the hydrolytic degradation of aliphatic polyesters derived from lactic and glycolic acids one can realized that degradation is very much dependent on chain structures, especially in the case of copolymers and stereocopolymers. The present understanding of water-sensitive polymers and copolymers will be recalled. It will be shown that the degradation of copolymer chains leads to deviation from cleavage at random, thus resulting in composition changes, formation of crystalline residues and of degradation products that are more resistant than partially degraded precursors of intermediate molecular weights. The cases of various copolymers and stereocopolymers will be presented, namely PLA stereocopolymers, PLAGA copolymers and poly(malic acid-co-benzyl malate) copolymers. A special attention will be paid to the effect of attaching a label to a degradable macromolecule in order to monitor the degradation mechanism. It will be shown that radioactive labelling by hydrogen-tritium isotopic exchange and labelling by binding a fluorescent dye to polymer chains do not lead to comparable results. The use of a chemical label can be the source of dramatic misinterpretation because of the influence of the dye on the physicochemical behaviour of partially degraded by-products. The chain structure-dependence also exists in the case of enzymatic degradation. It will be shown that selective enzymatic degradation can be used to create porous structures and to investigate the intimate structure of blends of enzymatically degradable polymers.

Biodegradable multiphase polymeric materials

11:45 - 12:05
oral

Anna Kozlowska[1)], **Marek Kozlowski**[1)], **Andrzej Iwanczuk**[1)]

1) Wrocław University of Technology, Wybrzeże Wyspiańskiego, Wrocław 50-370, Poland

Biodegradable composites prepared by melt blending were investigated. The blends were composed of synthetic and natural macromolecules, including poly(vinyl alcohol), aliphatic-aromatic polyester, granular starch and thermoplastic starch. Mechanical properties of the composites, their microstructure, melt rheology and thermal characteristics have been presented. Influence of water on the properties as well as degradation rate of the materials have been estimated as a function of their composition. Such materials can find applications in medicine and biology as polymeric scaffolds, drug delivery systems etc.

Lunch break

12:30 - 14:00

Afternoon session

14:00 - 15:30

Main Building, room 213

Cells and scaffolds for tissue engineering - what is needed for success?

14:00 - 14:30
invited oral

Malgorzata Lewandowska-Szumiel[1)]

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Tissue engineering is a relatively new branch of medicine which has been enthusiastically announced as a new tool in reconstructive surgery. Eight years ago it was being compared to genetic engineering, as an extremely promising area in medical treatment[1]. Bone reconstruction was indicated as potentially one of the first major application of tissue engineering, as published in Science in 2000[2]. In the last two volumes of Tissue Engineering however, two reviews have been published in which the current contribution of tissue engineering to healthcare is critically discussed[3,4]. According to the published data, only 4 TEPs (tissue engineering products) have been approved by FDA until now and the progress in clinical application of TEPs is below expectations. There are several reasons for this, but one of them suggested resolution - coming back to the basic science in tissue engineering research. One of the critical points is the ability of effective cell and tissue culture in vitro on scaffolds made from biomaterials of a controlled behavior at the preimplantation stage and after implantation. In the present analysis the potential sources and maintaining of cells which can be used in the reconstruction of the skeletal system are being discussed as well as the key expectations toward biomaterials which are the basis for effective scaffolds for cell and tissue transplantation.

This work was supported by the State Committee for Scientific Research (grant 05/PBZ-KBN-082/2002/06).

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2. R. F. Service, Tissue engineers build new bone, Science 289, 2000, 1421-1640;
3. T. Hardingham, Regional Perspectives on Tissue Engineering, View from a Small Isand, Tissue Engineering 9, 2003, 1063-1064;
4. M. J. Lysaght, A. L. Hazlehurst, Tissue Engineering: the End of the Beginning, Tissue Engineering 10, 2003, 309-320.

Alginate hydrogel-candidate support for cell transplantation - preliminary observation in human chondrocyte culture

14:20 - 14:40
oral

Piotr Woźniak[1)], **Marek Kozicki**[2)], **Janusz M. Rosiak**[2)], **Jacek Przybylski**[1)], **Malgorzata Lewandowska-Szumiel**[1)]

1) Medical University of Warsaw, Department of Biophysics and Human Physiology, Chałubińskiego 5,

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2) Technical University of Lodz, Institute of Applied Radiation Chemistry (IARC-TUL), Wroblewskiego 15, Łódź 93-590, Poland

Alginate hydrogels are being taken into account as a potential 3-D support for tissue engineering in skeletal reconstruction[1−3].
The aim of the present study was to investigate the influence of alginate hydrogel on human chondrocytes in vitro.
Hydrogels were prepared by crosslinking natural polymer, sodium alginate, with divalent cations (Ca^{2+}). Chondrocytes were encapsulated into hydrogel in the form of either beads or films and were incubated under standard conditions. Cells seeded on TCPS (Tissue Culture Polystyrene) served as a positive control. Morphological observations were carried out and chondrocytes viability was examined by means of Neutral Red cytotoxicity quantitative assay (NR).
In microscopy examination of chondrocytes, cells were visualised in the whole 3-D structure of hydrogel. The results of NR assay for encapsulated chondrocytes were higher, as compared to the cells cultured on TCPS.
These results show the positive effect of alginate encapsulation on human chondrocytes in vitro.
It might be concluded, that this kind of alginate hydrogels might be considered as a potential support for cells transplantation and this system needs further investigations.

This work was supported by the State Committee for Scientific Research (grant 05/PBZ-KBN-082/2002/06).

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2. Rowley JA, Madlambayan G, Mooney DJ. Alginate hydrogels as synthetic extracellular matrix materials. Biomaterials 1999;20(1):45-53.
3. Alsberg E, Anderson KW, Albeiruti A, Franceschi RT, Mooney DJ. Cell-interactive alginate hydrogels for bone tissue engineering. J Dent Res 2001;80(11):2025-9.

Electrochemical coating of metallic medical devices

14:30 - 15:00
invited oral

Abraham J. Domb[1], **Galit Shustak**, **Zehava Weiss**, **Stanislaw Slomkowski**[2], **Mariusz Gadzinowski**[2], **Dani Mandler**[1]

1) The Hebrew university of Jerusalem (HUJI), Ein Kerem Campus, Jerusalem 91120, Israel

2) Polish Academy of Sciences, Center of Molecular and Macromolecular Studies (CMMS-PAS), Sienkiewicza 112, Łódź 90-363, Poland

Electropolymerization of medical devices such as cardiovascular stents may posses advantages including: simple and reproducible process with the ability to control the thickness, adherence and composition of the coating by the duration and intensity of the applied current, the monomer composition and concentration, the solvent and the reaction conditions. The properties of the polymer can also be controlled by copolymerization of different monomers, grafting substituents to a functionalized polymer, and by entrapping biomolecules. The synthesis of a range of pyrrole based monomers and their electrocoating onto stainless still surfaces was investigated. N-substituted pyrrole monomers with C1 to C18 alkyl chains and polyethylene glycol chains were synthesized in good yields and purity. Electropolymerization of these monomers provided uniform coatings with different hydrophobicities. Current studies focus on the incorporation of drugs in the coated device for the release from the surface.

Natural Materials, Molecular Recognition and Rapid Prototyping: Three Ingredients for a Successful Recipe in Tissue Repair

15:00 - 15:30
invited oral

Gianluca Ciardelli[1]

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The technology of molecular imprinting permits recognition sites to be inserted into a polymeric material through the polymerization of a monomer in the presence of a template. In this way, advanced intelligent systems to be applied in the biomedical field as drug release devices or selective membranes can be realised. Cross-linked methylmethacrylate-methacrylic acid nanospheres were obtained directly through polymerisation. These nanoparticles have a capacity to recognise and rebind the template which is a function of the amount of functional groups in the copolymer. These results open the way to the realisation of systems with tuneable release and rebinding properties by varying the chemical composition of the copolymer. Another approach consists in developing an imprint matrix by the phase inversion precipitation technique. Recently, we applied this approach to realise porous membranes containing specific sites for molecules of clinical interest or proteins.
Tissue engineering (TE) and guided tissue repair are very rapidly developing new areas of science. These

techniques generally require the use of three-dimensional (3D) supports for initial cell attachment and subsequent tissue formation. Two new developing rapid prototyping techniques (Selective laser sintering and pressure assisted microsyringe) were applied to fabricate polyester based degradable structures for tissue regeneration, with a spatial resolution that can be regulated down to about 10 . microns. Cell attachment to microfabricated structures was higher than to membrane samples, indicating that surface topography and roughness have a positive influence on adhesion.
The two research lines are intended to meet by envisaging the creation of scaffolds for the growth of tissues and organs based on polymers imprinted with specific adhesion peptides or proteins.

The work was carried out in the framework of the STReP-project (HIPERMAX/ NMP-3-CT-2003-505790) funded by the European Commission

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Coffee break

15:30 - 15:50

Afternoon session - continued

Main Building, room 213

15:50 - 17:20

HYDROGEL-BASED ANTI-ARRYTHMIC CARDIAC DRUG DELIVERY

15:50 - 16:20
invited oral

Arthur Coury[1], Michael Philbrook[1], Robert Miller[1], Kevin Skinner[1], Jude Colt[1], Rubina Corazzini[1], Li-Ping Yu[1], Kenneth Messier[1], Peter Jarrett[1], James Burns[1]

1) Genzyme Corp., 500 Kendall Street, Cambridge 02142, United States

Atrial fibrillation (AF) is a common and severe complication of thoracic surgeries including coronary artery bypass, heart valve replacement and lung resection. Prophylactic treatment of surgery patients with anti-arrythmic drugs is not widely used because of complications from systemic delivery and coordination requirements between the patient's cardiologist and surgeon. A safe, effective anti-arrythmic, prophylactic drug applied at surgery would potentially find broad application among cardiac surgeons. The approach described here uses a photopolymerized, tissue-adherent, resorbable hydrogel containing the anti-arrythmic drug, amiodarone applied to the epicardium for sustained release. The hydrogel is a member of a family of compositions based on a macromer comprising a poly(oxyethylene) core, flanking oligomers of hydrolytically degradable groups and end-caps of acrylate ester. These hydrogels have successfully released and expressed a variety of substances including small molecules, proteins and genes. The current application technique involves deposition of a primer on the tissue, brushing in and dripping on the drug-containing topcoat and illuminating with visible light to produce an adherent composite for programmed drug release into the tissue. To date, in vitro studies have established that drug release should achieve the targeted two-week minimum delivery. In vivo, one-week canine studies have shown that tissue levels of amiodarone expected to be therapeutic were achieved. Longer-term canine studies indicated sustained elevation of atrial effective refractory period (AERP) in the treated cohort. AERP elevation is a surrogate marker for potential suppression of post-surgical AF. Future studies will focus on gel clearance and tissue healing.

Functional PEO as new building block for biomaterials

16:40 - 17:00
oral

Jutta Rieger[2], Katrien Bernaerts[1], Filip Du Prez[1], Christine Jérôme[2], Robert Jérôme[2]

1) Department of Organic Chemistry, Division Polymer Chemistry, Ghent University (U-Gent), Gent 9000, Belgium

2) Center for Education and Research on Macromolecules (CERM), University of Liège (ULg), Liege 4000, Belgium

Poly(ethylene oxide) (PEO) chains were capped at one end by ϵ-caprolactone (ϵ-CL), which is polymerizable by ring opening polymerization (ROP). These macromonomers (γPEO.CL) have been prepared by controlled anionic ring-opening polymerization (ROP) of ethylene oxide (EO) initiated by the potassium alkoxide of 1,4-dioxaspiro[4.5]decan-8-ol leading to PEO with a monomodal molecular weight distribution and low polydispersity (1.1). The acetal has been hydrolyzed into a ketone, followed by the Baeyer-Villiger oxidation of it into the seven-membered lactone.

After purification, macromonomers have been characterized by 1H-NMR, SEC, IR and MALDI-Tof. It must be noted that the ω-hydroxyl-end-group of PEO has been previously methylated in order to prevent ROP of ϵ-CL to be initiated by this function.

This type of macromonomer is well-suited for the synthesis of amphiphilic comb-like copolymers consisting of a biodegradable hydrophobic backbone of PCL and hydrophilic PEO grafts. First attempts of copolymerization of γPEO.CL with ϵ-CL have been successfully achieved using aluminum alkoxide as initiator- either in solution or attached on a solid surface. Characterization of the amphiphilic graft copolymers is under current investigation.

In addition, an α-bifunctional PEO has been easily prepared by hydrolysis of the lactone end-group into acid-alcohol. These COOH and OH groups are now available for the synthesis of mikto-armed ABC star-shaped copolymers.

ϵ-CL-terminated PEO is thus a promising building block of surfactants to be used in biomedical applications, for drug delivery and surface modification of biomaterials.

17:00 - 17:20
oral

Carbon Fibers - Polymer Composites in Human body

Reza Eslami Farsani[2,3], **Ali shokuhfar**[2], **Arman Sedghi**[1]

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2) Faculty of Mechanical Engineering, K.N.Toosi University of Technology, Tehran, Iran

3) Islamic Azad University, Tehran-South Branch, No.1182,1th Sepehr, Marzdaran Blvd.,Jandarmery Shahrac, Tehran 14638, Iran

Biomaterials used in human body for supplement and replacement must have special properties based on the type and place of them in body. These materials should not have any negative interaction with the body components and must compatible with tissues of body. In addition, these materials must not produce any toxic substances in body and the consumption of medical drugs should not have the negative effect on it. These conditions show that the application of biomaterials in body is very complicated. Polymer matrix composites with reinforcement of carbon fibers are suitable candidates for medical applications.

In this investigation, initially properties and special advantages of carbon fibers-polymer composites described, and their using in different parts of body (in hard and soft tissues) is studied. They are used as limbs, implants, devices and filler materials for replacement, supplement and fixation of body organs. After that, this study reveals various carbon fibers-polymer composites can replaced instead of other biomaterials (e.g. metals, ceramics and polymers) in the many applications, because of special properties (such as low weight, similar stiffness of hard tissues, high strength, and resistance against fatigue and corrosion), compatible with the modern diagnostic methods (such as MRI and CT) and no negative effect on tissue. These composites have desired properties and haven't many disadvantages of other biomaterials.

Wednesday, September 8th

09:00 - 10:30

Morning session

Main Building, room 213

09:00 - 09:30
invited oral

Magnetic colloids: preparation and biomedical applications

Hamid ELAISSARI[1]

1) CNRS-bioMerieux (UMR-2714), ENS-Lyon, 46 allee d'Italie, Lyon 69364, France

In recent years, increasing interest has focused on the preparation of magnetic latex particles for diagnostic applications. The pioneer work in this field was performed by Ugelstad (Prog. Polym. Sci. 1992) by reporting the preparation and the biomedical of polystyrene based magnetic microspheres. Then, several approaches have been investigated as evidenced from the numerous reported papers. The elaborated and manufactured magnetic latexes are not totally suitable in some specific biomedical applications such as nucleic acids detection and amplification or basically to be used in automated systems. The selected magnetic colloids should be compatible with the desired application. For instance, in the case of nucleic acid area, the cationic character of the particle surface is favorable for the adsorption but dramatic for enzymatic amplification process. The objective of this work is to present recent works on the elaboration, the colloidal characterization of magnetic colloids and there use for specific and non-specific capture, extraction and concentration of biomolecules. The magnetic colloids were prepared from well controlled oil in water submicronic magnetic emulsion.

Novel medical diagnostic test based on electrophoretic mobility of microspheres

09:30 - 09:50
oral

Teresa M. Basinska[1], **Stanislaw Slomkowski**[1], **Magdalena Chmiela**[2], **Monika Wisniewska**[2]

1) Polish Academy of Sciences, Center of Molecular and Macromolecular Studies (CMMS-PAS), Sienkiewicza 112, Łódź 90-363, Poland

2) University of Łódź, Department of Infectious Biology, Inst. of Microbiol. and Immunol., Łódź 90-237, Poland

Suspensions of colloidal polymer microspheres found variety of applications in medical diagnostics. Recently, we developed a model diagnostic test for determination of anti-HSA in blood serum based on simultaneous control of size of formed latex particle aggregates and electrophoretic mobility of latex particles. This method is based on an assumption that charge of particles with bound antigens changes after binding of complementary antibodies. In this work we report on the model test for determination of Helicobacter pylori antigens in patients sera.
For this purpose monodisperse poly(styrene/alpha-tert-butoxy-omega-vinylbenzyl-polyglycidol) particles (P(S/PGL), D_n=220 nm, D_w/D_n=1.02) containing hydrophilic polyglycidol segments with hydroxyl groups in the surface layer were synthesized. The hydroxyl groups were used for covalent binding of H. pylori antigens via hydroxyl groups of polyglycidol activated with cyanuric chloride. It was found that fraction of adsorbed antigen was negligible and essentially the whole amount of attached antigen was covalently bound onto P(S/PGL) microspheres with the maximal surface coverage equal 1.61 mg/m^2. H. pylori antigens were isolated from glycine acid extract obtained from H. pylori strain NCTC 11637 (CCUG 17874). Sera with and without H. pylori antibodies were obtained from children patients.
We found that the presence of anti-H. pylori antibodies in the blood serum added to suspension of P(S/PGL)-H. pylori microspheres results in significant change of electrophoretic mobility of particles and leads to some particle aggregation. The aggregation is visualized by a rapid increase in the size of microspheres (from 372.9 nm to 432.4 nm). The degree of these changes depends on concentration of the anti-H. pylori antibodies. The novel diagnostic test allowing quantitative determination of anti-H. pylori antibodies in blood serum can be based on these effects.

Novel Higher Sensitivity Silicone Based Capacitive Pressure Sensors For Biomedical Applications

09:50 - 10:10
oral

Khalil Arshak[1], **Deirdre Morris**, **Essa Jafer**, **Olga Korostynska**, **John Harris**, **Clifford Seamus**, **Lyons Gerard**, **Arshak Arous**

1) University of Limerick (UL), Plassey Technological Park, Limerick 02098, Ireland

Pressure measurement is an important tool in the diagnosis and treatment of injuries and disease. For example, after a serious accident, monitoring intracranial pressure can give information on haemorrhaging that may occur1. In minimally invasive surgery, pressure sensors are used to compensate for the surgeons loss of tactile sensation. Thick films and similar technologies can be used for the fabrication of cost effective sensors for a wide range of medical applications. Research in this area has recently focused on the implementation of capacitive sensors with silicone rubbers as the dielectric layer2. However it is noted that a continuous elastomer layer is not sensitive enough and more complex sensor designs are commonly required2, thus affecting the cost of fabrication. In this work an investigation into the pressure sensing properties of a RTV silicone rubber (Notcutt Ltd) was carried out. The silicone was used as the dielectric material of a metal-insulator-metal capacitive design. Small amounts of Carbon Black (CB) are added to the silicone during fabrication so that its sensitivity to pressure may be improved. It was thought that this should eliminate the need for complexity in sensor design. It is found that adding CB to the material resulted in changes of both electrical and mechanical properties. Adding 6 wt.% CB increases the relative permittivity of the silicone by a factor of two without causing undesirable increases in dissipation factor. Similar improvements in the pressure sensing properties of these materials have been observed when tested using a Lloyd Instruments LR50K over the range 0- 80 kPa. For samples with 6 wt.% C B a four-fold increase in sensitivity has been recorded. The improved sensitivity may eliminate the need for complexity in the sensor design.

1Flick, B. et al., (2000), IEEE Trans. Biomed. Eng, 47, p. 12-16
2Cristalli C. et al., (1995), IEEE-EMBC and CMBEC, p. 1541-1542.

Poly-N-vinylpyrrolidone amphiphilic derivatives: microaggregates forming

10:10 - 10:30
oral

Mikhail I. Shtilman[1], **Andrey N. Kuskov**[1], **Aristidis M. Tsatsakis**[2], **Manolis A. Tzatzarakis**[2], **Igor A. Yamskov**[1], **Vladimir P. Torchilin**[3]

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2) University of Crete, Iraclion 71409, Greece

3) Northeastern University, Boston 02115, United States

Amphiphilic poly-N-vinylpyrrolidones, which contain fragments of water-soluble polymer and hydrophobic long-chain end groups, were synthesized. On varying of the reaction conditions, polymers with different molecular weight (Mn=1500÷14000) and with high yield were obtained.
Obtained polymers were soluble in water and as it was shown in the experiment with the use of spin probe they formed associates with the compounds, which contains hydrophobic fragments. ESR-spectra of the hydrophobic spin-probe, nitroxyl radical N-oxyl-2-hexyl-2-(10-methoxycarbonyl)decyl-4,4'-dimethyl oxazoline, in the presence of amphiphilic PVP demonstrated good accessibility of terminal stearyl groups for the interaction with other hydrophobic ligands.
All tested amphiphilic PVP derivatives, formed aggregates in water solutions with the average size between 50 and 200 nm and narrow size distribution as follows from the particle size measurement. The influence of polymer molecular weight on critical concentration of aggregation was studied. Spontaneous micellization and low CAC values (in a low molar weight range) were found for amphiphilic PVP derivatives using the pyrene method. Using dynamic light-scattering and pyrene probe it was shown that length of hydrophilic and hydrophobic fragments influences greatly on polymers ability for aggregation. It was ascertained that in physiological solution size of aggregate was smaller than in distilled water. Using transmission electron microscopy it was shown that obtained aggregates were of spherical form and had certain size distribution, depended on hydrophilic and hydrophobic fragments length.
Mechanical stability of polymeric microaggregates was studied. Using transmission of microparticles through the microfiltering membrane, it was shown that decreasing size of particles after additional ultrasound processing recovers to initial value. It point to thermodynamical stability of particles with definite size, determined by polymer structure.

Coffee break

10:30 - 11:00

Morning session - continued

11:00 - 12:30

Main Building, room 213

Enhancement of sensitivity and selectivity in SPR detection of DNA point mutation by polymeric microspheres

11:00 - 11:30
invited oral

HARUMA KAWAGUCHI[1]

1) Science and Engineering, Keio University, Hiyoshi Yokohama, Japan

Polymeric microspheres were used to enhance the sensitivity and selectivity in the detection of DNA point mutation by SPR biosensor. First, Single-stranded DNA probes were immobilized onto epoxy group-derivatized gold surfaces and the hybridization of DNA targets was monitored. The SPR response was small. The subsequent interaction with DNA-carrying microspheres enhanced the response due to the significant increase of mass bound to the targets. After this, the flow rate of the buffer solution was increased during the event of dissociation. The increase in shear stress resulted in the detachment of DNA-carrying microspheres hybridized with the mismatched pair and so the increase in the ability to discriminate a point mutation. The same effect was observed by the increase in the viscosity of buffer solution. Thus, the polymeric microspheres contributed to the enhancement of sensitivity and selectivity in detection of DNA point mutation.

11:30 - 12:00
invited oral

BIOMIMETIC SURFACES OF POLYMERS FOR TISSUE ENGINEERING

Frantisek Rypacek[1), **Dana Kubies**[1,3), **Stepan Popelka**[1,3), **Vladimir Proks**[1,3), **Elena Filova**[2), **Lucie Bacakova**[2), **Ludka Machova**[1)

1) Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovsky Sq.2, 162 06 Prague, Czech Republic, Prague, Czech Republic

2) Institute of Physiology, Academy of Sciences of the Czech Republic, Vídeňská 1084, Prague, Czech Republic, Prague, Czech Republic

3) Center for Cell Therapy and Tissue Repair, 2nd Faculty of Medicine, Charles University, V Uvalu 84, 150 00 Prague, Czech Republic, Prague, Czech Republic

Trends in cell therapy and tissue engineering ask for polymer scaffolds which reflect requirements for tuned mechanical properties, suitably designed three-dimensional architecture as well as demands on the specific interaction between biomaterial and living cells. Adhesion, proliferation and differentiation of cells on polymer substrates can be modified by providing solid-state signals to the cells through specific structures exposed on the polymer surfaces.
Surface properties of polyester-based biomaterials were modified by amphiphilic block copolymers composed of hydrophobic polyester and hydrophilic poly(ethylene oxide) (PEO) blocks. The polyester blocks served to stabilize the copolymer layer on the polymer support while the hydrophilic blocks allowed introduction of functional groups, either nonspecific or cell-specific, on the polymer surface. The end-functionalized PLA-b-PEO copolymers were prepared by controlled polymerization of lactide using the semitelechelic PEO with protected carboxyl or amino groups as co-initiators. The selected peptide sequences were attached to the functional copolymers using the solid-phase techniques based on building a protected peptide on polymer support.
Several approaches were studied in preparation of functional polymer surfaces with controlled distribution of cell-adhesion structures. The effect of surface modifications on adhesion and growth of vascular smooth-muscle and endothelial cells on polymer films was evaluated. Thus, functional amphiphilic block copolymers can be used as a versatile modular system providing different types of bioactive patterned surfaces of polymer biomaterials, exhibiting selective interactions at biomaterial-cell interfaces.

Acknowledgment: Support from the Grant Agency of the Academy of Sciences of Czech Republic (grant No. A4050202), Grant Agency of CR (grant No. 304/02/0579) and the Ministry of Education of CR (grant No. LN00A065) is acknowledged.

THE TREATMENT OF PATELLA FRACTURES BY THE METHOD OF CONTROLLED EXTERNAL FIXATION

12:00 - 12:20
oral

Antonov A. Alexandr[1)

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THE TREATMENT OF PATELLA FRACTURES BY THE METHOD OF CONTROLLED EXTERNAL FIXATION

V.N.Pasternak, A.A.Antonov
Donetsk state medical university. Ukraine

It is developed the technique of controlled external fixation of patella fractures, which corresponds to modern anatomic and byomechanical requirements. The external design consists of two modules - compressive and fixing one on the patella and base one on the top third of shin. Modules are connected among themselves by hinges and provide the unloading of patellofemoral joint. The technique assumes open reposition, restoration extensive apparutus and fixationg of patella fragments. Reposition and fixing of them was made openly. 24 patients were operated on with good result in all cases.
Practical application of a technique has allowed to provide early function of a knee joint with an opportunity of static and dynamic loading of lover extremity and to conduct in time the fracture consolidation period with the rehabilitation one.

Lunch break

12:30 - 14:00

Afternoon session

Main Building, room 213

14:00 - 15:30

14:00 - 14:30
invited oral

Double stimuli-sensitive ABA block copolymers

Christo B. Tsvetanov[1), **Philip A. Dimitrov**[1), **Erol A. Hasan**[1)

1) Institute of Polymers, BAS (IP BAS), Acad G.Bonchev St. 103A, Sofia BG-1113, Bulgaria

Thermoassociative block copolymers usually consist of a water-soluble segment and a temperature-responsive one. In this study novel thermally sensitive ABA blockcopolymers were obtained carrying a central polypropylene oxide block (PPO) with molecular weight of 2000 D and outer blocks of poly(N-isopropylacrylamide) (PNIPAAm) or poly(ethoxyethylglycidyl ether) (PEEGE). Ceric ion redox method and ATRP were applied for the synthesis of PNIPAAm-b-PPO-b-PNIPAAM by using PPO as a precursor. The PEEGE-b-PPO-b-PEEGE blockcopolymers were prepared by sequential anionic polymerization using Cs alkoxides as initiators. Hence the resulting copolymers were comprised of blocks with different lower critical solution temperatures in aqueous media, which allowed us to obtain thermoassociative blockcopolymers characterized by two-step phase transition. This attractive behaviour will allow the development of nano-particles or micro-aggregates with two different cores. Such advancement could potentially provide the groundwork for a unique drug delivery system capable of carrying two biologically active compounds with different drug release profiles.

14:30 - 14:50
oral

Surface functionalization by smart binary polymer brushes to tune physiko-chemical characteristics at biointerfaces

Petra Uhlmann[1), **Nikolay Houbenov**[1), **Sergiy Minko**[2), **Manfred Stamm**[1)

1) Institute of Polymer Research, Dresden 01069, Germany

2) Clarkson University, Potsdam, NY, United States

Polymer brushes consist of an assembly of polymer chains that are attached by one end to the surface with sufficient grafting density. Binary brushes constituted from two incompatible polymers can be used in the form of ultrathin polymeric layers as a versatile tool for surface engineering to tune physico-chemical surface characteristics as wettability, surface charge, chemical composition or morphology, and furthermore to create responsive surface properties1. It is also possible to fix surface structures obtained in this way by (photo)crosslinking of the layers.
Mixed brushes of oppositely charged polyelectrolytes are representing a special case of responding surfaces which are sensitive to changes of the pH value in aqueous environments2.
Examples for the influence of the surface characteristics (charge, hydrophobicity/ hydrophilicity, extent of swelling) of symmetrical mixed polyelectrolyte brushes as well as of additional salt amounts in the protein buffered solution on the substrate anchorage and conformation of model proteins will be presented.

[1] A. Sidorenko, S. Minko, K. Schenk-Meuser, H. Duschner, M. Stamm, Langmuir 1999, 15, 8349
[2] N. Houbenov, S. Minko, M. Stamm, Macromolecules 2003, 36, 5897-5901

14:50 - 15:10
oral

Cell growth on plasma immersion ion implanted polymer surfaces

Alexey V. Kondyurin[1), **Manfred F. Maitz**[2), **Irina V. Kondyurina**[2,3)

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A wide number of polymer materials has well-known applications as prosthetics materials, but the application of polymers in the body often induces inflammatory reactions and/or fibrosis, if the growth of specialized cells is not favoured Therefore it is important to check in vitro the performance of cells from the target implant site on the material.
In the present paper we present our results of the modification of polyethylene, polyurethane and polytetrafluorethylene surfaces by plasma immersion ion implantation.
The polymer surfaces were treated by nitrogen ion fluxes. The surface properties were analysed by drop shape analysis for the surface energy, FTIR spectroscopy, XPS, optical microscopy and AFM. The growth of endothelial cells on polymer surfaces was analysed by the Alamar blue^{TM} redox assay, statistical evaluation of the cell distribution on microphotographs and by FTIR spectra.

Ion implantation caused chemical activity (oxygen containing groups, unsaturated groups and free radicals) of the polymer and made the surfaces more hydrophilic. The cell growth was more homogeneous on ion implanted polyethylene and polytetrafluorethylene surfaces in contrast to the untreated surfaces, where a very spotted cell growth was found. This indicates that the adhesion of cells was sufficient for an equal distribution over the surface. As result, the cells formed bigger colonies 2 days after seeding on the modified than on the initial surfaces. In conclusion, the polymer surfaces after ion implantation become more acceptable for the cells, what can be useful polymer prosthetics.

Metabolic distresses at the patients with polymer materials using at a polytrauma.

15:10 - 15:30
oral

SERGEY N. KRIVENKO[1)], **ANATOLIY K. RUSHAY**[1)], **KONSTANTIN A. BODACHENKO**[1)], **TATYANA A. KOLOSOVA**[1)], **VALERIY Y. BORISOV**[1)], **ROMAN V. CHUCHVAREV**[1)]

1) Donetsk State Medicine University, Scientific Research Institute for Traumatology & Orthopeadics (DonIT&Or), 106, Artema St, Donetsk 83048, Ukraine

Treatment of the patients with multiple diaphyseal fractures of bones of extremities - urgent problem, as this kind of traumas is one of the most often causes, which result in physical inability.
Stuffs And methods. With the purpose of research of pathogenetic aspects of a multiple trauma in conditions of research R&D Institute of Traumatology and Orthopedy of Donetsk State Medical University named after M. Gorky term 2000 -2003 years we carry spent complex clinic-laboratory inspection 140 patients.
The summary. The state of metabolic processes in an organism of the injureds was investigated in 1, 7, 14 and 21 days after a trauma. The mathematical processing of results by a method of the main components has allowed to reveal intrinsic frame of metabolic processes of the acute term of a multiple trauma of extremities with polymer materials using and to define its integrated parameters.
Conclusion. It is necessary to note, that since the moment of damage, the injureds with multiple fractures of bones of extremities with polymer materials using have complex metabolic changes, both in a place of fracture, and in an organism as a whole for phylum of a defense reaction on unfavorable environmental factors. Greatest information for an explanation of general metabolic reaction of an organism at a multiple trauma of bones of extremities have the parameters albuminous, carbohydrate and enzyme of exchanges.

Coffee break

15:30 - 15:50

Afternoon session - continued

15:50 - 17:20

Main Building, room 213

Macroscopic and microscopic hydrogels synthesized by radiation technique and their selected biomedical applications

15:50 - 16:20
invited oral

Piotr Ulanski[1)], **Janusz M. Rosiak**[1)]

1) Technical University of Lodz, Institute of Applied Radiation Chemistry (IARC-TUL), Wroblewskiego 15, Łódź 93-590, Poland

Among various classes of polymeric products used for biomedical purposes, much attention is attracted by hydrogels - two-component systems consisting of a permanent, three-dimensional network made of covalently bound chains of hydrophilic polymers and water filling the pores. At our Institute since mid-eighties several technologies have been developed to synthesize hydrogels for medical use by radiation technique (e.g. fabrication of hydrogel wound dressings, implemented on an industrial scale, production volume exceeding one million pieces per year). This paper is a brief review of our current research activities in this field.
Radiation techniques, based on crosslinking of polymer chains initiated by ionizing radiation, have many advantages over conventional synthesis methods. No monomers, crosslinking agents and other harmful chemicals are used, so there is no need for any additional purification steps. The process can be performed at any temperature, and the crosslink density can be precisely controlled. Materials can be irradiated in their final, sealed packages. Crosslinking and sterilization occur in single technological step.

By choosing appropriate irradiation conditions one can control the structure and properties of the products. In particular, it is possible to form a continuous, macroscopic hydrogel, or small gel particles of desired dimensions (nanogels, microgels).
Our current projects on the biomedical applications of hydrogels include: system for healing of endometrium cancer by precise, local drug delivery, encapsulation of living cells, construction of hybrid organs, intervertebral disc implants, hydrogel phantoms for three-dimensional radiation dosimetry in radiotherapy, synovial fluid substitute, temperature-sensitive gels and membranes, and dietary additives based on natural and synthetic polymers.

This work has been financed in part by the International Atomic Energy Agency (projects POL/6/007 and 11513/RO) and NATO (grant 980622).

16:20 - 16:40
oral

IN VIVO WEAR OF POLYETHYELNE GLENOID COMPONENTS IN TOTAL SHOULDER ARTHROPLASTY

Wojciech Swieszkowski[1), **Mark Frankle**[2), **Harald E. Bersee**[3), **Krzysztof J. Kurzydlowski**[1)

1) Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland

2) Florida Orthopaedic Institute, Florida, United States

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Introduction
Loosening of the glenoid component after a total shoulder arthroplasty (TSA), leading to pain and the need for a revision operation, accounts for one third of all shoulder replacement complications. It has been shown that glenoid loosening could be a result of osteolysis of periprosthetic bone induced by polymeric wear debris.
The aim of this study is to determine the amount and pattern of in vivo wear of polyethylene glenoid components by examining a set of so called retrievals using laser scanner technique and scanning electron microscopy.

Methods
Six glenoid components were retrieved and examined (five are all-polyethylene and one metal-backed). The average time of functioning of these components in human bodies was 10 years with the range of values from 7-14 years.
Each component was scanned using a laser scanner. The results of measurements have been used to generate geometrical models of the retrievals using CAD software - GEOMAGIC. These models have been subsequently used to determine the maximum depth and the volumetric of wear for each component. The retrievals were also examined using the scanning electron microscope (SEM).

Results
The maximum wear rate and wear depth for the analyzed retrievals was 30 mm3/yr and 0.2 mm/yr, respectively. From the SEM analysis of the retrievals it was found that prominent inferior wear areas and fine multidirectional scratches were dominant in all retrievals. Random scratches were also observed, most probably due to the third body wear (cement particles). Two implants were found to have surface micro-cracks, believed to result from subsurface fatigue.

Discussion
The observed wear rates and depths in the glenoid prosthesis are within the average value observed clinically in hip arthroplasty. The significant abrasive and fatigue wear observed in the study might be the result of high surface and and subsurface stresses acting in TSA and multidirectional component relative movement.

16:40 - 17:00
oral

Structure and biocompatibility of TiN coatings on polyurethane produced by laser ablation

Roman Major[1), **Elzbieta Czarnowska**[2), **Agnieszka Sowińska**[2), **Roman Kustosz**[3), **Jűrgen M. Lackner**[4), **Michal J. Wozniak**[5), **Tadeusz Wierzchoń**[5), **Bogusław Major**[1)

1) Polish Academy of Sciences, Institute of Metallurgy and Materials Sciences (IMIM PAN), Reymonta 25, Kraków 30-059, Poland

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4) Joanneum Research Forschungsgesellschaft mbH, Laser Center Leoben, Steyrergasse, Graz A8010, Austria

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Warszawa 02-507, Poland

TiN coatings on polyurethane (PU) were produced by pulsed laser deposition using a system working with a Nd:YAG laser for ablation of titanium target. Nitrogen environment was applied in the reactive chamber in flow of 30sccm. Structure examinations X-ray diffraction (XRD), atomic force microscopy (AFM) and transmission electron microscopy (TEM) were performed to study surface morphology (AFM) and microstructure of the cross-section (TEM) as well as crystallographic texture and residual stresses (XRD). AFM results revealed diminishing of the roughness of the surface with rise of the coating thickness in the range from 0.25 via 0.5 and 1 up to 3m. Dominating contribution of kinetic processes in the formed morphology could be suggested together with the thickness rise due to appearance of the characteristic features on the surface leading to the polycrystalline fine grained microstructure. Extend of the lattice parameter was stated in XRD measurements with the increase of the coating thickness which could be explained by the change of deposition mechanism. Crystallographic texture measured in TiN layers presented close to random preferred crystallographic orientation as well as pole figures of the residual stress distribution suggested isotropic character. Thin foils prepared from the cross-section using microtom method showed a form of anchoring of the TiN deposited layer to the PU substrate with possible local remelting of substrate by the first deposited particles. Residual stress measured in TiN layer was in the range of about -2GPa and its value diminished together with the rise of the coating thickness. Biological tight examinations of coating are carried out in the range of cell proliferation, death and adhesion.
Financial support of the work by project PBZ-KBN-082/T08/2002/11

STUDY ADSORPTION OF PROTEIN WITH LANGMUIR AND FREUNDLICH MODEL

17:00 - 17:20
oral

SAJJAD SEDAGHAT SHEREJINI[3], OMID MORADI[1], MOHAMMAD YARI[2]

1) Chemistry groups, Department of chemical Engineering AmirKabir University of Technology, Tehran, Iran

2) Islamic Azad University Islamshaher Branch, Tehran, Iran

3) Islamic azad university, Shahryar-Shahre gods branch, Tehran, Iran

Abstract
Adsorption of proteins, albumin and lysozyme on polymer surfaces; Poly Acrylic Acid (AA) and 2-hydroxyethyl methacrylate (HEMA) has been investigated by UV spectroscopy. The results have been treated by Langmuir model and the parameters of this model have been evaluated. The Freundlich model has also been utilized to determine the Gibbs free energy of adsorption for the proteins and polymers used in this study.
The protein adsorption models which are applied to the protein solutions include the Langmuir and the Freundlich isotherm model which are designed for the calculation of colloid particles with the surface and kinetic adsorption. In this research, the adsorption of the proteins albumin and lysozyme on the polymer surfaces of HEMA and AA was determined using the UV spectroscopy method in the wavelength of 280nm, and the parameters of Langmuir equation, and the surface, which was covered during the adsorption, are calculated. Also Freundlich equation is model to calculate the free energy change of adsorption. Also the results indicated show the average adsorption free energy for lysozyme on HEMA and AA surfaces. As it is seen from this figure the average adsorption free energy of lysozyme on AA surface is greater than HEMA surface. The reason for this can be attributed to the electrostatic attraction between lysozyme and AA surface.

Poster session 2

19:00 - 21:00

Thursday, September 9th

Morning session

09:00 - 10:30

Main Building, room 213

09:00 - 09:20
oral

Determination of the ions present in the eye tear by flame photometer spectroscopy on contact lenses

OMID MORADI[1)]

1)) Chemistry groups, Department of chemical Engineering AmirKabir University of Technology, Tehran, Iran

Application of contact lenses is being extended due to the several facilities. For instance, in people who have problem in their natural eyesight can use these contact lenses in substitution for glasses. Some lenses are applied for the control and relaxation of the drugs. But the use of lenses also has some problems, included the opacity and decrease in patients eyesight. Of the other problems in using eye lenses, is the infection of corneal as the result of biologic contamination and incomplete access to oxygen on corneal surface. The most important reason for the opacity of lens surface is the adsorption of proteins and ions in the eye tear. From these ions, Na, K and Ca are the most important factors in the eye opacity. In this research, adsorbed ions on the both sides of contact lens based on Acrylic Acid (AA) and 2-hydroxy ethyl methacrylate (HEMA) were measured by flame photometer spectroscopy for the specification of interferences result by these ions in lens opacity.
After the determination of concentration values of adsorbed ions on the AA and HEMA lens surfaces, the following results were obtained:
On AA surface:
Ca2+ adsorbed > Na+ adsorbed > K+ adsorbed
On HEMA surface:
Ca2+ adsorbed≈ Na+ adsorbed ≈ K+ adsorbed
According to the amounts resulted on the AA surface, it is obvious that the ions adsorption is dependent on surface charge. On AA surface this dependence is due to the negative surface charge produced by carboxylic groups. But the HEMA surface, because of the absence of polar groups which do not posses surface charge, the amount of each adsorbed ions are approximately same.

09:20 - 09:40
oral

Poly(epsilon-caprolactone)- and poly(methyl methacrylate)-based scaffolds in human bone-derived cell cultures in vitro

Radosław M. Olkowski[1)], **Katarzyna Filipczak**[2)], **Anna Chróścicka**[1)], **Piotr Woźniak**[1)], **Piotr Ulanski**[2)], **Janusz M. Rosiak**[2)], **Jacek Przybylski**[1)], **Malgorzata Lewandowska-Szumiel**[1)]

1) Medical University of Warsaw, Department of Biophysics and Human Physiology, Chałubińskiego 5, Warszawa 02-004, Poland

2) Technical University of Lodz, Institute of Applied Radiation Chemistry (TUL), Wroblewskiego 15, Łódź 93-590, Poland

Poly(methyl methacrylate) (PMMA) and poly(epsilon-caprolactone) (PCL) are synthetic polymers already used in medical applications. They are both taken into account as candidate scaffolds for cell transplantation in reconstructive surgery by means of tissue engineering. The aim of this work was to verify differences in morphology and vitality of Human Bone-Derived Cells (HBDC), cultured on PMMA and PCL. Polymers used for experiments were prepared in the form of 1mm high cylinders, 6.2mm in diameter, and placed at the bottom of a 96-well culture dish. Samples of PMMA were smooth, samples of PCL were either smooth or porous. Cells used for experiment were isolated from postsurgery bone tissue, which would be otherwise discarded. HBDC were cultured under standard conditions directly on the samples of PMMA and PCL and on the tissue culture polystyrene (TCPS) as a control. To assess HBDC vitality, XTT assay was performed. Morphological observations of CFDASE fluorophore stained cells in contact with biomaterials were carried out in reflected light and ultraviolet.
Vitality of HBDC cultured on the PMMA and PCL samples was found to be dependent on the mode of samples preparation and their porosity. Fluorescently stained HBDC cultured on both tested polymers were numerous and well spread. They differed in shape dependending on the support. Cells cultured on PCL were elongated and uniform; cells on PMMA had irregular shape.
Both biomaterials tested were found to be biocompatible in contact with human osteoblast-like cells. The influence of their surface and structure characteristics on cell function in vitro needs further investigations.

This work was supported by the State Committee for Scientific Research (grant 05/PBZ-KBN-082/2002/06).

09:40 - 10:00
oral

New approach for the explanation and control of the unique biocompatibility of the zwitterion-based polymers

Georgi Georgiev[1)], **A. Tzoneva**[1)], **E. Vassileva**[1)], **I. Kamenova**[1)], **E. Kamenska**[1)], **S. Iliev**[1)]

1) University of Sofia, Faculty of Chemistry, 1 J. Bourchier Avenue, Sofia 1164, Bulgaria

A new approach is proposed for the explanation of the unique bio- and haemocompatibility of the homo- and copolymer zwitterions (2-(methacryloyloxyethyl)phosphorylcholine, O-methacryloyl-L-serine, N,N-dimethyl(methacryloylpropyl)ammonium propane sulfonate, etc.), used for the production of the cardio-vascular prostesis, blood filtration membranes, coronary guidewires and stents, catheters, biolubricants, soft contact lens, cosmetic creams and lotions. The relationship between the salt- and hydrophylicity of the polyzwitterions (PZ) and their antipolyelectrolyte ability and lack of the Donnan effect in their aqueous solutions is elucidated. The specific dipole-dipole interaction between PZ segments results in a formation of domains from the opposite oriented dipoles. The equilibrium between the salt aqueous solution and these domains is realized when $(c_{s,o} - x)^2 = k^2x^2$ (Eqn (1)), where $c_{s,o}$, x and k are respectively the initial salt concentration, increment of this concentration at a contact between PZ and salt solution, and the volume ratio between the aqueous and PZ phases ($x = V_{w,eq}/V_{PZ,eq}$). The Eqn (1) solution is $x = c_{s,o}/(1+k)$, and the salt concentration in the both phases is $c_{s,eq} = k_{cs,o}/(1+k)$. From the salt balance relationship the PZ swelling could be obtained as a ratio of the equilibrium and initial PZ phase volume: $V_{PZ,eq}/V_{PZ,o} = [V_{PZ,eq}/V_{w,eq} + \Delta/V/V_{w,o}]V_{w,o}/V_{PZ,o}$ (Eqn (2)), where Δ/V is an increment of the both phases after PZ swelling, $V_{w,o}$ is an initial water volume. In most cases $V_{w,o}/V_{PZ,o}$ »1. So, the equation (2) proves the above mentioned relationship, and could be considered as a new rigorous substantiation of the experimentally established high free water fraction in PZ hydrogels. Formation of the mentioned above hydrophilic PZ dipole-dipole ordered clusters on the hydrophobic domains of the protein macromolecules during the protein unfolding suppresses protein aggregation.

Prolonged ageing polymers modified by plasma carbon black

10:00 - 10:20
oral

Tomasz Zieliński[1], **Jacek Kijeński**

1) Industrial Chemistry Research Institute (ICRI), Rydygiera 8, Warszawa 01-793, Poland

The use of new kinds of modifiers for polymers can create possibilities of finding new ecological safety and stable for thermal-mechanical and aging processes compositions. The new kind of polymers were made by modification of plasma carbon black, which can be use as an antioxidant and pigment. The using of plasma carbon black can improve economical part of low density and high density polyethylene production. The decreased amount of plasma carbon black in polymer, beside the economical profits of production, gives better properties of oxidation induction time, what can elongate the time of use. The paper presents the thermal-mechanical and oxidation induction time tests of LDPE and HDPE modified by changeable content of plasma carbon from 0.1 to 1.0% w/w. The investigations were based on SEM images, microscope images and XRD studies. Properties of plasma carbon black were measured by physical and chemical test like BET adsorption, IA and DBF numbers, etc. The results of ageing tests showed the increased oxidation induction time, 57 min., for 0.5% w/w of plasma carbon black content in the composition. The results were compared to commercial cable polyethylene modified by furnance carbon black.

Symposium C

Science and Technology of Nitrides and Related Materials

Introduction

Workshop organized as a part of: Center of Excellence CEMOS Work Package 6: "Research on optoelectronic application of nitride semiconductors"

Organisers

- Jacek Baranowski, Warsaw University, Poland
- Stanislaw Krukowski, High Pressure Research Center, Polish Academy of Sciences, Warsaw, Poland
- Krzysztof Korona, Warsaw University, Poland

Proceedings

Papers will be published in Physica status solidi.

Acknowledgements

Symposium is supported by Center of Excellence CEMOS (European Commission Contract GMA1-2002-72053).

Tuesday, September 7th

Tuesday afternoon

14:00 - 15:30

Main Building, room 206

MOCVD growth of Group III Nitrides for high power, high frequency applications.

14:00 - 14:45
invited oral

Marie-Antoinette di Forte-Poisson[1)]

1) Thales Research and Technology (TRT), orsay 91404, France

This paper reports on the LP-MOCVD growth optimisation of bulk GaN, GaAlN materials and GaAlN/GaN heterostructures grown on Sapphire and Silicon Carbide substrates for MESFET and HEMT applications, and on the device performances obtained with these structures.
High purity GaN grown on sapphire and Silicon Carbide has been obtained, with carrier concentration lower than 1013 cm-3.
GaN/Al2O3 MESFETs based on such high purity GaN buffer layers, have exhibited very promising static and microwave performances : high beakdown voltage 200V, ft = 12GHz, fmax = 25GHz and CW output power in excess of 2.2W/mm at 2GHz.. They have shown the best low frequency noise performances, with the lowest Hooge's parameter as compared to the values reported in the literature for different GaN- based FETs (HFETs and HEMTs).
The critical impact of some growth parameters on the physical properties of the GaAlN/GaN epilayers grown on SiC has been identified and studied using High Resolution X-Ray diffraction (HR-XRD), AFM, C-V and Eddy current probe measurements.
The devices performances related to our first GaAlN/GaN HEMT structures grown on Sapphire and Silicon Carbide have confirmed the high potentiality of GaN and related alloys for high power microwave transistors.
Load-Pull measurements performed at 2 GHz on devices related to GaAlN/GaN/Al2O3 HEMT structures, have shown a remarkably high output power density (4.4W/mm) and absolute power level (3.5W for 1mm devices). These power level results for devices on sapphire substrates measured on wafer, are well in agreement with the international state of the art.
Nevertheless, the thermal effects, which lead to a significant reduction of the power density with the increase of the transistor size, have been found to be more pronounced for devices on sapphire.
Devices related to GaAlN/GaN/SiC HEMT structures have been measured at 10 GHz using a load pull system. They exhibited a CW output power in excess of 4 W/mm (Lg= 0.25 mm).

[ABSTRACT TRUNCATED TO 2000 LETTERS]

Optical in-situ monitoring of III-Nitride epitaxial growth

14:45 - 15:30
invited oral

Thomas Zettler[1)], **K. Haberland**[1)], **E. Steimetz**[1)]

1) LayTec GmbH (LayTec), Helmholtzstr. 13-14, Berlin D-10587, Germany

In-situ monitoring tools for III-Nitride MOVPE are typically based on optics - because photons can penetrate the gas-phase easily and can sense the actual growth status even for complex or very fast wafer rotation configurations. The physical wafer-related parameters that can be detected today in-situ are: wafer temperature, growth rate, material composition, and - if present - wafer curvature and surface roughness. In addition, complete finger-printing of device growth (e.g., stop-band wavelength and cavity dip of laser structures) by means of spectroscopic in-situ sensors is increasingly used.
This talk will focus on the physics background of the optical in-situ methods presently in use for monitoring III-Nitride growth: emissivity corrected pyrometry, spectroscopic reflectance, and laser beam deflection. Based on this we will discuss how the optimum wavelength range of a sensor can be chosen with respect to the material grown in the actual III-Nitride process.
We will compare the different techniques regarding their applicability to process development, process calibration, process monitoring and control. Here the accuracy and reproducibility of the different methods will be discussed and the related sensitivity limits will be estimated. It will be demonstrated that the over-all performance of a specific in-situ sensor depends not only on the sensor's degree of sophistication but also on the application conditions at the very different types of epitaxial growth systems.
Finally, we will review very recent results on actually challenging in-situ applications like the effect of wafer curvature and wafer doping on the true wafer temperature, absolute wafer temperature calibration for process transfer between different epitaxial growth systems and the quantitative analysis of in-situ optical data measured on structured and masked substrates.

Coffee break

15:30 - 15:50

Afternoon session - continued

15:50 - 17:20

Methods of Stress Reduction in the MOCVD Epitaxial Growth of GaN on Silicon

16:00 - 16:20
oral

M. B. Charles[1)], **M. J. Kappers**[1)], **R. Datta**[1)], **C. J. Humphreys**[1)]
1) University of Cambridge, Pembroke Street, Cambridge CB2 3QZ, United Kingdom

The use of silicon substrates for GaN based device structures is attractive for many reasons, particularly in terms of cost and scale, but there are also inherent drawbacks. In addition to the large lattice mismatch between silicon and GaN, which causes a high dislocation density, there is a particularly large thermal expansion coefficient mismatch between the two materials. This introduces tensile stress, on cooling from the growth temperature of around 1000C, and can result in wafer bowing and cracking of the GaN.
Using guidance provided by XRD, AFM and TEM analysis, MOCVD growth schemes incorporating the use of AlN nucleation layers and interlayers, AlGaN graded layers and AlN/GaN superlattices have been used to reduce tensile strain in the GaN, producing uncracked surfaces and virtually flat wafers. In addition, SiN interlayers have been integrated into the structures to reduce dislocation density. Using these we have grown GaN films on Si which have an AFM roughness down to 0.11nm, with pit density of 4×10^8 cm^{-2}, and have XRD rocking curve FWHM of 500 and 550 arcsec for the (002) and (101) reflections respectively. A functional InGaN/GaN LED structure has also been realised on such a template.

Performance of III-nitride epitaxy in a low V-to-III gas-flow ratio range under nitrogen ambient in a hot-wall MOCVD system

16:20 - 16:40
oral

Anelia Kakanakova[1)], **Alexander Kasic**[1)], **Christer Hallin**[1)], **Erik Janzen**
1) Dept. of Physics and Meas. Techn., Linköping University, Linkoping, Sweden

Much of the best GaN material grown today is produced in cold-wall MOCVD reactors by running TMGa and NH_3 in a very high V-to-III gas-flow ratio, 10^3 and up to 40000, since a high NH_3 partial pressure is necessary to alleviate nitrogen loss during the growth.
The aim of this work is to explore the growth of AlN, AlGaN and GaN on SiC substrates in a lower V-to-III gas-flow ratio range, which may have advantages in avoiding the excess ammonia supply, reduced adduct formation and less toxic exhaust while achieving layers of device quality material. The growth runs are performed in a hot-wall MOCVD system, which is a new approach to the MOCVD growth of III-nitrides, though for the growth of device quality SiC epitaxial layers the situation is different. Today, the hot-wall reactor design dominates the SiC CVD world market and it is proven to supply very good heating efficiency, temperature homogeneity and uniform characteristics of the layers.
In the present experiments, with nitrogen as a carrier, TMAl and TMGa are added to NH_3 at N-to-Al and N-to-Ga gas-flow ratio of 50 and 250, respectively. The NH_3 flow is 50 ml/min and the precursors are delivered jointly.
High speed growth of epitaxial AlN and $Al_{0.2}Ga_{0.8}N$ layers are achieved, 1.5 and 3 μm/h, respectively, at a growth temperature of 1200^{o}C. The data analysis of the IR spectroscopic ellipsometry response of a 380 nm thick AlN, 55 nm thick $Al_{0.2}Ga_{0.8}N$, and 580 nm thick GaN layer provides the following results: E_1(TO) phonon mode broadening values of 5cm^{-1}, 4.2cm^{-1} and 4.6cm^{-1}, respectively. Small E_1(TO) broadening value indicates high compositional homogeneity and high crystal quality.
As a next step, we will show results from epitaxial growth under same growth conditions but using H_2 as a carrier gas. For example, relatively higher E_1(TO) broadening value, 5.7cm^{-1}, is measured for an AlN layer with similar thickness, 340 nm, grown however in 60 min when in H_2 ambient.
[ABS
[ABSTRACT TRUNCATED TO 2000 LETTERS]

16:40 - 17:00
oral

A New Single layer antireflection coating on PET substrates for the Display applications

Gowtham Manoharan[1)], **Bojan Karunagaran**[1)], **Devanesan Mangalaraj**[1)], **Chang Ki Seo**[1)], **Myung Suk Shim**[1)], **Jinsu Yoo**[1)], **Junsin Yi**[1)]

1) School of Information and Communication Engineering, Sungkyunkwan University, 300 Chunchun-dong, Jangan-gu, Suwon 440746, Korea, South

Single layer antireflection coating(SARC) is found to be the alternate for the current multilayer antireflection coatings . Titanium Nitride(TiN)is found to be appropriate for its good mechanical properties and optical properties. Recently very thin TiN films were found as an antireflection(AR) and antistatic(AS) layer for display applications. TiN films are fabricated by r.f. magnetron sputtering and the optical, electrical and compositional properties were investigated. The oxygen content is found in the XPS measurements revealed that our TiN films were actually titanium oxynitiride ($TiN_x\ O_y$) which is found to play an important role in AR properties .The optical properties TiN_xO_y films usually vary with the stoichiometry and crystallinity . so the experiment is carried out for different ratios of Ar/ N_2 to vary the optical property of the film. Spectroscopic ellipsometer (SE MF-1000) and UV-Vis spectrophotometer (SCINCO) were used for the optical measurements such as refractive index , transmittance and reflectance measurements.

Wednesday, September 8th

09:00 - 10:30

Wednesday morning

Main Building, room 206

09:00 - 09:45
invited oral

solar blind detectors based on AlGaN grown on sapphire

Jean-Yves Duboz[1)], **Nicolas Grandjean**[3)], **Franck Omnes**[1)], **Jean Luc Reverchon**[2)], **Mauro Mosca**[2)]

1) Centre de Recherche sur l'Hétéro-Epitaxie et ses Applications (CRHEA-CNRS), Rue Bernard Grégory, Valbonne - Sophia-Antipolis 06560, France

2) Thales Research and Technology (TRT), orsay 91404, France

3) Centre de Recherche sur l'Hétéro-Epitaxie et ses Applications (CRHEA-CNRS), Rue Bernard Grégory, Parc Sophia-Antipolis, Valbonne 06560, France

Solar blind detectors are key devices for applications where a small ultraviolet signal must be detected with a large solar background. In order to fabricate array that can be read by a hybridized Si read out circuit, we developed devices that can be illuminated from the back side. AlGaN heterostructures, with an active region with 43% Al and a window layer with 63% Al were grown on sapphire by Molecular Beam Epitaxy and Metal Organic Chemical Vapor Deposition (with different processes but similar results). Metal-Semiconductor-Metal (MSM) and Schottky diode detectors have been fabricated. Photoresponse spectra were recorded and show solar blind characteristics with cut off wavelengths in the range of 270-290 nm. The visible and near UV rejection ratio reaches 5 decades and the cut off slope is 4 nm per decade, which is the current state of the art for solar blind detectors. The effect of internal photoemission will be discussed. In MSM detectors, we reached state of the art detectivities. For a band width of 50 Hz, the detectivity D equals 4E14 /W corresponding to a noise equivalent power NEP=2.5 fW. This corresponds to a photon flux of 500/s per pixel which is among the best values ever reported in AlGaN solar blind detectors. Schottky diode AlGaN solar blind detectors exhibit a larger dark current due to parasitic leakage currents on the mesa edges. Some limitations in the charge collection were observed, due to the difficulty to get a highly conductive AlGaN with 65% Al and also due to the internal piezoelectric field. As a result, the performance of Schottky diodes, although comparable with published values, remains for the time being, slightly below the one obtained in MSM detectors. Preliminary results obtained in MSM detector arrays illuminated from the back side will possibly be given.

Properties and Applications of Group-III-Nitrides Solution-Gate Field-Effect Transistors

09:45 - 10:30
invited oral

Martin Eickhoff[1), Georg Steinhoff[1), Barbara Baur[1), Martin Stutzmann[1)

1) Technische Univ. München, Walter Schottky Institut, Am Coulombwall 3, Garching D-85748, Germany

Field effect transistors based on AlGaN/GaN heterostructures are of great interest for chemical and biochemical sensor applications. In addition to their high temperature stability, which has been exploited in the realization of gas sensitive devices for the detection of hydrogen and hydrocarbons up to temperatures of 600C [1,2], AlGaN alloys are chemically inert in aqueous solutions and non-toxic to living cells, which are basic requirements for the application as a substrate material for biosensors [3].
Recently, the deposition of highly mobile lipid membranes on hydrophilized III-nitride surfaces by vesicle fusion was demonstrated [3]. This allows the design of biosensors based on ultrathin lipid membranes deposited directly on the nonmetallized gate regions of AlGaN/GaN transistors. These devices allow the electronic detection of ligand binding to specific receptors in the lipid membrane [4] as well as electrochemical detection of transmembrane transport. A different approach for the realization of biosensors is the cultivation of living cells directly on the gate area and the measurement of their ionic response to chemical or physical stimuli [5].
We have investigated the response of AlGaN/GaN transistors and transistor arrays to changes in the concentration of specific ions in the ambient electrolyte. The potential drop at the interface between the gate surface and the electrolyte solution was measured and used as a sensor signal. A linear sensor response of approximately 56 mV/pH was found for variations in the H+-concentration between 10^{-1} and 10^{-13} mol/l, which is close to the theoretical Nernst limit, determined by the native oxide layer present on the surface [3,6]. The sensitivity towards Na^+, K^+, Ca^{2+} and Cl^- ions, which give the main contribution to cell action potential and long term stability of the transistor devices in aqueous solutions were also investigated. As the limiting factors for the detection of relatively small cell sig
[ABSTRACT TRUNCATED TO 2000 LETTERS]

Coffee break

10:30 - 11:00

Morning session - continued

11:00 - 12:30

Main Building, room 206

Electrical Properties of GaN/AlGaN Hetrostructures

11:00 - 11:20
oral

Wlodek Strupinski[1), Dariusz Lenkiewicz[1), Ewa Dumiszewska[1), Marek Wesołowski[1), Agata Jasik[1), R. Jakieła[1,2)

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GaN and AlGaN electrical transport properties were investigated in undoped and intentionally doped layers using Hall measurements. GaN/AlGaN films grown by MOCVD exhibited strong variations in resistivity as a result of changing MOCVD growth conditions in controlled experiments. The explanation of high compensation in GaN is connected to carbon impurity acting as a acceptor, substitutional oxygen predicted to act as donor, association of threading dislocations with charge centers, gallium vacancies and VGa-O complexes (deep acceptors). In our experiments we tried to recognize the most efficient source of n- and p-type carriers in undoped GaN and mechanisms of compensation by impurities and defects creation. The influence of AlGaN defects structure, with various Al content, on GaN electrical properties was examined detailed. Highly resistive and highly conductive GaN films were produced as a result of our investigations. GaN/AlGaN structures were applied for HEMTs and photodetectors.

Modeling of elastic, piezoelectric and optical properties of vertically correlated GaN/AlN quantum dots

11:20 - 11:40
oral

Grzegorz Jurczak[1), S. P. Lepkowski[2), Paweł Dłużewski[1), T. Suski[2)

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We theoretically investigate elastic, piezoelectric and optical properties of wurtzite GaN QDs, having hexagonal pyramid-shape which are stacked in the multilayers. [1] We solve the boundary-value problem using the nonlinear theory of anisotropic hyperelasticity based upon the general strain measure. [2] Calculated strain field is used to determine piezoelectric polarization. The spontaneous polarization is taken into acccount. The distribution of the electrostatic potential is obtained by solving the Poisson equation while the electronic states are obtained by using 8x8 kˇp hamiltonian of the wurtzite crystal.
We perform calculations in two steps. First, we calculate the stress and strain distribution, the piezoelectric fields and the electrostatic potential for the sequence of five GaN/AlN QDs placed one on another in the direction of growth. Second, for the centrally located QD, we calculated electronic states. This procedure allows us to examine the correlations of strain and piezoelectric fields between QDs in the multilayers.
Calculations have been performed for structures having different height of QDs and different thickness of the AlN spacers. We observe that the magnitude of the strain in the plane perpendicular to the direction of growth increases in the QDs and decreases in the spacers with increase of the thickness of the spacer. Additionally, electric field in the QD increases with the increasing the distance between the dots which results in the variation of the energy emission on the thickness of AlN spacer. We predict that the energy emission for 4nm height QDs and separated by 10nm-thick AlN layers exhibits a red-shift as large as 200 meV comparing to the energy emission for the same QDs grown with the 5nm-thick AlN spacers.

[1] N. Gogneau, F. Fossard, E. Monroy, S. Monnoye, H. Mank, B. Daudin, Appl. Phys. Lett., 84, 4224, (2004)
[2] P. Dłużewski, G. Maciejewski, G. Jurczak, S. Kret, J.Y. Laval, Comp. Mat. Sci., 29, 379, (2004)

11:40 - 12:00
oral

Low Temperature Deposition of Silicon Nitride Layers by Plasma Enhanced CVD For Large Area High Efficiency MC-Si Solar Cells

Bojan Karunagaran[1], **Jinsu Yoo**[1], **Kim Do Young**[1], **Kyunghae Kim**[1], **Suresh Kumar Dhungel**[1], **Devanesan Mangalaraj**[1], **Junsin Yi**[1]
1) School of Information and Communication Engineering, Sungkyunkwan University, 300 Chunchun-dong, Jangan-gu, Suwon 440746, Korea, South

Silicon nitride (SiN) deposition using PECVD is a proven technique for obtaining layers that meet the needs of surface passivation and AR coating.In addition, the deposition process appears to provoke bulk passivation as well due to diffusion of atomic hydrogen.A further advantage of PECVD is that the process takes place at a relatively low temperature of 300C.This paper deals with the fabrication of multicrystalline silicon solar cells with PECVD SiN layers combined with high-throughput screen printing and RTP firing. Using this sequence we were able to obtain solar cells with an efficiency of 14% for mc-Si wafers of size 125 mm square. $POCl_3$ doped polished silicon wafers with a junction depth of about 0.5 m and an emitter sheet resistance of 35 ohm/sq were selected for the cell fabrication.The mean cell efficiency, fill factor and Voc for the cells prepared in the present study were found to be 14%, 0.76 & 0.602V respectively. SiN deposition was performed using a horizontal PECVD reactor system consisting of a long horizontal quartz tube that was radiantly heated.Special and long rectangular graphite plates served as both the electrodes to establish the plasma and holders of the wafers.The electrode configuration was designed to provide a uniform plasma environment for each wafer and to ensure the film uniformity. These horizontally oriented graphite electrodes were stacked parallel to one another, side by side, with alternating plates serving as power and ground electrodes for the RF power supply.The plasma was formed in the space between each pair of plates.The optimized flow rates of N_2, NH_3& SiH_4 for the deposition of SiN were 70, 50 & 10 sccm respectively.Working pressure was maintained at 650 mtorr.The SiN layer deposited under these optimized condition were found to have a thickness of approximately 70 nm and a refractive in 1.9 at 630nm.Currently we are on the process designing a new PECVD system which can be used for mass production.

12:30 - 14:00

Lunch break

14:00 - 15:30

Wednesday afternoon

Main Building, room 206

Cathodoluminescence Microscopy of Nitrides

14:00 - 14:45
invited oral

Juergen H. Christen[1)]

1) Otto-von-Guericke-University Magdeburg, Universitaetsplatz 2, Magdeburg 39016, Germany

Nitride-based Surface Acoustic Waves Devices and Applications

14:45 - 15:30
invited oral

Fernando Calle[1)], **Jorge Pedrós**[1)], **Tomás A. Palacios**[1)], **Jesús Grajal**[1)]

1) Universidad Politécnica de Madrid, Ciudad Universitaria, Madrid 28040, Spain

Bulk and surface acoustic wave (SAW) devices are a convenient solution for high frequency filters in mobile communication systems due to their stability, reliability and compactness. In addition, SAW filters are ideal for gas sensing, with many industrial, environmental and biomedical applications. Furthermore, SAW sensors offer the additional feature of wireless transmission, and therefore the feasibility of operation in harsh environments. Whereas acoustic wave devices are typically fabricated on quartz or $LiNbO_3$, other piezoelectric materials where devices could exhibit novel or improved characteristics are highly desired. III-nitrides, particularly AlN, combine high SAW velocity and electromechanical coupling coefficients, while showing excellent thermal and chemical stability. These properties pave the way for the development of SAW devices operating at frequencies higher than 2 GHz, a requirement of modern telecomm applications. Moreover, the semiconductor character and direct bandgap of AlGaN enables the integration of SAW devices with electronics and optoelectronics.

In this work a review of the fabrication techniques of nitrides for SAW applications and the device properties will be done. Several acoustic modes are observed in the transfer functions of the filters: besides the Rayleigh wave, guided modes (Sezawa) arise when the sound velocity in the nitride layer is lower than in the substrate (like in GaN/sapphire), and new pseudobulk modes may also appear. The effect of the substrate characteristics (sound velocity and thickness) will be addressed, including the anisotropy found in devices grown on sapphire due to the crystal structure mismatch. Finally, two novel devices based on surface acoustic waves will be discussed: a SAW-assisted photodetector, based in the integration of a SAW generator and a UV photodetector, and a DC controlled SAW filter, obtained by the fabrication of a SAW device on a 2-DEG AlGaN/GaN heterostructure.

Coffee break

15:30 - 15:50

Afternoon session - continued

15:50 - 17:20

Main Building, room 206

Novel Noncontact Thickness Metrology for Backend Manufacturing of Wide Bandgap Light Emitting Devices

16:00 - 16:20
oral

Wojtek J. Walecki[1)], **Kevin Lai**, **Vitalij Souchkov**, **Phuc Van**, **SH Lau**, **Ann Koo**

1) Frontier Semiconductor (FSM), 1631 N 1st Street, San Jose, CA 95112, United States

Low coherence optical interferometry [1] has been proven to be an effective tool for characterization of thin and ultra-thin semiconductor Si wafers [2]. Purpose of this paper is to present an extension of this method to characterization of ultra-thin compound wide bandgap wafers mounted on insulating carriers.

The metrology of thin and ultra-thin compound materials wafers has been identified very early as one of the technology gaps of the industry. Most commonly employed metrologies include capacitance and air pressure techniques. These two competing technologies have been proven reliable and quite accurate methods of measurement of thickness, bow, warp and related parameters for relatively thick and well conducting materials. Capacitance method however is not suitable for measuring thickness of semi-insulating and insulating materials such as sapphire, or SiC, and very thin wafers (thinner than 100 um). Air pressure based sensors are able to measure insulating materials, however they cannot be directly applied to wafers mounted on carriers. Both these competing technologies require access from both top and bottom sides of the wafer. Very small standoff distance makes difficult to integrate these metrologies in in-situ or ultra-clean environments.

In this paper we present alternative technique, which does not suffer from above discussed limitations, and can be easily integrated in the production tools, and provide accurate measurement of samples while they are being processed.

[1] D. Huang, E. A. Swanson, C. P. Lin, J. S. Schuman, W. G. Stinson, W. Chang, M. R. Hee, T. Flotte, K. Gregory, C. A. Puliafito, J. G. Fujimoto, Science 254, 1178-1181 (1991).

[2] W.J. Walecki, R. Lu, J. Lee, M. Watman, S.H. Lau, A. Koo, 3 rd International Workshop on Thin Semiconductor Devices - Manufacturing and Applications November 25, 2002, Munich, Germany

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16:20 - 16:40
oral

The p-i-n photo detectors for UVA and UVB regions made of GaN/AlGaN

Lech Dobrzanski[1)], **Dariusz Lenkiewicz**[1)], **Krzysztof Góra**[1)], **Andrzej Kozłowski**[1)], **Andrzej Jagoda**[1)], **Krystyna Przyborowska**[1)], **Beata Stańczyk**[1)], **Urszula Bielińska**[1)], **Artur Wnuk**[1)]

1) Institute of Electronic Materials Technology (ITME), 133 Wólczyńska, Warszawa 01-919, Poland

In this contribution we report on fabrication and testing of front side and backside illuminated UV p-i-n detectors. Short description of epitaxial structure, layout construction and device processing will be introduced followed by device characterization. Detector design trade offs will be discussed focused on differences between front side and backside-illuminated devices. The former exhibit uneven spectral response due to shallow light absorption in the p-type region and subsequent diffusive transport of generated carriers towards intrinsic region of device. For these reasons this devices are sensitive to the p-doping process deviations. In contrast device illuminated from the sapphire substrate side are immune towards p-region doping problems and have better responsivities, which values are as high as 0.15-0.20A/W. Spectral response of these diodes is even and resembles characteristics of a good band pass filter. We achieved this feature using "window" layers made of AlGaN in the vicinity of sapphire interface. Sensitivity of our devices has been estimated on basis of low frequency noise measurements. It appeared that its value is higher than 2 10^12 cm $Hz^{\frac{1}{2}}$ W^-1.
We presented development of semiconductor devices, which can find many important applications

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16:40 - 17:00
oral

Room temperature stimulated emission from self-organized GaN nano-columns grown on (111) Si substrate

Makoto Tada[1)], **Akihiko Kikuchi**, **Katsumi Kishino**

1) Sophia University, 7-1, Koi-cho, Chiyoda-ku, Tokyo 102-8554, Japan

High optical quality self-organized GaN nano-columns were successively grown on (111) Si substrates by an rf-plasma assisted molecular beam epitaxy. The intensity of room temperature photoluminescence (PL) of the nano-columns was 500 times stronger than that of typical GaN film grown by MOCVD. Furthermore, room temperature stimulated emission was observed with a very low threshold excitation power density of 350kW/cm^2. This superior optical property of GaN nano-columns on Si is comparable to that of the optimized GaN nano-columns on (0001) sapphire reported recently [1].
GaN nano-columns with a diameter, density and height of 100nm, 5 12x10^9/cm^2, and 1.6μm, respectively, were grown on (111) Si substrate without native oxide (sample A), and with native oxide (sample B). After a Ga deposition, active nitrogen was irradiated for 60s to form GaN dots as nucleation layer at 530^{o}C, then GaN nano-columns were grown at high temperature for 60min. The c-axis of nano-columns was perpendicular to the substrate surface for sample A and randomly tilted to the perpendicular of the substrate surface for B.
Strong PL emission was observed at 363 364nm from both samples for low excitation condition (1.3W/cm^2). The peak intensity was 500 times stronger than that of a 3.7μm-thick GaN films grown by MOCVD on a (0001) sapphire with a dislocation density of 3 5x10^9/cm^2. For higher excitation condition, stimulated emission was observed at 369nm with a threshold of 350kW/cm^2 for sample A. While no stimulated emission was observed up to 6MW/cm^2 for sample B. For reference, the threshold of stimulated emission of the MOCVD-GaN film and optimized GaN nano-columns on (0001) sapphire were 1.6MW/cm^2 and 200kW/cm^2, respectively.
These results suggesting that high performance light emitting devices on low-cost conductive substrate

can be realized by GaN-based nano-columns on Si substrates.

[1] A. Kikuchi and K. Kishino, Int. Symp. on Blue Laser and LED, B3-1, March 2004.

Electrochemical Etching and CV-Profiling of GaN

17:00 - 17:20
oral

Thomas Wolff[1)], **Michael Rapp**[1)], **Thomas Rotter**[2)]

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2) Universität Erlangen, Lehrstuhl für Elektronische Bauelemente (LEB), Cauerstrasse 6, Erlangen 91058, Germany

We report on the implementation of a robust and reproducible electrochemical CV (ECV) characterization for the (Al,In)GaN material system. A Schottky-like contact is formed by electrolyte, wetting the area of the semiconductor surface delimited by a sealing ring. In reverse bias with common CV technique the concentration of donors and acceptors can be evaluated. Using a newly developed etch procedure, which we call "cyclic oxidation" nitrides can be etched (photo-)electrochemically (PEC) to yield reproducibly etched surfaces with mirror-like surface morphology at high etch rates (3 μm/h). This new etch procedure is not restricted to n-type nitrides, but works also for p-type nitrides. In the first time cycle the nitride semiconductor is electrochemically oxidized: UV illumination and forward voltage is applied to oxidize n-GaN and p-GaN, respectively. During this time cycle the electrolyte at etch area impoverishes. The established thin oxide film - essential for smooth etching - is dissolved by jet-pumping with fresh electrolyte during the complementary time cycle. The influence of the process parameters on the etch rate is discussed. The application of this new etch procedure to characterize various MOVPE and HVPE grown samples by CV-Profiling is presented.

Posters session

18:00 - 21:00

Theoretical model of transport characteristics of AlGaN/GaN High electron mobility transistors

poster
C-01

Asghar Asgari[1,2)], **L Faraone**[2)], **M Kalafi**[1)]

1) Tabriz University, 29 Bahman BLV, Tabriz 56544, Iran

2) The University of Western Australia, Perth, Australia

A realistic AlGaN/GaN heterostructure field-effect transistor model has been developed to predict the drain-source current and small-signal parameters such as drain conductance, transconductance, cut-off frequency and transit time with using nonlinear polarization effects, fully and partially occupied sub-bands in interface quantum well in self-consistent solution of Schrödinger and Poisson equations, taken into account self-heating, linearly voltage drops in ungated regime at device, more accurate mobility model and simulated electron drift velocity. The results out-coming from simulation have a good agreement with exist experimental data especially at linear regime.

Argon ion beam voltages influence the changes of microstructure and chemical composition of aluminum nitride films in dual ion beam sputtering system

poster
C-02

Hong-Ying Chen[2)], **Sheng Han**[1)], **Han.-C Shih**[2)]

1) Department of Finance, National Taichung Institute of Technology, Taichung 402, Taiwan, P.O.C.

2) Department of Materials and Science, National Tsing Hua University, Hsinchu, Taiwan, P.O.C.

Aluminum nitride films were prepared at room temperature by varying argon ion beam voltages from 400 V to 1200 V in a dual ion beam sputtering system. The X-ray diffraction spectra showed that ploycrystalline aluminum nitride films were synthesized above 800 V and the films consisted of both (100) and (002) crystallographic planes. The surface morphology of the films was nanoparticle-like morphology, which was observed by the field emission scanning electron microscopy, and the relative flat roughness ranged in 2-3 nm, which was measured by atomic force microscopy. The cross sectional photos of field emission scanning electron microscopy demonstrated that the nano-scaled granular structure was found above 600 V. The films thickness and its corresponding deposition rate increased with argon ion beam voltages. Regardless of whether the argon ion beam voltages changed, secondary ion mass spectroscopy

spectra indicated that the uniform chemical composition in aluminum nitride films. Nevertheless, from X-ray photoelectron spectroscopy measurement, the atomic concentration in aluminum nitride films was concentrated in aluminum-rich phases, and the aluminum concentration markedly increased with argon ion beam voltages below 1000 V, above which the concentration decreased slightly. Overall, aluminum nitride films can be prepared above 600 V at room temperature and the correlation between the microstructure and composition changes of aluminum nitride films and argon ion beam voltages is also discussed.

Charge transfer and thermodynamic stability of ternary nitride solid solutions

poster C-03

Vitalij Deibuk[1)], **Oleksandr Voznyy**[1)]

1) Chernivtsi National University (ChNU), 2 Kotsubinsky Str., Chernivtsi 58012, Ukraine

During the past years remarkable progress has been made in the development of optical and electronic devices based on the group-III nitrides. Using their alloys one can in principle obtain a material with a bandgap from 0.7 eV (InN) to 6.2 eV (AlN) with an intermediary value 3.44 eV (GaN). But it is impossible to make an alloy of group-III nitrides with any composition due to large miscibility regions. Thermodynamics of bulk and biaxially strained AlGaN, GaInN and AlInN alloys was investigated in "delta lattice parameter" (DLP) model. Calculated values of critical thickness for the films grown on GaN substrate agree well with the experimental data and Helmholtz mixing energy is calculated. Obtained T-x phase diagrams show critical temperature Tc=107K and its lowering under biaxial strain for AlGaN, which means the stability of these alloys. For GaInN Tc=1344K. At growth temperatures T=1000K the alloy is fully miscible only up to 5% composition of InN but it is metastable up to 20% of InN. Biaxial strain in thin films broadens the metastable region up to 76% of InN. For AlInN calculated critical temperature is Tc=1450K and it doesn't lowers under biaxial strain. At T=1000K the miscibility gap is 16%< x(In)<70% and becomes smaller under biaxial strain. Valence charge density distributions were calculated using model pseudopotential method in 32-atom supercells approach to take into account internal deformations, compositional disorder and structure relaxation. This allowed to understand the processes which take place during alloy formation. Stability of the solid solution is determined by two main factors: destabilizing charge redistribution under strain due to lattice mismatch of pure binary compounds and stabilizing charge transfer from less ionic bond to more ionic due to compositional disorder. Biaxial strain strongly affects the deformation induced charge redistribution, while it doesn't have effect on chemical charge transfer, thus stabilizing the system.

$Al_xGa_{1-x}N$ bulk single crystals: Temperature dependence of Al solubility

poster C-05

Janusz Karpinski[1)], **Peter Geiser**[1)], **Jan Jun**[1)], **S. M. Kazakov**[1)], **Peter Wägli**[1)], **Leonhard Klemm**[2)], **Bertram Batlogg**[1)]

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2) Isotope Geochemistry and Mineral Resources ETHZ, Zurich, Switzerland

Bulk $Al_xGa_{1-x}N$ and GaN single crystals have been grown, using (Ga,Al) alloys and pure Ga under high nitrogen pressure. Gas (up to 15 kbar) and solid pressure medium setups (up to 35 kbar) are used to provide the pressure required for phase stabilization. The solubility of Al was studied by growing crystals at various temperatures (1400 - 1750C). Mass spectrometric analysis reveals a rapidly increasing Al solubility at higher temperature. Thus, the growth temperature, together with the composition of the starting materials, serves as a parameter to control the Al content. For the maximum temperature of the gas autoclave (T=1600C) an upper limit of 2% Al is determined. Using the solid pressure medium setup (T_{max}=1750C) $Al_xGa_{1-x}N$ crystals with x=0.3 and a size of up to 0.6 x 0.4 x 0.2 mm^3 are synthesized. X-ray diffraction investigations confirm the growth of the single crystalline $Al_xGa_{1-x}N$ phase. Room temperature photoluminescence spectroscopy shows a blue-shift by up to 0.4 eV of the band gap related peak, further confirming significant Al substitution.

Influence of n-type doping on light emission properties of GaN layers and GaN-based quantum well structures

poster C-06

Marek Godlewski[1,7)], **Vitalii Y. Ivanov**[1)], **Elżbieta Lusakowska**[1)], **R. Bozek**[2)], **Saulius Miasojedovas**[3)], **Saulius Jursenas**[3)], **Karolis Kazlauskas**[3)], **A. Zukauskas**[3)], **Ewa M. Goldys**[4)], **Matthew R.**

Phillips[5)], **T. Bottcher**[6)], **S. Figge**[6)], **Detlef Hommel**[6)]

1) Polish Academy of Sciences, Institute of Physics, al. Lotnikow 32/46, Warszawa 02-668, Poland

2) Warsaw University, Faculty of Physics, Hoza 69 Str., Warszawa 00-681, Poland

3) Institute of Materials Science and Applied Research, Vilnius University (IMSAR, VU), Sauletekio 9, building III, Vilnius LT-2040, Lithuania

4) Division of Information and Communication Sciences, Macquarie University, Sydney, Australia

5) University of Technology (UTS), Broadway, Sydney 2007, Australia

6) University of Bremen, Institute of Solid State Physics, P.O. Box 330440, Bremen 28334, Germany

7) Cardinal S. Wyszynski University, College of Science, Warszawa, Poland

In this communication we discuss effects of n-type doping of GaN epilayers and InGaN/GaN quantum well structures. We evaluate the influence of n-type doping on a structural quality of the samples (using atomic force and scanning electron microscopy), on light emission intensity and on in-plane emission intensity variations. Possible mechanisms responsible for strong enhancement of light emission from doped samples are discuss based on the results of cathodoluminescence, photoluminescence (PL), PL kinetics and PL in-plane variations.

This work was partly supported by the DENIS program of European Union (G5RD-CT-2001-00566).

Annealing Behaviors of Void-like Defects in SiO_2/SiC Probed by Slow-Positron-Beam

Min Gong[1)], **Jing Yuan**[1)], **Haiyun Wang**[2)], **Weng Huiming**[2)], **Xudong Chen**[3)], **S. Fung**[3)], **C. D. Beling**[3)] poster C-07

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3) The University of Hong Kong, Hong Kong, Hong Kong

Silicon carbide has been realized to be one of powerful semiconductors. Various kinds of devices, including Schottky diodes, bipolar-transistors, MOSFETs and some IC units with good properties, have been manufactured using SiC. In these devices, SiO_2 films play important roles. However, since the existence of carbon atoms, qualities of thermal oxidation formed SiO_2 films on SiC wafers were far from as good as those on Si. The effects of impurities on the C-V characteristics of SiO_2/SiC have been investigated by using atoms sensitive probes such as the secondary ion mass spectrometry (SIMS) and the x-ray photoelectron spectroscopy (XPS). These analyzing techniques are not adequate for full understanding of characteristics of SiO_2/SiC interface and the structure of SiO_2 film since a large of void-type defects will form during thermal oxidation and post-annealing due to the removal or escape of C atoms and CO molecules.

In this work, the technique of Doppler broadening of positron annihilation spectroscopy (PAS) has been used to reveal information on void-type defects of SiO_2/SiC system. Variable-energy positron beam makes positrons to different depth in the sample. The value of the S parameter, which reflects the number of positrons annihilated with low momentum electrons, increases since the reduced electron density at open-volume defects narrows the momentum distribution.

The SiC materials used in the experiments were obtained from Cree. The wafers were 6H-SiC (0001) having basic nitrogen and aluminum dopant of 110^{17} cm^{-3} in n- and p-type samples, respectively. Dry oxidation was carried out at 1150C for 6 hours. Post-annealing was done at 1100C in nitrogen gas. The thickness of the SiO_2 film was about 0.6 nm measured by ellipsometry. Variable energy (0-20 keV) positron beam made the positrons stop and annihilate at different depth from the SiO_2 surface to the SiC bulk. The measurement results obviously showed that the S-parameters

[ABSTRACT TRUNC

[ABSTRACT TRUNCATED TO 2000 LETTERS]

Microstructure of homoepitaxially grown InGaN/GaN, violet light emitting laser diodes.

Lucja Gorczyca[1)], **P Prystawko**[1)], **Robert Czernecki**[1)], **Mike Leszczynski**[1)], **T. Suski**[1)], **Till Riemann**[2)], **Juergen H. Christen**[2)], **Piotr Perlin**[1)], **Sylwester Porowski**[1)], **Izabella Grzegory**[1)] poster C-08

1) Polish Academy of Sciences, High Pressure Research Center (UNIPRESS), Sokolowska 29/37, Warszawa 01-142, Poland

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In this work we present the optical micro-analysis of violet light emitting laser structures grown on bulk GaN substrates. These lasers, because of high structural quality and low defect concentration have a great potential as a high power sources of violet and UV light. It is however, an open question whether the reduced density of dislocation influences homogeneity of InGaN quantum wells and what degradation mechanisms are important for aging processes in these devices.
We carried out our investigation using new and degraded (subdue to aging precedure) laser diodes grown by MOVPE method on high-pressure synthesized bulk GaN crystals. We compare the results with these obtained by MBE on identical substrates. The active region of our lasers consists on an InGaN/InGaN multiple quantum well (MQW) emitting blue light around 405nm, placed between GaN or InGaN guiding layers and GaN/AlGaN superlattices as n- and p-cladding. Laser stripes are 600μm long of width between 5μm and 20μm. The microscopic properties of these completely processed laser structures and MQW are analysed by spectrally resolved cathodoluminescence microscopy (CL). The individual layer sequence of the laser was revealed by cross-sectional CL, showing, e.g., the luminescence of the cladding layers, the MQW, and the p-GaN. The lateral homogeneity of the whole laser was measured by highly spatially resolved plan-view CL imaging. We studied structures containing InGaN quantum wells of various widths (from 3 up to 17 nm). We demonstrate an outstanding homogeneity of the light emission from the above mentioned structures which may imply the reduced In composition fluctuations in the high crystalline structures. Finally, we will also comment on the determination of post-aging defects present in our laser structures.

Microstructure Strength Relationship in Microalloyed Cast Steels

poster C-09

Barbara Kalandyk[1)]

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The staircase test block with 20, 45 and 75mm wall thickness were performed on low alloyed Mn-Ni cast steels microalloyed by V or V + Nb additions. Precipitations of carbo -nitrides in these alloys are related to the different cooling rate and segregation during solidification process.
The effects of V + Nb nanoparticles and heat treatments increased yield strength up to 850-950 MPa at the elongation above 8-10 %. Particle size changes from 10 to 60nm and depends on the cooling rates (0,15 - 0,9 0C) and the process of microalloying. Carbo - nitrides are distributed mainly in one phase of mikrostructrue.

Thermally stable Ru-Si-O gate electrode for AlGaN/GaN HEMT

poster C-10

Eliana Kaminska[1)], **Anna Piotrowska**[1)], **Artur Szczesny**[1,5)], **Radoslaw Lukasiewicz**[1)], **Andrian V. Kuchuk**[1)], **Krystyna Golaszewska**[1)], **Renata Kruszka**[1)], **Adam Barcz**[1,2)], **R. Jakieła**[2,4)], **Elzbieta Dynowska**[2)], **Anna Stonert**[3)], **Andrzej Turos**[3,4)]

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Reliable Schottky contact for AlGaN/GaN high electron mobility transistor (HEMT) should use low resistivity, large work function metal. Moreover, the metallisation for this application should withstand high-temperature treatments during device processing (realisation of self-aligned HEMT) without change of structure, electrical conductivity and composition, and be stable in contact with the semiconductor. Recently, several studies have demonstrated the applicability of RuO_2 as Schottky contact to n-GaN. Ru and RuO_2 are high melting point materials, characterised by low resistivity and work function > 5 eV.
With an eye on high temperature applications we have chosen to study thermally stable, electrically conducting, amorphous Ru-Si-O films being a combination of conducting RuO_2 and SiO_2. We compare Ru, RuO_2 and Ru-Si-O Schottky contacts fabricated on n-GaN and AlGaN/GaN HEMT heterostructure. Ti/Al ohmic contacts were prepared for this study. Ru, RuO_2 and Ru-Si-O layers were deposited by sputtering, using either Ru or RuSi target, in a mixture of Ar and O_2. Heat treatments were done at 400-1000^{0}C in either O_2 or N_2 flow. The electrical properties of contacts were extracted from I-V and C-V characteristics. Contact microstructure was analysed by high-resolution XRD, SIMS and RBS.
Crucial point during the deposition was to optimise the O_2/Ar ratio and the working pressure with regard to thin film resistivity and stress.
Of three investigated metallisations, Ru films yielded the lowest potential barriers. Although barrier

heights of RuO2 and Ru-Si-O Schottky contacts were very similar, amorphous Ru-Si-O contact exhibited significantly lower reverse leakage current and superior thermal stability. We will discuss in detail the behaviour of Ru-based contacts in terms of electronic interactions at either crystalline or amorphous metallisation/semiconductor interface.
Work supported by the grant from the State Committee for Scientific Res.3 T11B 008 026.

TaSiN, TiSiN and TiWN diffusion barriers for metallization systems to GaN

poster C-11

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The wide band-gap nitrides are ideally suited for high-speed high-temperature applications. The field of nitride processing technology is still very much in its infancy and a large number of novel process steps are being investigated. In particular, successful development of such devices requires reliable contact technology.

The objective of this work was to develop diffusion barrier for thermally stable metallization systems to GaN. Since gold overlayer is a commonly used component of metallizations, fabrication of efficient barrier layer against Au migration/reaction was of primary concern.
High melting point, conducting thin films of of Ta-Si-N, Ti-Si-N and Ti-W-N were compared as barrier materials. They were deposited by reactive magnetron sputtering in Ar/N_2 atmosphere, from Ta_5Si_3, Ti_5Si_3 and 10%Ti-90%W targets, respectively. The effects of sputter-deposition parameters on the resistivity and the microstructure of barrier layer have been investigated. Applicability to both p-type (Au/Pd and Ni/Au) and n-type (TiAl) metallisations to GaN has been analysed. Heat treatments were performed in a rapid thermal annealer under flowing N_2. Electrical characterisation of metal/semiconductor contacts involved measurements of I-V characteristics and specific contact resistance. Reactions at metal/semiconductor interface were analysed by Rutherford backscattering method, secondary ion mass spectroscopy, x-ray diffraction and TEM.
We show that for appropriate sputter deposition conditions, amorphous Ta-Si-N, Ti-Si-N and Ti-W-N films can be obtained. Moreover, they remain in amorphous phase after annealing up to 750-900^{0}C, effectively suppressing the interaction between GaN and Au.
This work was carried out with support from EC under grant G5RD-CT-2001-00566-DENIS

GaN growth by Sublimation Sandwich Method

poster C-12

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Sublimation Sandwich Method (SSM) [1] has proven successfully in the growth of both bulk AlN and SiC [2,3] and shows promise for growth of bulk GaN crystals as well. In our investigations, GaN layers were grown by the SSM. Experiments were carried out in a tubular quartz reactor with induction heating at temperatures from 1100OC to 1250OC. GaN layers, grown on Al2O3, obtained by MOCVD were used as the substrate. The area of deposition was 10x10mm. Monocrystaline GaN layers were obtained under atmospheric pressure during a deposition time from 5 to 60 minutes. GaN powder was used as the source of gallium and ammonia as the source of nitrogen. GaN powder and the substrate were placed in a quartz boat on top of a graphite cylinder, which was the heating element. To ensure gallium transfer, temperature gradient was employed between the gallium source and the MOCVD substrate. The obtained GaN layers possessed irregular surface morphology with a thickness range up to 1mm. Raman spectroscopy and X-ray studies were used to investigate the films.

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Recombination Dynamics in GaN/AlGaN Low Dimensional Structures Obtained by SiH_4 Treatment

poster C-13

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We present optical properties of low dimensional quantum dot-like GaN/AlGaN structures, which were obtained in a low-pressure MOVPE reactor. A primarily grown AlGaN layer had been exposed to SiH_4. On the SiH_4-treated surface GaN grew on distinctly separated island sites and was capped with a second AlGaN layer.
Photoluminescence (PL) shows two bright PL bands (P1, P2) and one weak (P3) PL band at energies of 3.48 eV, 3.44 eV and 3.35 eV, respectively. Micro-photoluminescence measurements reveal that these bands consist in fact of many sharp lines coming from small spots on the sample. Such behavior is characteristic for quantum dots or islands.
Time-resolved PL shows that the P1, P2 and P3 bands have lifetimes of about 0.1 ns, 0.5 ns and 1.3 ns, respectively. The P2 and P3 bands show significant spectral shifts with time. For example, the P2 band shifts from 3.445 eV at t = 0.1 ns down to 3.430 eV at t = 2.5 ns. As confirmed by power dependent measurements, the spectral shifts are partially due to state filling effects. State filling is usually observed in QDs due to their low density of states. During few hundreds of ps, electrons relax from higher to lower states and the average energy of the QD band decreases with time. Then PL emission from the ground states of QDs can be measured and analyzed. For the P2 band, at about 3.43 eV, a ground state decay rate of about 2.4 ns^{-1} has been determined.
Temperature dependent PL measurements show S-shape dependence of the PL energy vs temperature for the P2 band. On the other hand, the P1 peak shifts monotonically to lower energy in agreement with the energy band-gap shrinkage. The time-resolved measurement shows the mechanism of this effect. Up to 50 K, increase of temperature leads only to promotion of some electrons to high-energy states. But above 50 K the decays are faster due to the thermal escape of carriers. Since the thermal escape is faster in the case of high-energy states, the average PL energy decrease.

Interaction of Mn and Ti atoms with GaN surface - a resonant photoemission study

poster C-14

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The aim of the reported work was investigation of Mn/GaN and Ti/GaN interface formation in order to reveal differences and similarities between interaction of these transition metals (TM) with GaN(000-1)-(1x1) surface. In both investigated systems doping with TM atoms leads to important modifications of properties. Annealing of Mn/GaN is considered as a technique suitable for fabrication of a ferromagnetic semiconductor with a Curie temperature higher than room temperature. Ti/GaN system is important as an element of ohmic contacts in nitride-based electronic devices. Thus, knowledge of details of interaction between these TM and GaN are crucial for applications as well as for basic research of electronic structure of open-shell atoms in nitrides. Resonant photoemission experiments were performed in order to compare interactions between Mn or Ti atoms and clean GaN surface, to reveal compounds formed at the interfaces and to relate them to changes in the density of states distribution in the valence bands of Mn/GaN and Ti/GaN formed under UHV conditions.
The clean surfaces of bulk GaN crystals were prepared in situ by repeated cycles of Ar+ ion sputtering and annealing. The sets of photoemission spectra were measured for clean GaN surface, as a function of TM coverage and after annealing of these systems. Contributions of TM 3d states to the valence band of Mn/GaN and Ti/GaN systems were derived from the spectra taken for photon energies near to TM 3p-3d excitation. Mn 3d contribution to the emission from the valence band turned out to be similar to that characteristic of Mn built into tetrahedrally coordinated semimagnetic semiconductors. Ti deposition and annealing led to formation of Ti-N compound - the valence band became similar to that observed for titanium nitride. Summarizing, the acquired results enabled us to prove strong interaction of Mn and Ti

with GaN, to observe GaN surface disruption and reactive interface formation in Ti/GaN and Mn/GaN.

Spontaneous Superlattice Formation in MOCVD Growth of AlGaN

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poster C-15

It has been found that AlGaN layers grown by MOCVD on sapphire substrates form superlattice (SL) along growth direction. Transmission electron microscopy (TEM), high resolution X-ray diffraction and atomic force microscopy (AFM) found the phenomenon. The amount of Al in AlGaN layer oscillates between a few percent to about 50%, thus by about one order of magnitude. The period of oscillations range from 30 nm to 50 nm depending on the growth condition. TEM and AFM reveal a homogenous lateral distribution of the SL. The vertical extension covers the total layer thickness.

It has been found that the appearance of SL depends on the thickness of the buffer layer on which the growth of AlGaN layer is initiated. The thinner buffer layer leads to the uniform growth of AlGaN layer without oscillating character. On the other hand the thicker buffer layer stimulate the oscillating growth, which persist throughout the whole growth process. The possible mechanism indicating oscillating character of reactions taking place on the surface of the grown AlGaN layer will be discussed.

HARDNESS AND LUBRICATION PROPERTIES OF CN_X THIN FILMS GROWN BY CLOSE FIELD UNBALANCED MAGNETRON SPUTTERING

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poster C-16

Carbon-Nitride (CN_x) film is a material that may successfully compete with DLC coatings, which have high hardness, high wear resistance, and a low friction coefficient. CN_x films were prepared on silicon substrate by a Close Field UnBalanced Magnetron sputtering with a graphite target and using the N_2-Ar mixture gas. It is obtained parameters on the deposition rate and investigated effect of negative DC bias voltage and N_2 Pressure. The Characteristic of the carbon-nitride films were investigated of the microstructure, chemical composition, surface morphology, surface free energy, and by physical properties by measurements of Raman spectroscopy, FT-IR(Fourier transform infrared), EDX(Energy Dispersive X-ray analysis), AFM(Atomic Force Microscopy), contact angle, nano-indentation and friction coefficient.

Nitridation of InP(100) surfaces studied by synchrotron radiation

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poster C-17

InN is the least studied of III-N materials which are currently the most promising semiconductors for opto- and micro-electronic applications. The devices performance strongly depends on the quality of the interface between layers. Thus a deep understanding of the early stages of nitridation and following nitride growth is required for improvement of devices efficiency. The nitridation process can be used to produce thin passivating layers and insulating films for fabrication of metal-insulator-semiconductor structures

(MIS)
We report results on the InP(100) surfaces nitridation. The nitridation process consist of two main steps : firstly the creation of metallic indium droplets by Ar^+ ionic bombardment of the InP(100) surface then the consumption of these droplets by the atomic nitrogen flow which entails the formation of one or two nitride monolayers. The nitrogen flow is produced by a glow discharge source (GDS).
This nitridated structures and its evolution under annealing at 450C and 500C have been studied with synchrotron radiation at the Elletra Material Science Beamline in Trieste (Italy). In_{4d}, P_{2p} and N_{1s} core levels have been specially observed as well as the evolution of the valence bands structures at different beam energies (hν = 50 and 190 eV).

Close-Spaced Crystal Growth and Characterization of BP Crystals

poster C-18

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The present study was undertaken to determine if BP crystals could be produced by a simpler technique, close-spaced vapor transport (CVST). This technique has proven very successful in achieving very high growth rates for a wide variety of materials including CdTe, Cu(In,Ga)Se_2, and GaP. Boron phosphide crystals were prepared on silicon and sapphire substrates using CSVT and characterized by Raman spectroscopy, scanning Auger microscopy, x-ray diffraction, and optical microscopy. Amber colour, polycrystalline BP crystals were produced by the sublimation of BP powder from 1050 to 1450 C in an argon atmosphere. The crystal size increased and the crystal density decreased with increasing temperature. Well-faceted crystals were produced at an intermediate temperature of 1200 C. A fibrous mass of fine whiskers, only loosely attached to the substrate were produce at the highest temperature. The peak position of the Raman LO mode of the BP crystals was shifted to higher wavenumbers than the BP powder source, suggesting that the crystals were compressively strained.

The atomic structure of defects formed during doping of GaN with rare earth ions

poster C-19

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Transmission electron microscopy (TEM) is an unique technique to perform structural investigations with atomic resolution. In this work we present our studies on structure changes of GaN doped with different rare earth ions (RE) by ion implantation and molecular beam epitaxy (MBE). Due to its wide and direct band gap GaN is an ideal host material for RE ions that have very interesting optical properties. Changing RE we can obtain luminescence covering the whole visible light spectrum. We present the influence of different doping conditions using each technique on the characteristic stacking faults formation. We take into account different RE and their concentration. For MBE doped layers, we notice that the increase of the RE concentration above a threshold leads to the disruption of the GaN stacking sequences. We investigate the connection of this disruption with possible RE segregation by measuring the local lattice parameter changes by HRTEM. During doping by implantation, typical stacking faults are formed around the projected stopping power. We present their detailed investigation and we analyze their evolution versus implantation dose (10^{14}-10^{16} at/cm^2) and energy (150-300 kV).

Transmission electron microscopy structural investigations of Tm implanted GaN

poster C-20

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For the last few years much work has been done in the field of semiconductors doped with different rare earth ions (RE) due to their interesting optical properties. By changing the RE one can obtain luminescence covering the whole visible light spectrum. Due to its suitable physical, chemical and mechanical properties GaN seems to be promising material as a host for RE. As a wide and direct band gap semiconductor significantly reduces thermal quenching of the RE luminescence. Ion implantation is one of the techniques that can be used for doping GaN with different RE ions. It was shown that GaN is a very resistant material to irradiation damage, nevertheless during the implantation a lot of damage is created in the implanted areas. Using transmission electron microscopy (TEM) we carry out a structural characterization of GaN implanted with Tm ions. Our aim is to determine optimal conditions of implantation process and further annealing. We present results from samples implanted with different energies (150-300 kV), fluences (0.2-2.2x10^{15} Tm/cm^2) and temperatures (20-500^{o}C). The influence of the dose, energy, temperature and the annealing on the structural quality of the layers will be discussed in detail.

Automated Electrochemical CV-Profiling of semiconductor structures on wafer scale

poster C-21

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A novel equipment tool to perform electrochemical CV profiling on semiconductor structures is given. The setup is PC controlled and fully automated to handle small sample sizes from some millimetre in diameter up to 6 inch wafers. Fully automated loading of the electrochemical cell, fluid handling, drying and unloading are incorporated into the setup. Using a wafer stepper as an option even surveys on wafer scale are feasible. Especially for the case to profile nitride semiconductors, the hardware makes use of a etch technique named "cyclic oxidation" recently developed by us. This new etch procedure results reproducibly in mirror-like etched surfaces for n-type as well as p-type material. Characterization of various semiconductor samples, including Silicon, III-V-heterostructures and III-Nitrides will presented - showing some typical epitaxial layer structures for LEDs, HEMTs or solar cells.

Thursday, September 9th

Thursday morning

09:00 - 10:30

Main Building, room 206

GaN Crystal Growth and Light Emitting Devices

09:00 - 09:45 invited oral

Shuji Nakamura[1)]

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Roughened surfaces of light-emitting diodes (LEDs) provide substantial improvement in light extraction efficiency. By using the laser lift off (LLO) technique followed by an anisotropic etching process to roughen the surface, an n-side up GaN-based LED with a hexagonal "cone-like" surface has been fabricated. The enhancement of the LED output power depends on the surface conditions. The output power of an optimally roughened surface LED showed a two to three-fold increase compared to that of an LED before roughening.

Nonpolar A- or M-plain GaN has been grown by hydride vapor phase epitaxy (HVPE). Using a lateral epitaxial overgrowth (LEO), an uniform mirror-like surface has been obtained. The device perforamnce grown on nonpolar GaN templates will be described.

09:45 - 10:30
invited oral

"Classic" and Novel Methods of Dislocation Reduction in Heteroepitaxial Nitride Layers

Jacek Jasiński[1)]

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One of the main problems of nitride-based technology is the lack of commercially available large native substrates. Commonly used substrates, such as sapphire or 6H-SiC, are poorly matched in terms of lattice parameters and thermal expansion coefficients. This leads to high densities of threading dislocations (typically in the range of 10^{10}-10^{11} cm^{-2}), which seriously limits the performance of nitride-based devices. Dislocations are believed to reduce the mobility and lifetime of electrical carriers, provide paths for diffusion of impurities and serve as leakage current pathways. They also seem to be responsible for the degradation of nitride laser structures. To address these problems several different methods of dislocation density reduction have been proposed in recent years. Early methods utilized growth of buffer layers and were aimed at controlling the number of nucleation sites and lowering the strain at the interface area. They brought down the dislocation density to the range of 10^8-10^9 cm^{-2}. However, further reduction was possible due to the development of other methods. First group of such methods, known as epitaxial lateral overgrowth methods, are designed to change the dislocation propagation from vertical to horizontal redirecting them from the active layer of the nitride structure. In other methods an insertion of intermediate layers or growth of thick nitride layers increases the probability of interactions between dislocations resulting in their combination and/or annihilation. There are also methods that attempt to combine these approaches. They include growth on porous substrates or growth interruption combined with in situ surface treatment with anti-surfactants. In this paper all different methods will be reviewed and compared. Their advantages and limitations, as well as, specific mechanisms of dislocation reduction will be discussed.

10:30 - 11:00

Coffee break

11:00 - 12:30

Morning session

Main Building, room 206

11:00 - 11:20
oral

Application of picosecond four-wave mixing and photoluminescence techniques for investigation of carrier dynamics in bulk crystals and heterostructures of GaN

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We studied defect-density governed photoelectric parameters in GaN heterostructures and bulk crystals by using the time-resolved techniques of picosecond four-wave mixing (FWM) and photoluminescence (PL). A few mm-thick GaN layers were grown on 6H-SiC or 4H-SiC substrates by hot-wall MOCVD with varied growth parameters, while the 270-mm-thick free-standing bulk crystal was grown by HVPE on a two-step epitaxial lateral overgrown GaN template on sapphire. FWM was realized by recording transient free carrier gratings at interband excitation at 355 nm wavelength and probing their kinetics by the delayed probe beam at 1064 nm. For spectrally and temporally resolved PL, the samples were excited at 266 nm

and luminescence was measured in backward geometry. The excitation density varied up to a few mJ/cm^2, what allowed us to study effects at nonequilibrium carrier density from 10^{18} up to 5x10^{19} cm^{-3}.
Simple correlation between photoelectrical and nonlinear optical properties of FWM allowed us to determine carrier lifetimes τ_R and diffusion coefficients D in differently grown samples. The τ_R increased value from 100-300 ps in the epilayers up to 3 ns in the bulk crystal, while the D value varied from 1.5-1.7 cm^2/s up to 2-2.8 cm^2/s, correspondingly. We attribute the enhanced values of D and τ_R to screening of potential barriers around dislocations and ability of carriers to avoid nonradiative recombination at dislocations.
We observed a novel feature of FWM in GaN, namely a complete saturation of its diffraction efficiency at the excitation energy 0.5 - 2 mJ/cm^2, dependent on sample. This peculiarity of FWM correlated with the spectra and intensity of stimulated PL, and pointed out that the origin of the FWM saturation is the favorable conditions for ultrafast stimulated recombination. The kinetics and spectra of PL are compared with the features of FWM to develop complementary characterization of the highly-excited nitrides.

Anomalous behaviour of the photoluminescence from GaN/AlGaN quantum wells

11:20 - 11:40
oral

Barbara Chwalisz[1], Andrzej Wysmołek[1], Krzysztof P. Korona[1], Roman Stępniewski[1], Czeslaw Skierbiszewski[2], Izabella Grzegory[2], Sylwester Porowski[2]

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Temperature and excitation power behaviour of the emission from low dimensional structures can provide important information about localisation effects, strain and electric field distribution. Usually it is difficult to separate the contribution of the particular effect on the observed photoluminescence. In order to understand the influence of those effects photoluminescence measurements in the temperature range 4.2-300K on GaN/AlGaN quantum wells (QW) of different width were performed.
The investigated structures consisted of several GaN QWs of nominal width: 1nm, 1.5nm, 2.5nm, 4nm and 6nm embedded in Al0.15Ga0.85N barriers. Energy positions of the emission observed for QW wells with different width vary from 3.14eV (for 6nm QW) up to 3.52eV (for 1nm QW) as the result of strong built-in electric fields. The increase of the excitation power results in the blue shift of the widest well and the red shift of the narrowest well emission. The magnitude and direction of the energy shift depends on the temperature.
Moreover, the temperature behavior of the QWs emission is entirely different from that observed for unstrained bulk GaN. The particular effect depends on the well width. The observed emission energies exhibit so-called S-shape like temperature behavior. Such dependence is usually interpreted as due to localization of excitons in the QW caused by well thickness fluctuations and/or structural disorder.
The observed results can be understand assuming that not only potential fluctuation but also built-in electric field and strain effects must be taken into account. The role of the particular mechanisms is discussed.

Resonant tunneling and intersubband absorption in AlN-GaN-superlattices

11:40 - 12:00
oral

Esther Baumann[1], Fabrizio R. Giorgetta[1], Daniel Hofstetter[1], H. Wu[2], W. J. Schaff[2], L. F. Eastman[2], Lutz Kirste[3]

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We report on intersubband absorption and vertical transport phenomena in regular GaN-AlN-based superlattice structures grown by MBE. We found that for barrier thicknesses larger than about 25 A, the optical intersubband absorption peaks at a much smaller energy than the photovoltage. A simple model based on the oscillator strength of the corresponding transition and the Wentzel-Kramers-Brillouin-method can qualitatively explain the experimental facts. For barrier thicknesses on the order of 20 A, a much smaller shift between the measured intersubband absorption and photovoltage peaks is observed. This energy difference is due to the strong barrier height dependence of the tunneling probability, which favors vertical transport at the upper edge of the minband formed by the excited states.
For the sample with the smallest well thickness of 17 A, we were able to detect light at 1.55 μm up to room temperature. Due to a considerable surface roughness, p- and s-polarized detector signals were almost identical in this particular device and a Gaussian line broadening of the photovoltage spectrum was observed.

Furthermore, the transient behavior of the DC component of the photovoltaic signal under strong illumination with a halogen lamp was investigated at different temperatures. Besides the intersubband absorption/tunneling process contribution to the signal, a strong influence of optical quenching and persistent photoconductivity due to midgap defects in GaN occurred under illumination of the sample with energies above 1.1 eV.
Similar investigations on lattice-matched InAlN/GaN MOVPE grown superlattice structures were carried out. They revealed valuable information about the conduction band discontinuity of this novel material combination.

12:30 - 14:00

Lunch break

14:00 - 15:30

Thursday afternoon

Main Building, room 206

14:00 - 14:45
invited oral

Characterisation of GaN grown by HVPE

Bo Monemar[1)]

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The Halide Vapor Phase Epitaxy (HVPE) Method is at the moment the most popular technique for the development of bulk GaN substrates. This process is still in a rather early stage, but the material produced is of interest for studies of the HVPE process as well as the physical properties of bulk GaN. The HVPE growth of GaN in different laboratories is so far essentially done on homemade growth equipment, meaning that growth conditions in different laboratories cannot be directly compared. We shall give some materials characteristics related to the growth conditions in our growth systems, related to structural defects but mainly optical properties. The residual impurities and their corresponding optical signatures will be discussed. In particular residual acceptors are of interest.

14:45 - 15:05
oral

Electroreflectance and photoreflectance studies of AlGaN/GaN heterostructure with a QW placed inside AlGaN layer

Aneta Drabińska[1)], **Krzysztof Pakuła**[1)], **Jacek Baranowski**[1)], **Ilona Frymak**[1)]

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The investigated $Al_{0.07}Ga_{0.93}N$/GaN heterostructure was grown on a thick GaN:Si layer by MOCVD. Inside the AlGaN barrier there was placed AlGaN quantum well. The structure was covered with a low temperature GaN cap layer. On the investigated structure there were performed photoreflectance (PR), electroreflectance (ER) and X-ray diffraction.
In the PR spectra there are present three features; one connected with transitions in GaN layer, second are Franz-Keldysh oscillations (FKOs) from AlGaN barrier, and the third line connected with transitions within AlGaN QW.
The ER measurement was performed for constant bias from 2 V to -7 V. In the spectrum there are also visible three features. For forward and low reverse bias there is visible line originating from AlGaN QW which due to the Stark effect is changing its position to lower energies. For low reverse bias there are visible two sets of FKOs from AlGaN barrier corresponding to two different values of electric field. This is due to the occupancy of the AlGaN QW and the presence of electric charge in AlGaN barrier. For higher reverse bias there are visible only one set of oscillations from AlGaN barrier, but in the spectrum appear FKOs from GaN layer. For this bias range the difference between calculated values of electric fields in GaN and AlGaN layers is connected with the concentration of polarization charge located in AlGaN/GaN interface which was found to be equal 2.5×10^{12} cm^{-2}. This charge is induced by spontaneous and piezoelectric polarization present in those layers.
From the X-ray diffraction there were obtained lattice constants of AlGaN and GaN layers which allow to calculate the piezoelectric part of polarization. Combining this with ER results it was possible to obtain the difference of spontaneous polarization between GaN and AlGaN layer equal to 0.0030 C/m^2. This value is in very good agreement with the theoretical predictions.

Built-in electric fields in group III-nitride light emitting quantum structures

15:05 - 15:25
oral

G. Franssen[1], T. Suski[1], Piotr Perlin[1], R. Bohdan[1], A. Bercha[1], P. Adamiec[1], F. Dybała[1], W. Trzeciakowski[1], L. Dmowski[1], S. P. Łepkowski[1], H. Teisseyre[1], Karolis Kazlauskas[2], G. Tamulaitis[2], A. Žukauskas[2], P Prystawko[1], Robert Czernecki[1], Mike Leszczynski[1], Izabella Grzegory[1], Sylwester Porowski[1]

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In light emitting devices based on GaN, InN, AlN and their alloys, the presence of a built-in electric field (caused by spontaneous and piezoelectric polarization effects) has a detrimental effect on the efficiency of the device. Indeed, built-in electric fields induce a spatial separation of electrons and holes in the quantum wells of the active region, thereby considerably reducing the radiative recombination rate and, ultimately, the device efficiency.
The aim of this work is the demonstration of the feasibility of high hydrostatic pressure experiments as a tool for the determination of the presence of electric fields in group III-nitride structures. Indeed, the presence of electric fields can be sensitively detected through a drastic reduction of the observed shift of the emitted light energy as a function of pressure with respect to the pressure evolution of the band gap in bulk material. This reduction can be used as a fingerprint of the presence of a built-in electric field.
In this work, we first discuss the behavior under the influence of built-in electric fields and pressure of a variety of quantum structures. After this, we proceed to a proposed design of laser diodes (grown on bulk GaN crystals) based on quantum structures with a reduced internal electric field. For that purpose the appropriate screening of the built-in electric fields by doping and/or injection of charges is applied. In these devices, we show a bulk-like value of the pressure coefficient in the high current injection regime. This result demonstrates the absence of built-in electric fields in our laser diodes, showing that the proposed laser diode design helps to avoid the detrimental effects of the presence of electric fields (such as the reduction of efficiency due to carrier separation and the reduction of laser gain). In the final part, we discuss the particular roles of electric field screening by injected carriers on one hand, and doping on the other.

Coffee break

15:30 - 15:50

Afternnon session - continued

Main Building, room 206

15:50 - 17:20

Monte Carlo simulation approach for a quantitative characterization of the band edge in InGaN quantum wells

16:00 - 16:20
oral

<u>Karolis Kazlauskas</u>[1], G. Tamulaitis[1], Saulius Jursenas[1], A. Zukauskas[1], M. Springis[2], Yung-Chen Cheng[3], Hsiang-Cheng Wang[3], Chi-Feng Huang[3], C.C. Yang[3]

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3) Graduate Institute of Electro-Optical Engineering and Department of Electrical Engineering, National Taiwan University 1, Roosevelt Road, Sec. 4, Taipei, Taiwan, P.O.C.

InGaN is the key compound of the state-of-the-art blue-UV light emitting diodes and laser diodes. InGaN layers have inherent compositional fluctuations resulting in potential fluctuations, which localize carriers/excitons so that their nonradiative recombination is inhibited and light emission efficiency is increased. However, such an inherent disorder obscures the absorption edge of InGaN, which is a fundamental optical property.
In this report we apply photoluminescence (PL), PL excitation, and photoreflectance spectroscopy to characterize the absorption edge of InGaN multiple quantum wells with different In content (20-30%) and propose Monte Carlo simulation of exciton hopping to quantitatively describe band-edge dynamics in the temperature range of 10-300 K and to estimate the scales of potential fluctuations in the alloy.

The simulation yielded a temperature dependence of the Stokes shift between the PL peak and the average exciton position as well as of the PL linewidth. We described quantitatively the experimental data by introducing a double-scale potential profile. One potential fluctuations scale reflects formation of In-rich regions with different average In content, while another scale corresponds to the variations of local indium content within a single In-rich region. Moreover, the Monte Carlo approach enabled us to estimate the band edge energy in the entire temperature range. The determined band edge was found to correspond to that obtained from the photoreflectance measurements within the experimental uncertainty. Increased indium content in InGaN alloy resulted in an increase of the both scales of potential fluctuations.

16:20 - 16:40
oral

The fundamental absorption edge of high crystalline quality GaN and that of amorphous GaN grown at low temperature

Pawel Trautman[1], **Krzysztof Pakula, Jacek M. Baranowski**

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The absorption coefficient of GaN immediately above the band gap is equal to 1.0x10^5 cm^{-1}. It implies that GaN layers of thickness ranging from 200 to 500 nm are required for optical transmission measurements with light of energy larger than the band-gap. A few hundred nm thick GaN layers grown on sapphire have a very high defect density due to lattice mismatch between GaN and sapphire. Therefore, the growth of GaN layers of thickness and quality suitable for measurements of optical absorption is very difficult. In order to overcome this obstacle, heterostructures consisting of a 2 μm thick $Al_{0.08}Ga_{0.92}N$ layer and, on top of it, of a thin GaN layer have been grown in a single run of a MOVPE reactor. The absorption spectra of these samples taken at 12 K show three well resolved excitons on the onset of the fundamental absorption edge of GaN. These spectra have the property of light-induced narrowing. The spectral range of absorption spectra of GaN grown on AlGaN layer is limited by the absorption edge of AlGaN. In order to measure the spectra in a broader spectral range and to investigate the influence of the growth temperature on properties of GaN, a 500 nm thick layers of GaN have been grown. The layers grown at 500C, 800C, and 1100C have mirror-like surfaces, and their thicknesses were determined from the spacing of the interference fringes in transmission spectra. The layer grown at 1100C has a step-like absorption edge at 3.5 eV with an excitonic structure. The layer grown at 800C has broad absorption edge at 3.5 eV and lacks the excitonic structure. The absorption coefficient of the layer grown at 500C increases approximately linearly with energy above 2.8 eV. The absorption coefficient for energies larger than 4.0 eV of the layers grown at 500C and 800C is much larger than that of the layer grown at 1100C. It seems that it is due to a relaxation of momentum selection rule for optical absorption in the amorphous GaN layers.

16:40 - 17:00
oral

Bowing of epitaxial structures grown on bulk GaN substrates

Marcin Sarzynski[1,3], **Marcin Krysko**[1], **Jaroslaw Domagala**[2], **Robert Czernecki**[1], **Grzegorz Targowski**[1], **Krzysztof Krowicki**[1], **P Prystawko**[1], **Boleslaw Lucznik**[1], **Izabella Grzegory**[1], **Sylwester Porowski**[1], **Mike Leszczynski**[1]

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The main activity of the HPRC Nitride Processing Lab is the fabrication of blue-laser diodes (LDs), and blue and UV light-emitting diodes (LEDs). Also, a fundamental research on the growth and physical properties of the nitrides is carried out.
In the present work, we investigated mechanical properties of bulk GaN substrate crystals and epitaxial structures grown on them. Growth methods were HVPE (Halide Vapor Phase Epitaxy) and MOVPE (Metalorganic Vapor Phase Epitaxy). Measuring techniques included Laser Profilometry for the curvature and X-Ray diffraction for the material parameters. Additionally, the EPD (Etch Pit Density) and the PL (Photoluminescence) were used. We developed a device that allows in-situ curvature measurements. It is based on the well-known MOS (Multi-beam Optical Sensor) technique. We also developed a simple, low cost laser profilometer for the ex-situ curvature measurements.
The aim of the present work was to establish relations between the material parameters such as the composition, lattice constant, layer thickness, dislocation density, and the bowing of structures. This is important, since large bowing and the stress can significantly affect the device parameters and is a big problem in device processing. Typically, epi-ready bulk GaN substrates have a radius of bowing of about 0.5 to 1.0 meters. This is due to the gradient of free-electrons concentration and the influence of polishing. Additional bowing is introduced by the growth of AlGaN and InGaN layers, due to the lattice mismatch. To give an example, 0.4μ m thick layer of $Al_{0.1}Ga_{0.9}N$ on bulk GaN substrate causes bowing of about 0.25

m. This is the value typically seen in our LD structures.
To reduce the value of the bowing, various techniques can be used. Currently, we focus on mechanical properties of bulk GaN substrate crystals thickened by the HVPE method, as well as the AlGaN/InGaN layers and their influence on the bowing.

Study of photo- and electro-luminescence related with Er^{3+} ions in GaN:Er

17:00 - 17:20
oral

Maciej Wojdak[2], **Alain Braud**[2], **Jean Louis Doualan**[2], **Richard Moncorgé**[2], **Tomasz Wojtowicz**[3], **Pierre Ruterana**[3], **Philippe MARIE**[3], **Alban Colder**[3], **Hock Min Ng**[1]

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3) SIFCOM, UMR6176, CNRS-ENSICAEN, 6 Bld Maréchal Juin, CAEN Cedex 04 14050, France

Semiconductors doped with erbium are attractive materials for optoelectronic devices due to the fact that characteristic Er^{3+} emissions meet technologically important spectral ranges, and semiconductor host provides the possibility of electrical excitation. Due to low thermal quenching of erbium luminescence, GaN:Er was recently extensively studied and devices based on this material were demonstrated. However, the optimization of the emission requires a better understanding of the excitation mechanisms.

We studied infrared and green erbium photoluminescence (PL) of MBE-grown GaN:Er with above- and below-band-gap excitation methods. In the latter case, the excitation wavelengths resonant and nonresonant with Er^{3+} transitions were also used. The PL spectra obtained in these conditions are similar, but the decay kinetics change with the excitation method. This enables us to distinguish emissions related with isolated and defect-coupled Er^{3+} centers.

To obtain the electroluminescence (EL) electrical contacts were made, and characteristic infrared and green emissions of Er^{3+} were observed. Electrical characteristics of this device and the dependence of its emission on the current and temperature were studied.

When electrical and optical excitations are combined, we observe that electroluminescence is altered by additional illumination. The below-band-gap illumination leads to a slight enhancement of EL, while with above-band-gap illumination very strong quenching of EL is observed. This indicates that both excitation mechanisms proceed via common steps within the excitation path, and as a result, they are perturbed by each other.

Friday, September 10th

Friday morning

Main Building, room 206

09:00 - 10:30

Giant traps in GaN and SiC: nanopores and dislocations

09:00 - 09:45
invited oral

David C. Look[2,3], **Zhaoqiang Fang**[2,3], **Stanislav I. Soloviev**[1], **Tangali S. Sudarshan**[1], **John J. Boeckl**[3]

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3) Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson AFB, Ohio 45433, United States

Porous SiC (P-SiC), is presently being investigated as a buffer layer for epitaxial SiC and GaN growth, an active layer for gas sensors, and a cell-friendly transistor for in vivo applications. Recently, a correlation between carrier concentration and pore density in n-type P-SiC has been observed, and this observation has been interpreted to mean that pores can act as electron traps. Traps in semiconductors can be conveniently studied by deep level transient spectroscopy (DLTS), and we have applied this technique to P-SiC. In comparison with the nonporous SiC case, most of the traps are the same, and indeed are common to various SiC materials studied by other workers in the past. However, we also find a new trap of very high concentration (6 x 10^{17} cm^{-3}), appearing only in P-SiC. The DLTS signal from this new trap displays abnormally slow and non-exponential saturation with filling pulse length (t_p), whereas most traps saturate rapidly and exponentially. Besides the unusual saturation behavior, the DLTS emission spectrum moves to higher temperatures as t_p increases, and also narrows with t_p. The standard DLTS modeling framework cannot explain these observances. It should be noted that similar effects have been observed in various semiconductors in which the traps lie along vertical threading dislocations, and thus form line charges. In this work, we present a single, general formalism that describes both capture and emission behavior for traps that exist on the inner surfaces or interfaces of spherical or cylindrical structures imbedded in semiconductor materials. Common structures of these shapes include pores, precipitates, and nanopipes. A very important case is cylindrical nanopipes (open-core screw dislocations) in GaN grown on Al_2O_3, which can sometimes generate states in the band gap, either due to dangling bonds or impurities that congregate nearby (the Cottrell atmosphere). Here, we will model dislocations in GaN as well as nanopores in SiC.

09:45 - 10:30
invited oral

Nitrides for Spintronics - Magnetic Moments and Spin Lifetimes in Nitrides

Jacek Majewski[1)]

1) Technische Univ. München, Walter Schottky Institut, Am Coulombwall 3, Garching D-85748, Germany

Theoretical predictions and later experimental findings of room-temperature ferromagnetism in Mn doped GaN have awoke considerable interest in nitrides as promising materials for spintronics. The ferromagnetic GaN:Mn could be a potential candidate for spin-polarization field emitter and might be useful in the development of all semiconductor spintronic devices. However, the physical mechanisms of possible room-temparature ferromagnetism in GaN:Mn are not well understood yet. Here, we provide critical review of existing theories and experimental data for GaN:Mn and discuss prospects of ferromagnetism in GaN doped with other transition metals.
Further, we discuss the problem of the spin decoherence in nitride heterostructures. In standard semiconductors, the electric field dependence of the spin splitting of energy bands (Rashba effect) has a marked influence on the spin dynamics and spin relaxation processes. This issue becomes much more relevant in nitride heterostructures. In view of their huge (of order few MV/cm) electric fields that originate in their strong piezo- and pyroelectric character, one may anticipate very significant spin splitting. In nitride heterostructures grown along the c-axis and in the neighborhood of the Γ point, the spin splitting of each energy band is dominated by the k-linear isotropic term. In AlN/GaN/AlN quantum wells, we find the spin splitting for the lowest conduction band to initially increase with increasing quantum well width but to saturate at well widths of 4 nm. We find that this limiting value is an order of magnitude smaller than in GaAs based heterostructures and agrees fairly well with recent experiments. These results indicate GaN heterostructures to be promising candidates for spintronic applications that require long electronic spin lifetimes.

Symposium D

Applications of Linear and Area Detectors for X-ray and Neutron Diffraction and Spectroscopy

Introduction

Symposium D is organized by the Institute of Physics, Polish Academy of Sciences, as a part of European Centre of Excellence "CEPHEUS" activities, in cooperation with European Materials Research Society and other scientific institutions. One of missions of the Centre of Photon, Electron and Ion Advanced Methods for Natural Science "CEPHEUS" is to spread and increase the knowledge of modern techniques for examination of new materials as well as to perform the research to increase the level of confidence in analysis. These goals perfectly converge with the subjects of Symposium D: i) presenting advanced diffraction and spectroscopy techniques based on the use of 1D, 2D and 3D detectors, and ii) overviewing the results of studies mploying such techniques in the material science and related fields. The symposium includes 26 invited lectures and 6 oral presentations by scientists affiliated in France, Germany, Israel, Italy, Netherlands, Poland, Portugal, Switzerland, Taiwan, United Kingdom and United States of America. The future of radiation detectors will be discussed during a panel discussion on Thursday 9th Sept. afternoon.

Welcome!

Organisers

- Wojciech PASZKOWICZ, Institute of Physics, Polish Academy of Sciences
- Jurgen HARTWIG, European Synchrotron Radiation Facility, Experiments Division
- Krystyna LAWNICZAK-JABLONSKA, Institute of Physics, Polish Academy of Sciences
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- Thomas WROBLEWSKI, DESY, HASYLAB
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- A.J. Wojtowicz, N. Copernicus Univ., Torun, Poland.

Proceedings

Papers will be published in Nuclear Instruments and Methods in Physics Research A

Acknowledgements

Symposium support:

- European Community: Program GIMA-CT-2002-4017, Centre of Excellence "CEPHEUS")
- State Committee for Scientific Research (Republic of Poland): Grant No. 72/E-67/SPB/5.PR UE/DZ 27/2003-2005
- Panalytical B.V.
- Hilgenberg GmbH

Monday, September 6th

Opening addressKrystyna Lawniczak-Jablonska

13:55 - 14:00

ADVANCED DETECTORS - GENERAL

Main Building, room 226

14:00 - 15:30

Past and present of semiconductor detectors

14:00 - 14:45
invited oral

Erik Henricus M. HEIJNE[1,2)]

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2) Nationaal Instituut voor Kern en Hoge Energie Fysika (NIKHEF), Kruislaan 409, AMSTERDAM 1098SJ, Netherlands

The first semiconductor particle detectors between 1943 and 1955 have been developed to serve as compact particle energy spectrometers. It soon became evident that with these devices improved energy resolution can be obtained in comparison with gaseous and scintillation-based detectors, and at a cost that is much lower than for the superior magnetic spectrometer systems. A variety of physics experiments and applications have become possible, in particular after 1970 with the high purity germanium detectors. The segmentation of semiconductor devices has been tried in parallel also since the early days but the need for matched readout electronics remained largely unfulfilled until 1990-2000. Then in the early 1980s a few people developed dense (C)MOS signal processing circuits for silicon detectors. This eventually allowed the exponential increase in the application of position sensitive detectors in 1, 2 and 3 dimensions. Several new fields of application have opened up, most notably tracking in elementary particle physics and space experiments, which at present are installing several hundreds of square meters of silicon detectors. For early imaging devices in 1971 the lack of electronics has been circumvented in the MOS charge coupled devices. Now the use of new approaches in silicon technology allow alternative techniques that become complementary to CCD for imaging over large parts of the wavelength spectrum. The continuous interaction between microelectronics development and semiconductor detector technology fuels progress and leads to new applications.

Area detectors for synchrotron radiation detection - applications in crystallography

14:45 - 15:30
invited oral

Heinz Graafsma[1)]

1) Europen Synchrotron Radiation Facility (ESRF), 6, Jules Horowitz, Grenoble 38000, France

Synchrotron radiation sources are have seen a spectacular increase in performance during the last decades, with an increase in brilliance of one order of magnitude every 3 years. This exponential increase in source performance has significant consequences for the way, as well as the type of science that is performed at these sources. Despite the fact that x-ray detectors used at synchrotron sources have seen a significant increase in performance over the last years, going from single detectors to imaging plates to CCD based systems, the detector remains very often the limiting factor in the experiment. Since storage ring sources are nearing perfection, the next significant gain is available via improved detectors.
An overview will be given of the current status of detectors at synchrotron sources. It will be shown how the detector is often limiting the experiment, and an analysis of what is needed will be given. Finally an overview of the perspectives, current and future developments will be given.

Coffee break

15:30 - 15:55

IMAGING: TOWARDS MICRO AND NANO SCALE
Main Building, room 226

15:55 - 17:05

Real time radiology in micro and nano scale

15:55 - 16:25
invited oral

Yeu-Kuang Hwu[1)]

1) Academia Sinica, Taipei, Taiwan, P.O.C.

Assisted by the high coherence of synchrotron X-rays, radiography has reached a new level of sophistication and power. Phase contrast due to the difference in the refractive index is added to the absorption as anther, yet much improved, contrast mechanism. Together with the improvement in the detecting system, we can now looking deep inside into matters with unprecedented precision and speed. Sub-μm or better resolution radiograph can now be obtained with ease and in many cases fast phenomenon can be observed in a real time fashion. The application of this new tool has already helped researches in materials science, biology and medicine. Ongoing developments in the instrumentation and reconstruction algorithms have generated even higher excitement with the recent demonstration of nanometer scale resolution in 3D. It is anticipated that with the new installation of X-ray free electron laser, X-rays can be used to "image" a single protein molecule with atomic resolution in the near future and to continue the legacy started by Röntgen. Review of this advent of this technology, its application to various domains in science, the relevance to the medicine, nano-science and -technology, and the future potential will be presented.

Nanotomography employing asymmetrical Bragg diffraction

16:25 - 16:55
invited oral

Marco Stampanoni[2)], **Gunther Borchert**[1)], **Rafael Abela**[2)]

1) Technischen Universität München, Forschungsneutronenquelle FRM-II (FRM2), Garching 85747, Germany

2) Swiss Light Source, Paul Scherrer Institut, Villigen 5232, Switzerland

High brilliance, third generation, synchrotron radiation sources push the spatial resolution of non-destructive X-ray tomographic investigations down to the micrometer or even submicrometer range while the coherent nature of the radiation extends the traditional absorption imaging techniques towards edge-enhanced or phase-sensitive measurements. Presently used detectors based on scintillation screens optically coupled to charge coupled devices (CCDs) are limited to a practical spatial resolution or 1 micrometer with efficiencies of a few percent. A recently developed new detector, called Bragg magnifier, exploits double asymmetrical Bragg diffraction from flat crystals to efficiently produce distortion- and aberrations-free X-ray images. For the present prototype, magnification factors as high as 150x150 can be reached, corresponding to a pixel size less than 100 x 100 nm^2.

X-ray imaging for applied and industrial research - applications in microelectronics and in micro system technology

16:55 - 17:40
invited oral

Tilo Baumbach[1,5)], **L. Helfen**[1,3)], **P. Mikulik**[1,6)], **P. Pernot**[1,4)], **D. Lübbert**[2)], **D. Kiel**[2)], **S. Keller**[3)], **P. Cloetens**[4)], **J. Baruchel**[4)]

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5) Forschungszentrum Karlsruhe GmbH, Institute für Synchrotronstrahlung, ANKA, Hermann-von-Helmholtz-Platz 1, Eggenstein-Leopoldshafen 76344, Germany

6) Masaryk University, Faculty of Sciences, Kotlarska 2, Brno 61137, Czech Republic

Development and production of new materials and their application in various branches of microelectronics and microsystem technology require information on their structural perfection. Of crucial importance are structural properties and their relations to technological steps involved with their production. Moreover, the investigation of structure-property relationships for component as well as entire devices is needed.
Beside laboratory methods a reliable availability of experimental set-ups/stations at SR sources with unique properties (high intensity, small focus, high brilliance, good coherence of radiation) opens up advanced possibilities for nondestructive material characterization and for nondestructive testing of components of applied and industrial research labs. The talk gives an overview illustrating x-ray imaging

inspection and defect analysis in this context by results from microelectronics and microsystem technology, such as

-ultra-thin Si for smart wafers, macrodefects in GaAs, dislocation density mapping
-growth and quality of GaN-ELO structures on sapphire and SiC
-metallization layers: stress migration in Cu conducting lines
-lasers: deformation fields in high-power laser bars
-interconnection technology: inspection of Al and Au wire bonding in glop-tops
-flip-chip technology: inspection of solder bumps in sensor arrays and pixel detectors
-microfluidics: hydrodynamical permeability of microfilters
-MOEMS (micro-opto-electro-mechanical structures): stress in micro-mirror arrays

Imaging techniques of absorption-, phase- and diffraction contrast (holo-tomography, micro-diffraction, rocking curve imaging) are employed. Results of computed laminography are reported which was developed and implemented with SR for the first time and can be considered as a successful extension of 3D imaging to flat, laterally extended devices such as microelectronic circuit boards. Conclusions for requirements to future detector development will
be given.

Poster session 1

19:00 - 21:00

Tuesday, September 7th

NEW MATERAIALS AND CONCEPTS FOR POSITION SENSITIVE DETECTORS, NEW APPLICATIONS

Main Building, room 226

11:00 - 12:30

Materials for semiconductor detectors: CdTe and CdZnTe

11:00 - 11:30
invited oral

Michael Fiederle[1], **Alex Fauler**[2], **Heiko Braml**[2], **Jens Ludwig**[2]

1) Materials forschungcentrum (FMF), Stephen Meier str. 21, Freiburg 79104, Germany

2) Univ.Freiburg, Freiburg, Germany

The properties of CdTe and CdZnTe favour these materials for the application as radiation detectors. These materials are the subject of scientific and industrial research for more than twenty years. Enormous improvements had been made of the material growth and fabrication of spatial resolving detectors. Nevertheless, there are still several limitations like inhomogeneity of the detector performance and availability of the crystals.
In this talk the state of the art of CdTe and (Cd,Zn)Te detectors will be discussed with the focus on the material parameters, detector performance and the development of spatial resolving detectors. The results of the leading scientific and commercial groups will be presented in comparison to the actual results of the detector development in the Freiburger Materialforschungszentrum. The activities in Freiburg include the growth of detector grade CdTe and CZT crystals, the material characterization and the processing of pixel detector by flip-chip bonding.

Novel materials and concepts for Neutron Image Plates

11:30 - 12:00
invited oral

Michael Schlapp[1,2], **Alexander Ioffe**[2], **Sergey Masalovich**[2], **Harald Conrad**[2], **Thomas Brückel**[2], **Hartmut Fueß**[1], **Heinz von Seggern**[1]

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Neutron image plates (NIPs) provide the means for two-dimensional, position-sensitive detection of neutrons. Commercially available NIPs consist of a mixture of the neutron converter Gd_2O_3 and the storage phosphor $BaFBr:Eu^{2+}$, dispersed in an organic binder supported by a flexible sheet. Since BaFBr is an excellent storage phosphor for X-rays, these NIPs are prone to the γ-background always present at neutron experiments. In this contribution we present a system of converter (^{6}LiF) and storage phosphor ($KCl:Eu^{2+}$ or $KBr:Eu^{2+}$) which shows a high efficiency for the detection of neutrons while at the same time features a low γ-sensitivity due to the low atomic numbers. It was found that storage phosphors mixed with LiF feature a signal per absorbed neutron that is twice as high as those samples containing GdF_3 as converter. This advantage results from a much higher usable energy output of LiF after a neutron absorption reaction. Combining the large signal with the γ-absorption of KCl, which amounts to about 10% of BaFBr, one obtains a neutron equivalent for $KCl:Eu^{2+}$-^{6}LiF image plates of 1/20 neutron per photon for soft γ-rays (< 300 keV) while the equivalent for hard γ-quanta (>300 keV) is 1/400 neutron per absorbed photon.
Three different morphologies of NIPs were fabricated based on $KCl:Eu^{2+}$-LiF: polymer supported (P-NIPs), ceramic (C-NIPs) and pixelated (Pix-NIPs) neutron image plates. Pix-NIPs represent a novel morphology in which the scattered light is confined to the cell of a honeycomb structure embedded in the image plate. Due to this confinement, the resolution of such an image plate is primarily independent of scattering properties of the NIP and is primary a function of the size of the honeycomb structure used.
Determining the Detective Quantum Efficiency DQE for a C-NIP consisting of $KCl:Eu^{2+}$-^{6}LiF resulted in a value of 38 % which corresponds to an efficiency comparable to commercially available NIPs.

12:00 - 12:30
invited oral

Stress and texture analysis with two-dimensional X-ray diffraction

Bob B. He[1)]

1) Bruker Advanced X-ray Solutions (Bruker AXS), 5465 East Cheryl Parkway, Madison 53711-5373, United States

Two-dimensional x-ray diffraction has many advantages in stress and texture analysis. This presentation introduces the recent progress in two-dimensional X-ray diffraction as well as its applications in stress and texture analysis. Two-dimensional X-ray diffraction provides far more information than the conventional one-dimensional diffraction. Therefore, two-dimensional diffraction requires new theories and approaches to interpret and analyze the two-dimensional diffraction data. The fundamental equations for both stress measurement and texture measurement are developed with the matrix transformation defined for the two-dimensional diffraction. Stress measurement is based on a direct relationship between the stress tensor and the diffraction cone distortion. The two-dimensional detector collects texture data and background values simultaneously for multiple poles and multiple directions. The presentation also shows the geometry convention, data collection strategy, data interpretation, and data analysis for stress and texture analysis. Several experimental examples have shown that area detectors can measure stress and texture with high sensitivity, high speed and high accuracy.

12:20 - 14:00

Lunch break

14:00 - 15:35

ADVANCED DETECTORS FOR IMAGING AND DIFFRACTION APPLICATIONS

Main Building, room 226

14:00 - 14:45
invited oral

X-ray imaging using 2D semiconductor detectors

Jean-Pierre Ponpon[1)]

1) CNRS, PHASE Laboratory, Strasbourg, France

Semiconductor nuclear radiation detectors are nowadays of current use for high resolution spectrometry in a number of fields, including those involving X-rays measurements. The significant advances achieved during the last ten years in materials properties, detector characteristics, and high quality electronic systems, make now possible to go one step further and to build 2D X-rays imaging systems based on semiconductor detectors. It is the aim of this paper to present the state of the art of X-rays imaging systems based on such devices.
We'll first focus on the basic principles involved. We'll try to discuss the main requirements (detector size,

spatial resolution, pixels number, dynamics, counting rate, etc.) and limitations (physical and experimental limitations), with respect to the applications envisaged (scientific, medical or industrial imaging). The major properties of the semiconductors of interest for such applications will be briefly summarized.
Then the working principles and main characteristics of existing systems based on various semiconductor materials and devices will be reviewed and compared to those of conventional X-rays imagers.
Finally, possible evolutions will be discussed in terms of new detector materials and new semiconductor devices, taking into account the increasing potential of microelectronics technology.

New array detector for protein crystallography at the Argonne National Laboratory

14:45 - 15:15
invited oral

Istvan Naday[1)], **Timothy Madden**[1)], **Gerold Rosenbaum**[2)]

1) Argonne National Laboratory (ANL), 9700 South Cass Avenue, Argonne, IL 60439, United States

2) University of Georgia, Athens, GA, United States

A new advanced CCD/fiberoptic array detector is being developed for the Structural Biology Beamlines at the Advanced Photon Source. The new detector, called Clematis-1330, uses a novel geometrical arrangement of the fiberoptic tapers resulting in a circular like imaging area with an equivalent diameter of 412 mm. Additional features such as selectable readout speeds, software controlled binning, gain and offset adjustments of the individual modules and self testing modes make this new generation fiberoptic taper / CCD array detector a flexible and reliable device for macro-molecular beamlines. The very large active area (1330 cm2) with the new geometry combined with high spatial resolution provides for a substantial increase in solid angle coverage significantly improving anomalous data collection for phasing at low energies, increasing the number of resolved orders per frame for large macromolecular assemblies, reducing the dose on the sample, i.e radiation damage, for the same resolution and completeness of data, and giving more leeway in detector distance for minimizing background. The added novel gain control feature makes this detector particularly suited for acquisition of very-high resolution data.. Independent read-out speed control allows balancing the opposing quests for low read-noise and short read-out times. An overview of the hardware and software design and specifications, as well as a comparison of its performance parameters with existing detectors will be given.

2D-multi-wire position-sensitive gaseous detectors for neutron and hard X-ray diffractometry

15:15 - 15:35
oral

Reinhard Kampmann[1,2)], **M. Marmotti**[2)], **M. Haese-Seiller**[1)], **R. Georgii**[3)], **V. Kudryashov**[1)]

1) GKSS Research Centre, Institute for Materials Research, Geesthacht, Germany

2) DENEX Detectors for Neutrons and X-rays GmbH, Lueneburg, Germany

3) Technische Universität München, ZWE-FRM-II (FRM-II), Lichtenbergstr. 1, Garching 85747, Germany

Delay-line based 2D-multi-wire position-sensitive gaseous detectors (MW-PSGD) have been developed for neutron scattering instruments SANS-2 and ARES at FRG-1, REFSANS and MIRA at the new German high flux reactor FRM-II and the hard X-ray diffractometers HARWI and PETRA-2 at DESY in Hamburg. Within the scope of the detector development the relative resolution (R_r) of these detectors, defined as the position resolution in percentage of the detector dimension, has been improved from 0.66% (ARES detector : active area: A_a = 500 mm x 500mm; wire pitch : p_w = 2mm) to 0.4% (REFSANS detector: A_a = 500 mm x 500mm ; p_w = 2mm). These R_r-values demonstrate substantial progress in the technology of 2D-MW-PSGDs because hitherto the actual limit of resolution for such detectors has been R_r = 0.8%. The performance of these detectors (design, detection probability, spatial resolution and discrimination of gamma-radiation) is presented and the count rate capability of these modern delay-line based detectors is discussed for the case where they are linked to modern multi-hit TDC based data acquisition systems. Finally, comments on the usage and future perspectives of these detector types are made.

Coffee break

15:35 - 15:55

15:55 - 17:35

2D DATA ANALYSIS; APPLICATIONS OF AREA DETECTORS IN SCIENCE AND INDUSTRY

Main Building, room 226

15:55 - 16:25
invited oral

X-ray holography using area detectors

Andrea Lausi[1)]

1) Sinchrotrone Trieste, Trieste, Italy

The atomic and molecular structures of crystalline substances can be mostly solved by means of electron and x-ray diffraction. In contrast to the diffraction, holographic imaging does not require translation periodicity and can be, in principle, applied also to non-crystalline samples (e.g. quasicrystals, doped systems, amorphous materials). Moreover reconstruction algorithms can also be applied to the scattering signal, allowing information on electron-density to be recovered using a single two-dimensional x-ray pattern. The fact that all the data needed can be collected in one shot has important practical consequences; reduced exposure time can resolve the problem of radiation damage of specimens and opens new possibilities for studies of fast processes in three dimensions.

16:25 - 16:55
invited oral

Using FIT2D software for data analysis

Andrew P. Hammersley[1)]

1) European Synchrotron Radiation Facility (ESRF), Grenoble 38043, France

FIT2D is a multi-purpose data reduction, visualisation, and analysis program. A brief overview will be presented, followed by more detailed explanation of detector calibration and correction procedures, and integration of powder diffraction data from 2-D detectors to 1-D 2-theta scans.

16:55 - 17:15
oral

Application of 2D detectors in X-ray diffraction based metrology in semiconductor industry

Krzysztof J. Kozaczek[1)]

1) Hypernex, Inc., 3006 Research Drive, State College 16801, United States

In recent years a significant progress has there been made in applying X-ray diffraction (XRD) for in-line measurement of crystallographic phase and texture in conductors for process monitoring. One of the enabling factors is the usage of a large area 2-D- detector which has the sensitivity, stability, and reliability suitable for in-line applications in semiconductor fabs. We present the principles of operation and a summary of results from using an automated XRD metrology in support of copper damascene production. The principles of operation include a model of a diffractometer that translates the detector space to the reciprocal space and subsequently through a series of corrections to the orientation distribution space of the crystallites.
The automated XRD tool equipped with a 2D detector is capable of rapid mapping of 200/300 wafers (with a throughput rate of up to 50 wafers/hour) and delivering quantitative information about the film crystallographic composition and texture.
The major applications of in-line XRD include process development for the 65 nm node and beyond, and BEOL process monitoring-control for 130 and 90 nm nodes. The presented examples concentrate on the TaN/Ta/Cu seed/ECP Cu processes. Monitoring of film microstructure has proven to be a sensitive indicator of deposition tool stability and a useful method in defining the process windows. The examples of applications, based on three years of experience in the fabs, show a clear correlation between the yield loss, poor parametrics, resistivity, electromigration and stress migration performance of copper interconnects and TaNx/Ta phase, Cu seed texture and ECP Cu texture. The microstructure of barrier layers, copper seed, and ECP copper may be tailored for improved reliability and monitored throughout the process by means of XRD on both blanket and patterned wafers with a spatial resolution down to 30 microns.

17:15 - 17:35
oral

Stabilization of Eu^{2+} in the storage phosphor CsBr:Eu^{2+} by Me^{+}-codoping

J. Zimmermann[1)], **Sabine Hesse**[1)], **M. Fuchs**[2)], **W. Knüpfer**[2)], **Heinz von Seggern**[1)]

1) Technische Universität Darmstadt, Institute of Materials Science, Petersenstr. 23, Darmstad 64287,

Germany
2) Siemens AG, Medical Solutions, Vacuum Technology, Erlangen 91058, Germany

Nowadays image plates (IP) are frequently used for 2D detection of x-rays in medicine and materials research. Commercial IPs thereby consists of the storage phosphor BaFBr:Eu^{2+} in form of a powder mixed with a polymer binder and applied evenly on a flexible substrate. The spatial resolution of those plates is limited by light scattering introduced by the difference of refractive index of the binder and the phosphor grains. For IPs with higher spatial resolution the X-ray storage phosphor CsBr:Eu^{2+} is a promising material since it can be grown in form of needles on a glass substrate using evaporation techniques. The higher resolution of those NIPs (needle image plates) thereby is achieved by a light guiding effect resulting from the thin needles exhibiting diameters in the ten-micrometer scale. The present problem with those NIPs is the low radiation hardness due to a missing spatial stability of Eu^{2+} in the CsBr-lattice. This poor radiation hardness can be explained by large colour centres (F_2 (M)- centers) generated during irradiation, which agglomerated with activator/vacancy dipoles (Eu^{2+} - V_{Cs}) thereby increasing the diffusivity of Eu^{2+}. This leads to larger Eu-aggregations, which loose their luminescence properties and explains the poor radiation hardness by loss of active Eu^{2+}. By means of thermally stimulated luminescence (TSL), photostimulated luminescence (PSL), and diffuse reflection spectroscopy it will be demonstrated that codoping with Me^+ ions reduces the Eu-aggregation and thus increases the radiation hardness.

Wednesday, September 8th

POSITION SENSITIVE DETECTORS: BIOLOGICAL APPLICATIONS AND CONNECTIONSLawniczak-Jablonska, Krystyna

Main Building, room 226

14:00 - 15:45

High resolution, high speed measurement of weak diffraction from crystals of biological molecules

14:00 - 14:45
invited oral

Zbyszek Otwinowski[1)]
1) University of Texas, Southwestern Medical Center (UT), 5323 Harry Hines Blvd., Dallas 75390, United States

Structure determination of complex biological molecules is the largest application of synchrotron X-ray radiation. About 1/4 of X-ray beam lines worldwide are dedicated to macromolecular crystallography. At the third-generation synchrotrons, radiation damage limits the crystal lifetime to minutes, making further improvements in X-ray source insignificant. With the fraction-of-second individual image exposure time, detection systems and data analysis are the main experimental limitations. Currently installed detectors can read a 36M-pixel diffraction image in one second, making it possible to acquire Gigabytes of data per minute, but in practice exceeding the capacity of data transport, analysis and storage systems.

The experimental problems arise from the necessity to measure the diffraction from marginal-quality crystals. The ability to measure the diffraction is constantly challenged by the biology advancing to study more complex, often imperfectly ordered, systems of molecules. The resulting diffraction is very weak, barely resolved and changing due to the radiation damage.

Data analysis has to provide the minimum error estimates of the diffraction signal and also to be computationally efficient. Determining the structure of macromolecules requires iteratively solving a highly convoluted series of sub-problems. The solutions are a combination of purely experimental approaches with calculations based on complex, theoretical thinking. The limitations of detection systems propagate throughout the analysis, with different detector characteristics limiting particular calculations.

Application of state-of-the-art 2D detectors in structural biology

14:45 - 15:15
invited oral

Jasper R. Plaisier[1)], **Jan Pieter Abrahams**[1)]
1) Leiden Univ., Leiden, Netherlands

The development of area detectors for structural biology is one of the driving forces behind the exponential increase in the number of structure determinations of biological complexes. X-ray crystallography has largely been responsible for this rise.

In recent years cryo-electron microscopy has become a rapidly emerging tool for determining structures of sub-nanometer resolution. In the latter technique, however, area detectors are still hardly used, most data is still collected on photographic film. With the increasing number of structures being solved using microscopy the development and usage of area detectors is on the rise as well.

The two techniques are based on fundamentally different principles: Diffraction of X-rays and direct imging using electrons. Comparison of the two indicates that each approach places different demands on a detector. Next to these differences, both techniques are also at a different stage in their development. Whereas in electron microscopy people are still working on constructing a detector that fulfills the basic demands, in X-ray diffraction development is focussed on refining and improving throughput.

In this survey these two techniques in structural biology and their demands on detectors are compared. An analysis of the current application of detectors is presented. Furthermore, current trends in development are shown.

15:15 - 15:45
invited oral

2D detectors technology and optics - relations to Nature

Jerzy B. Pełka[1)]

1) Polish Academy of Sciences, Institute of Physics, al. Lotnikow 32/46, Warszawa 02-668, Poland

2D detector systems are amongst the most important tools of science and technology. Myriads of particular applications of the systems in medicine, industry, earth and space exploration or basic research generate specific technical problems in the subject.

Recent rapid progress in electronic circuitry, mechanics on the micro- and nanoscale, and design of new materials has a direct impact on development of 2D detector systems. They are becoming more and more sophisticated, resembling, in some cases, the complexity of the natural solutions formed evolutionary in biological systems.

Main aim of the present lecture is to discuss the question of relations between "state of the art" in 2D detectors and the natural vision systems.

15:45 - 16:00

Coffee break

16:00 - 17:20

1D AND 2D DETECTORS: APPLICATION IN X-RAY X-RAY DIFFRACTION AND ABSORPTION STUDIES

Main Building, room 226

16:00 - 16:30
invited oral

Quality of X-ray diffraction data collected at one-dimensional PSD: application for thin epitaxial layer systems

Olivier Masson[1)], **Alexandre Boulle**[2)], **René Guinebretiegrave;re**[2)], **André Lecomte**[2)], **Alain Dauger**[2)]

1) Laboratoire Science des Procédés Céramiques et de Traitements de Surface - UMR 6638 CNRS - Université de Limoges, 123 avenue Albert Thomas, Limoges 87060, France

2) Laboratoire Science des Procédés Céramiques et de Traitements de Surface - UMR 6638 CNRS - ENSCI, 47 avenue Albert Thomas, Limoges 87065, France

Over the past two decades, position sensitive detectors (PSDs) have found increasing use in many fields of X-ray powder diffractometry. Their great potential has been demonstrated not only for time- and temperature-resolved powder diffraction studies but also for applications ranging from conventional structure characterisation to pole figures measurement. In most cases, one takes advantage of the significant reduction of the acquisition time resulting from the ability of PSDs to simultaneously record a much larger region of the pattern than conventional counters.

One important issue concerning PSDs is data quality. Data quality not only depends on the detector specifications (linearity, uniformity of response, spatial resolution, stability...) but also on combined effects of the detector and the geometry of the used set-up. In the present work, this point is illustrated within the framework of the study of thin epitaxial layer systems, which represents a new field of application of PSD. We first present a versatile homemade set-up which is particularly well suited to the study of thin epitaxial layers. It is based on a rotating anode generator, a four bounce (220) Ge monochromator and a curved position sensitive detector (INEL CPS120). We then describe how PSDs can be advantageously used to allow fast reciprocal space mapping, which is especially interesting when analysing poor crystalline and defective layers as usually observed with oxides and ceramics films. We finally present some aspects of the quality of data collected with this instrument. In particular the effects of PSD on peak position and intensity precision, instrument resolution and corrections that must be applied to raw data are discussed.

Fast high resolution characterization of powders by utilizing image plate Guinier camera

16:30 - 16:50
oral

Joseph Gal[1], Dimitry Mogiliansky[1], Michael Nippus[2], Giora Kimmel[1], Jacob Zabicky[1]

1) Ben-Gurion University of the Negev, P.O.Box 653, Beer-Sheva 84105, Israel

2) Huber Diffraktion Technik GmbH, Rimsting, Germany

A new Huber Guinier Camera 670 was installed on an Ultrax 18- Rigaku X-ray rotating Cu anode source. A monochromator (B=360 mm) attached to the source providing $K\alpha_1$ radiation. The camera is used for powder diffraction utilizing transmission geometry. An image plate makes the position sensitive detection measurement. This configuration enables fast scanning with high resolution.

In order to evaluate the camera quality we collected data of some classical reference materials like silicon, quartz and some standards supplied by NIST USA and organic complexes. Each sample was measured at 4kW for 1 to 2 minutes at 2θ between 0 to 100 degrees. The results were compared with previous references. It was found that the relatively high instrumental background can be easily dealt-with and do not pose difficulty in the analysis of the data.

Detectors for EDE experiments.

16:50 - 17:20
invited oral

Giuseppe Salvini[3], Jon Headspith[3], Stephen L. Thomas[2], Gareth Derbyshire[2], Andy Dent[3], Trevor Rayment[5], John Evans[1], Richard Farrow[3], Sofia Diaz-Moreno[2,4], Cyril Ponchut[4]

1) Department of Chemistry, University of Southampton, Southampton SO17 1BJ, United Kingdom

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3) CLRC Daresbury Laboratory (DL), Daresbury, Warrington WA4 4AD, United Kingdom

4) Europen Synchrotron Radiation Facility (ESRF), 6, Jules Horowitz, Grenoble 38000, France

5) Department of Chemistry, University of Cambridge, Cambridge CB2 1TN, United Kingdom

EXAFS, X-ray absorption spectroscopy fine structure, has been an important tool within synchrotron radiation science for some years. It has been used extensively in step scanning mode to provide information on the local environment within both static and slowly changing samples.
Energy dispersive EXAFS (EDE) allows similar information to be collected in a significantly shorter time frame, enabling the study of truly dynamically changing samples. The technique uses a bent crystal monochromator to focus an energy dispersed x-ray beam onto a sample which then impinges upon an array detector positioned behind the sample. This allows the absorption over a range of energies to be collected in a very short period. Until recently only few systems have existed for this technique, typically employing commercially available detectors originally constructed for other applications. These presented limitations in speed, energy resolution, linearity and dynamic range and could only follow changes in the millisecond range.
Using UK ESPRC grant funds, a new detector has been developed (XSTRIP) which shows great improvements over the above limitations. This has opened whole new areas of science to researchers.
This talk will present the technique, some of the historical limitations, the performance increase afforded by the XSTRIP system and an overview of the future direction of detectors for this most exciting and important technique.

Poster session 2

19:00 - 21:00

Main Building, Main Hall (Duża aula)

Application of Si-strip detector in X-ray crystallographic texture measurement

poster D-01

Leszek Tarkowski[1)], **Jan Bonarski**[1)]

1) Polish Academy of Sciences, Institute of Metallurgy and Materials Sciences (IMIM PAN), Reymonta 25, Kraków 30-059, Poland

Traditionally applied method registration of a pole figure by means of the the X-ray diffraction technique is based on the usage of a single slit detector (point counter) at the fixed 2-theta position. However, examination of the crystallographic texture of multi-phase and lower symmetry materials requires registration of wider diffraction spectra when compared to e.g. pure metals. This procedure can be done by scanning the chosen range of the 2-theta angle with the single-slit detector (pseudo-PSD mode) or by applying the position-sensitive (linear) detector, or an area detector.
The work presents application of the linear Si-strip detector in the classic X'Pert system equipped with texture attachment. Full integration of the new detector with existing hardware enabled to use the new measurement possibilities and reduction of the pole figures registration time. Various examples of measured profiles and pole figures are presented.

Design optimisation of silicon strip detectors for position-sensitive measurements of X-rays

poster D-02

Piotr Wiacek[1)], **Wladyslaw Dabrowski**[1)]

1) AGH University of Science and Technology, Faculty of Physics and Nuclear Techniques (AGH), al. Mickiewicza 30, Krakow 30-059, Poland

In the paper we present a comprehensive simulation method to evaluate X-ray imaging response of a silicon strip detector with particular emphesis on the charge sharing effects. The simulation steps include:
- generation of parameterised charge distribution in the detector sensitive volume based on cross sections for basic mechanisms: photoabsorption, Compton scattering and coherent scattering,
- transport of generated charge in the detector volume, taking into account drift in the electric field and diffusion,
- generation of charges induced in the readout strips,
- adding random electronic noise to the electronic signals,
- discrimination of electronic signals including the electronic noise,
- determination of count efficiency vs position of incident photons as a function of the discrimination threshold.

The developed simulation tools are used for optimising the design and operating parameters of a silicon strip detector to be used as 1-D position sensitive device in experimental techniques like X-ray powder diffraction, X-ray high-resolution diffraction, and small angle X-ray scattering, using laboratory X-ray sources. The response of the detector as a function of the detector bias and discrimination threshold has been investigated for two geometrical configurations: photons incident from the strip side and from the back side. The simulation results for a particular detector design are discussed and comparison with measurements of the detector response is presented.

Ceramic and structured neutron image plates based on KCl:Eu^{2+}-LiF

poster D-03

Michael Schlapp[1,2)], **Alexander Ioffe**[2)], **Sergey Masalovich**[2)], **Harald Conrad**[2)], **Thomas Brückel**[2)], **Hartmut Fueß**[1)], **Heinz von Seggern**[1)]

1) Technische Universität Darmstadt, Institute of Materials Science, Petersenstr. 23, Darmstad 64287, Germany

2) Forschungszentrum Jülich, IFF, Streumethoden, Jülich 52425, Germany

Neutron image plates have found widespread application as neutron detectors for single-crystal and powder diffraction, small-angle scattering and tomography. After neutron exposure, the image plate can be read-out by scanning with a laser. Commercially available neutron image plates (NIPs) consist of a powder mixture of BaFBr:Eu^{2+} and Gd_2O_3 dispersed in a polymer matrix and supported by a flexible polymer sheet. Since BaFBr:Eu^{2+} also is an excellent X-ray storage phosphor, these NIPs are particularly prone to γ-radiation which is always present as a background radiation in neutron experiments. In this contribution we present results of NIPs consisting of KCl:Eu^{2+} and LiF which were fabricated into ceramic image plates hence eliminating the necessity for an organic binder phase. An advantage of this type of NIP is the significantly reduced γ-sensitivity. However, the much lower neutron absorption cross section of LiF compared to Gd_2O_3 demands a thicker image plate to obtain comparable neutron absorption. This increased thickness inevitably leads to a loss in spatial resolution of the NIP. However, the reduction in resolution can be restricted by a novel image plate concept in which a ceramic structure with square cells is embedded in the NIP resulting in a pixelated image plate (Pix-NIP). In such a NIP the read-out light is confined to the respectively illuminated pixel decoupling the spatial resolution from the optical properties of the image plate material and morphology. In this contribution, a comparison of experimentally determined and simulated spatial resolutions of pixelated and unstructured image plates for a fixed read-out laser intensity is presented as well as simulations on the properties of these NIPs at higher laser powers.

Diamond-based X-ray detectors

Daniele M. Trucchi[1)], **Paolo Ascarelli**[1)], **Gennaro CONTE**[2)], **Emilia Cappelli**[1)] poster D-04

1) CNR-IMIP, Via salaria km 39,200, Rome, Italy

2) DIE University Roma Tre (DIE), Via Vasca Navale, 84, Rome 00146, Italy

Due to the radiation damage resistance and to the tissue-equivalent properties, diamond is considered one of the most suitable active material for the realization of x-ray detectors, especially for medical applications. The development of enhanced CVD techniques made possible an effective tailoring of the material properties in an effort to meet the requirements of specific applications where the substitution of the rare and costly natural diamond was solicited. CVD diamond shows a polycrystalline structure in which the material quality largely influences the photoconductive response of the resulting detectors. The control of the material properties during the growth process and the optimal design of the final detector represent the main aspects we considered. We realized x-ray dosimeters with different diamond film morphology and tested them in DC and AC conditions by a beam generated by a standard Copper tube (CuKα at 8.05 keV). The analysis of the $\mu\tau$ product, affecting the detector collection efficiency, and of the density of shallow states in the band-gap in proximity of the valence band, affecting the response time and intensity, were correlated with important parameters as the crystal grain quality and the grain boundary contamination. Moreover, a study regarding the influence of an irradiation bias on the detector response and an operative definition of the priming process were performed.

Diamond photoconductive structures for X-rays beam monitoring

Giovanni Mazzeo[1)], **Giuseppe Prestopino**[1)], **Gennaro CONTE**[1)], **Victor Ralchenko**[2)] poster D-05

1) DIE University Roma Tre (DIE), Via Vasca Navale, 84, Rome 00146, Italy

2) General Physics Institute, Vavilov Str. 38, Moscow 117942, Russian Federation

Diamond is considered the elective material for electronic devices operating in extreme environments. In particular, its wide band-gap and high thermal conductivity make diamond the best candidate for detectors able to work with UV and X-ray sources. The use of photoconductive CVD diamond devices for monitoring pulsed UV sources in the field of ULSI photolithography and micro-machining has been recently proposed. For such kind of applications the principal request is for a fast and sensitive detector in order to control the photoresist dosimetry. Such kind of application requires not only the intensity but also the position of the beam. The field of position sensitive detectors (PSDs) has recorded many contributions on 1D and 2D detectors based principally on amorphous and crystalline silicon. With the aim of contributing in understanding potentiality and performances of CVD diamond detectors, we propose a 1D-PSD based on the voltage division scheme to be exploited in deep-UV and X-ray beam centring and monitoring.
High quality, 8x8 mm2 large and 0.8 mm thick, polycrystalline diamond deposited by a microwave CVD process has been used in this work. Chromium deposits have been realized by physical vapour deposition. Fine line lithography has been then used to define structures with resistance values in the kW range. A Neweks PSX100 ArF laser (4.5 mJ per pulse, FWHM=3 ns, 10-100 Hz) has been preliminary used to test the performance in respect of the lateral sensitivity. The output voltage signals have been recorded by using a Le Croy Wavepro 960 digital sampling oscilloscope. The performance to X-ray irradiation has been tested by using a sealed-off 8.06 keV Copper tube typically used in X-ray diffraction. To improve the signal/noise ratio, the beam has been frequency modulated by using a mechanical iron-modified chopper. We present and discuss the results in the framework of the photoconductive response of 1D-PSD as a function of beam dimension and intensity.

Silicon carbide for room and high temperature X-ray detectors

Giuseppe Bertuccio[1,4)], **Stefano Caccia**[1)], **Roberto Casiraghi**[1)], **Claudio Lanzieri**[2)], **Antonio Cetronio**[2)], **Filippo Nava**[3,5)] poster D-06

1) Politecnico di Milano, Department of Electronics Engineering and Information Science (Polimi-DEI), *P.za L. da Vinci, Milano 20133, Italy*

2) Alenia Marconi Systems (AMS), Via Tiburtina km12.400, Rome 00131, Italy

3) University of Modena and Reggio Emilia, Via Campi 183, Modena 41100, Italy

4) Istituto Nazionale di Fisica Nucleare - Sez. Milano (INFN - MI), Via Celoria 16, Milano 20133, Italy

5) INFN - sez. Bologna, Bologna, Italy

Several prototype devices have been manufactured and tested showing very promising or even outstanding results compared to other semiconductors.
In this presentation we show the results of our research activity, whose aim was to deeply understand the physical and electronic characteristics of 4H-SiC available for device construction and, at the same time, to develop a technology able to realise high performance radiation detectors.
For this purpose we have designed and manufactured several types of device, test structures and detectors on epitaxial 4H-SiC, 30 to 70 μm thick, furnished by different foundries, with doping concentrations ranging from 5x10^{13} to 10^{15} cm^{-3}. Residual doping in the epitaxial layer should be as low as possible in order to deplete thick layers at adequate voltage, so maximising the detection efficiency at low reverse current and reasonable charge collection times. The detector Schottky contacts with Au and Ni_2Si have been tried, giving barrier heights around 1.2-1.6 eV, ideals to made negligible thermionic emission currents, so achieving low noise. Specifically, on our best devices we have measured dark currents as low as 5 pA/cm^2 at 27C and 0.5nA/cm^2 at 100C, which are from two to three orders of magnitude lower with respect to state of the art junctions on silicon or other semiconductors suitable for radiation detectors, such as GaAs, CdTe, CdZnTe. Such ultra-low dark current densities of our SiC detectors allow to reach superior performance in a wide temperature range.
Noise levels as low as 17 electrons r.m.s. at room temperature and 43 electrons r.m.s. has been measured with a pixel detector operating at room temperature and at 100C, respectively, still limited by the noise of the silicon-based front-end electronics.

Performance study of monolithic line radiation detector based on semi-insulating GaAs using X-rays source

poster
D-07

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During last decade a great effort has been concentrated to development of radiation detectors based on bulk semi-insulating (SI) GaAs due to its low cost coupled with good properties in detection of X- and gamma-radiation [1, 2].
Digital X-ray testing and imaging present the most perspective field of its application. The main advantages include: i) higher sensitivity in comparison to photographic film due to better absorption, ii) suppression of low-frequency noise by pulse-processing front-end electronics, iii) linear behaviour over entire dynamic range, iv) setting of a threshold allows to discriminate (not only) noise from signal, and also photon energies, v) multiple thresholds can be implemented, which open qualitatively new kind of X-ray imaging at various photon energies [3].
Our effort is devoted to development of X-ray testing and imaging insturmentation based on the SI GaAs (InP) monolithic line detectors with 1D scanning system.
In this work, results of experimental performance study of SI GaAs monolithic line detector are demonstrated. SI GaAs based chip consists of 32 strip detectors with pitch 0.25 mm and strip area 0.2*1.25/2.5 mm^2. Chip can be irradiated from the edge or the face - contact side. 24 strip detectors are directly coupled to 24 channel electronic read-out system. We study the response of SI GaAs line detector to X-ray radiation (including focused beam) with emphasize to evaluate detection efficiency, spatial resolution and interstrip crosstalk following its imaging ability.

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Two-dimensional X-ray diffraction for micro-area and thin film

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X-ray diffraction analysis on micro-area or thin films is always a challenge task due to weak diffraction and poor statistics, especially when dealing with samples containing large grain size, inhomogeneous phase distribution and preferred orientation. Two-dimensional x-ray diffraction has many advantages in microdiffraction and thin film analysis. This presentation introduces the recent progress in two-dimensional X-ray diffraction as well as its applications in microstructure and residual stress analysis on small samples, micro-area on large samples or thin films. The two-dimensional X-ray diffraction provides far more information than the conventional one-dimensional diffraction. Therefore, two-dimensional diffraction requires new theories and approaches to interpret and analyze the two-dimensional diffraction data. The presentation shows the geometry convention, data collection strategy, data interpretation, and data analysis for various applications, such as phase identification, stress and texture analysis.

The fundamental equations for both stress measurement and texture measurement are developed with the matrix transformation defined for the two-dimensional diffraction. Stress measurement is based on a direct relationship between the stress tensor and the diffraction cone distortion. The structure information, such as grain size and preferred orientation, can be observed directly on the two-dimensional diffraction image. Phase identification can be done by integration over a selected range of diffraction rings. The integrated data gives better intensity and statistics, especially for those samples with texture, large grain size, or small quantity. The two-dimensional detector collects texture data and background values simultaneously for multiple poles and multiple directions.

Some experiments with silicon strip detector

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The X-Ray powder diffraction is, at present, the main application area of the silicon strip detector. Several prototypes of the detector dedicated to diffraction applications were developed by Dąbrowski, Gryboś and others [1], [2]. The presented results are obtained with the 128-channel strip silicon detector (with strip pitch 100 μm) installed at XPert diffractometer [3].
Experiments with powders were performed with use as follows: Ni-filtered Cu-radiation, Bragg-Brentano geometry, and Si and LaBi6 standard samples. Experiments were focused on the analysis of the diffraction peaks profile [4], [5]. The presented results will show: (a) effect of defocusing of the diffraction peak resulting from its registration off the focusing point (noticeable for small diffraction angles only), (b) the importance of Soller slits for reducing the effect of axial aberrations, and (c) measurement of the peak width as a function of the diffraction angle. The value obtained at small angles amounts about 0,05 deg. The standard LiF 200-oriented crystal was used for single-crystal experiments. The scan through 002 and 004 inverse lattice points demonstrate the high dynamic range of the detector, since the counts change in the range between 20 imp/s and 50 000 imp/s. The high reflectivity of the crystal allows to reach experimentally the limit of the counting rate of the examined silicon strip detector. (In experiments with polycrystals and thin films the detector counting rate will always be sufficient.)

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Sensitivity of a genetic algorithm to the mutation rate parameter value: results for a crystallographic test

Wojciech Paszkowicz[1)] poster D-10

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Genetic algorithms (GAs) represent a family of powerful global-search methods applicable to solving high-complexity optimisation tasks in science, technology and everyday life. The global-optimisation strategies based on the genetic approach mimic the evolution of living organisms. Applications in materials science,

physics, chemistry, crystallography, technology, industry, medicine, economy, communication can be found in literature. In crystallography and related fields, the GAs are used e.g. for molecular design, for structure prediction, and for solving structures. Moreover, they constitute an important tool for image analysis, e.g. in medicine, and can be used for analysis of various kinds of data collected at 2D detectors.
Mutation is one of operators employed in GAs. Typically, it consists of flipping a single bit with a small probability (mutation rate, M). Using this operator ascertains that whole parameter space is searched. The value of M is either fixed at the level 1% - 5%, or is adjusted during calculations. In the present study, the role of M value for the success and for the calculation speed is studied on a test example of powder-diffraction data of an orthorhombic crystal. The convergence of the algorithm was determined for 20000, 30000, 60000 and 100000 function calls (during 200-400 generations) on the basis of multiple test calculations. The probability of finding the global optimum is found to be strongly influenced by the M value. When M equals 1.8%, the chance for successful finding the global optimum is 0.2, only (in remaining cases the algorithm converged to some local minimum). The process of reaching the global minimum is fast then (stopping criterion of 20000 calls is sufficient). For the M value being twice as high (3.7), the chance for success increases to 0.8, but at expense of calculation time (stopping criterion of 100000 calls). The study demonstrates how sensitive is the algorithm to the value of the mutation rate.

Rietveld refinement of powder diffraction data collected with a laboratory diffractometer equipped with a linear X-ray detector

poster D-11

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Advantages of using a strip detector in the X-ray Bragg-Brentano diffraction geometry are presented. The instrument setting (described in detail in [1]) includes a semiconductor strip detector permitting for data collection with high counting rate and very good resolution. The installed detector (of construction related to those earlier reported [2-5]) is a commercial one with 127 active strips of 0.05 mm width. The X-ray beam is conditioned by selecting either an X-ray filter or a Johansson-monochromator. The latter option offers a high spectral purity and low background at the expense of reduced intensity. Nevertheless, the data collection using this setting is several times faster than that available at classical instruments. The data reveal peaks of even 0.1% intensity, enabling i) improved analysis results for minority phases in bulk polycrystalline samples, ii) detailed phase analysis of very thin polycrystalline layers and iii) diffraction studies of multilayer systems. The diffraction data of polycrystals are suitable for structure refinement by the Rietveld refinement. Refinement applications for various materials will be demonstrated. The applied modification of the Bragg-Brentano setting is concluded to create new quality in diffraction measurements.

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X-ray diffraction studies of thermal-expansion with the use of 1D detectors installed at synchrotron beamlines

poster D-12

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Thermal expansion studies using powder diffraction methods require long measurement time at classical sources. This can be improved by using combination o synchrotron X-ray source with a position sensitive counter. Experimental setting of this type should enable wavelength calibration, in order to eliminate possible, even small, wavelength instabilities: this goal can be achieved using a suitable internal standard [1]. In this presentation, examples of unit-cell size dependence on temperature determined at synchrotron beamlines with the use of linear imaging plate detectors will be demonstrated. The measurements were carried out at powder diffractometers at the B2 beamline at Hasylab/DESY (Hamburg, Germany) [2] and at I711 beamline at MAXlab Laboratory (Lund, Sweden) [3]. For structure refinement, the Fullprof program [4] was applied. Using the position sensitive detectors is found to ascertain a fst and accurate determination of thermal expansion behavior.

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Characterization of intermediate phases of Y-RE oxides by using image plate Guinier camera

Giora Kimmel[1], **Jacob Zabicky**[1], **Elena Goncharov**[1], **Dimitry Mogiliansky**[1], **Joseph Gal**[1] poster
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In a project of formation and characterization of intermediate phases between Y_2O_3 and RE_2O_3 (RE=rare earth element), we collected data using a new image plate Guinier camera installed (670 Huber) on a rotating Cu anode source (Ultrax 18 Rigaku), with a monochromator attached to the source providing $K\alpha_1$ radiation. This configuration enables fast scanning with high resolution. However, there are some limitations like: (a) the angle range is limited; (b) it is impossible to filter inelastic scattering; (c) in transmission mode only a small amount of powder can be loaded.
In order to evaluate the instrument quality we collected data from two sets of binary oxides $Dy_{2x}Y_{2-2x}O_3$ and $Gd_{2x}Y_{2-2x}O_3$ (0<x<1). The materials prepared by sol-gel technique, providing almost ideal samples for powder diffraction. The xerogel products were fired at different temperatures from 200 to 1400C resulting in powders with grain size from nano to micro. Nine intermediate phases were prepared. The crystal data were refined by the Rietrveld method. The scanning range was $5<2\theta<100$. The results were compared with previous references.

In spite of the camera limitations excellent results were obtained. The cell parameters found to be highly accurate. The RBragg for the intensities were between 0.02 and 0.06. The intensity quality for crystal refinement was better for the Y-rich samples, due to lower fluorescence emission and after firing at temperatures between 700 and 1000C due to optimal grain size for powder diffraction. A comparison of the above results with a conventional Bragg-Brentano diffractometer will be given for selected samples.

Microstructure of dislocation slip-band in p/p+ Si (001) by white beam diffraction topography and x-ray diffractometry

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We investigated the misfit dislocation(MD) nucleation and the dislocation morphology in lightly boron-doped Si epitaxial layers (20 Ωcm) on heavily boron-doped Si (001) wafer (0.015 Ωcm) (p/p+ Si) using white beam diffraction topography (WBDT) and high resolution x-ray diffractometry (XRD). The strain-relaxing MDs start to nucleate from the wafer edge and proceed to the center. Interestingly a dislocation slip-band morphology together with an orthogonal array of <110> type dislocations is able to be observed by WBDT, which has not been reported by conventional x-ray topography. The dislocation slip-bands are misoriented each other as measured by XRD. The misorientation gradually increases with approaching to the wafer edge. The existence of lattice misorientation is also confirmed by black-and-white dislocation contrast in x-ray topographs. These results indicate that the formation of cross-hatch patterns in p/p+ Si is caused by multiplication mechanism in MD nucleation, eventually enabling the strain field of MDs to extend to the top surface of the epitaxial layer.

Grain orientation-location measurement by combined use of x-ray topography with diffractometry

poster D-15

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Nondestructive probe with sensitivity to both orientation and location of individual grain has been strongly required due to the importance of local microstructure in studying structural dynamics of a material or its physical properties.
We developed a new x-ray diffraction microscopy technique capable of coupling grain orientation with its spatial location in textured materials. The grain orientation-location measurement is based on angular-resolved orientation contrast by combined use of x-ray topography with x-ray diffractometry using monochromatic, collimated x-rays.
By applying it to Y_2O_3/Ni, we demonstrated the capability of grain orientation-location measurement for the textured materials. Its useful applicability for local microstructural analysis was also demonstrated with the observation of the grain-on-grain microstructural correlation between the Y_2O_3 film grains and the Ni substrate grains. As a result, we found that on surface orientated Ni grains, Y_2O_3 film grains preferred growing along the crystallographic direction of the Ni(002) grains. On the contrary, on large misoriented Ni grains, Y_2O_3 grains grew along the surface direction rather than the crystallographic direction of the Ni(002) grains. This result indicates the possibility of different growth mechanisms of Y_2O_3 film grain, depending on misorientation of substrate Ni grain. This technique is expected to contribute further to understanding of mesoscale phenomena such as phase transformation and plastic deformation of textured materials.

Total electron yield X- ray absorption applied for hard materials studies

poster D-16

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The cubic boron nitride (c-BN) Ti composites are multiphase materials attractive due to combined high hardness and low friction, high corrosion resistance, suitable thermal and electrical properties. These materials are synthesized at high-pressure and high-temperature. Chemical reactions between activators (e.g. Ti compounds) and c-BN powder occur resulting in the formation of several phases. Some correlations between amount of these phases and mechanical properties were found. Due to existence of several phases with similar crystal structure and high hardness of these materials, quantitative analysis by powder X- ray diffraction failed. Nevertheless, the X-ray absorption method appears to be good tools for quantitative phase analysis of these hard materials. Most of the X-ray absorption studies (XAS) are performed either in transmission or fluorescence detection. In fluorescence one should avoid the self-absorption therefore the content of analyzed element should be around 1 at%. In transmission there is strict requirement for thickness of the samples, which imposes sample preparation (grinding, pellet pressing, etc.). It results in samples unrepresentative of the active state of materials in industrial practice. In such a case total electron yield (TEY) detection offers a good solution of problems. Highly concentrated as well as inhomogeneous materials can be investigated reliably. Studied samples were electrically isolated from the spectrometer and the drain current from the samples was measured. The edges of several elements were measured for all compounds formed in Ti composites and for composites. The studies were performed at HASYLAB (A1) in Hamburg and at Advanced Light Source (6.3.1) in Berkeley.
Acknowledgements
This work was supported in part by Polish State Committee for Scientific Research (Grant No 2P03B10625 and 2P03B05524) and by the IHP-Contract HPRI-CT-2001-00140 and G1MA-CI-2002-4017 (CEPHEUS) of the European Commission.

Application of a CCD detector for pulsed x-ray radiography of a gas jet target for laser-matter interaction experiments

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CCD detectors are commonly used in various applications such as digital cameras, spectrographs, sky telescopes, etc. Special type, back-thinned silicon CCD camera detectors, without entrance window, are sensitive to electromagnetic radiation in a wide range of wavelengths from IR to x-rays below 1 nm. Their sensitivity is linear in a wide range of photons number, unlike classical detectors such as photographic films. If cooled, such a detector keeps a charge induced by radiation for a relatively long time. It makes possible to obtain images with low level of noise. A CCD detector was applied for pulsed x-ray radiography of gas jet targets. The radiography method, with the use of a laser-plasma x-ray source was developed at the Institute of Optoelectronics, Warsaw. This paper presents results of the investigation of gas jet targets created from xenon or argon performed with the use of a CCD camera (Reflex s.r.o.). To produce gas jet targets, a commercial electromagnetic valve (Parker Instr.) was used. The x-ray radiograms of the target were obtained using radiation at the wavelength of about 0.75 nm, produced in krypton plasmas and filtered by 20-μm thick Si and 10-μm thick Be filters. A single shadowgram was taken by multiple 1 Hz exposition of a CCD sensor during about 20 s. The parameters of gas jet targets were determined. Spatial distributions of the particle density at the nozzle axis and the particle density profiles perpendicularly to the axis for various backing pressures and time delays between x-ray pulse and opening valve are presented. The characterized gas jet targets will be used in the experiments on interaction of ultra-short, high-intensity laser pulses with gases.

Analysis of stress in buried Ge layers by means of X-ray fluorescence

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The use of transmission EXAFS for concentrated systems is well established. In some cases, when the systems under investigation become increasingly dilute in the absorbing atom there is a point where the signal to noise (S/N) ratio favors alternative techniques which measure signals characteristic of the absorbing species (X-Ray fluorescence and Auger electron detection, for example). Auger emission and fluorescence are competing processes. Their relative strengths depend on the atomic number of the absorber. In light elements Auger emission is more probable, while for heavy elements fluorescence becomes more likely.
When energy discrimination is required, as for our samples, a fluorescence detector, single photon counting is necessary. Only the solid state and gas scintillation proportional detectors have resolutions sufficient for separating a fluorescence line from the background. The real need for energy resolution in the detector is to isolate interfering fluorescence lines from a multicomponent sample.
Samples for our studies were grown by molecular beam epitaxy of Ge and Si layers utilizing the Stranski-Krastanov growth mode on Si (001) substrates. We would like to present some EXAFS spectroscopy results for Ge single layers (with different thickness) buried in Si matrix at different temperatures of Ge layer deposition (about 210-250 and 700-750^{o}C).
These measurements were done with using of X-Ray fluorescence 7 element Si detector at the A1 station (HASYLAB), which is equipped with high energy resolution monochromator. To reduce a temperature disorder we prefer to perform the measurements at LN temperatures.
Using these techniques we observed the changes in atomic order around the Ge, and respectively Si, atoms in investigated samples depending on the growth conditions and both the Ge and Si layer thickness and compared the formed atomic order with that in crystalline Ge and Si, and solid solution with different concentrations of Ge (x=0.1-0.9).

Structural analysis of reactively sputtered W-Ti-N thin films

poster D-19

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The work is devoted to relationships between structural, electro-physical and diffusion barrier properties of W-Ti-N thin films, prepared by reactive dc magnetron sputtering from W-Ti (30 at.%) target in Ar-N_2 gas mixture. A dc power density of 1.7 W/cm^2 was applied to the target and the partial pressure of nitrogen was varied from 0 to 3.5x10^{-3} mbar at a total gas pressure of 5x10^{-3} mbar.
Phase composition and crystallite size were studied using X-ray diffraction method (Philips X'Pert MPD diffractometer with CuKα_1 radiation, equipped with a Johansson monochromator and a linear semiconductor strip detector). Surface morphology and root-mean square (RMS) roughness was examined using atomic force microscopy (NanoScope IIIa Dimension 3000 TM). The conductivity, stress and composition of W-Ti-N films were investigated using four-point probe sheet resistance measurements, stress measurement optical system and Rutherford backscattering spectrometry.
About ten layered samples were studied differing by nitrogen partial pressure applied during deposition. With increasing nitrogen partial pressure, the deposition rates decreased, what may be explained by lower efficiency of the nitrogen atoms with regard to argon atoms. Between the values of $p_{N2} = 0.2$ and 0.5x10^{-3} mbar, the deposition rate drops more steeply, which is indicative of changes in the sputtering mode (transition from a metallic to a nitride target), as well as in the film structure (from amorphous to polycrystalline films).
The resistivity of pure $W_{88}Ti_{22}$ film was 100 $\mu\Omega$cm and rose slowly up to 365 $\mu\Omega$cm for the ternary $W_{42}Ti_{12}N_{46}$ film. When the nitrogen partial pressure reaches $p_{N2} = 3.5\text{x}10^{-3}$ mbar, the resistivity of $W_{34}Ti_{11}N_{55}$ film is 850 $\mu\Omega$cm, which may be attributed to the reduction in crystalline size.

Phase relationships in annealed Cu-Al-O layers

poster D-20

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Complex materials structures based on Cu-Al-O layer on silicon and fused silica were studied. The Al-O and Cu-O film was deposited by reactive sputtering method. We used a CO_2 laser and furnace methods to change the structure of the Cu-Al-O layer.
X-ray diffraction method was used ex situ to study the change of Cu-Al-O structure caused by post-deposition thermal treatment. The diffraction patterns were recorded on a state-of-the-art diffractometer (Philips X'Pert MPD, with CuKα_1 radiation; $\lambda = 0.15406$ nm) equipped with a Johansson monochromator and a linear semiconductor strip detector.
The optical constants and film thickness were determined using commercial software for data collected at an ellipsometer (WVASE 32).
For investigation of the influence of process-dependent properties of film morphology, the tapping-mode atomic force microscopy was used. Chemical analysis of the interface region was conducted by X-Ray Photoemission Spectroscopy (XPS).
Samples with silicon substrate after post-deposition annealing in furnace in the temperature range of 873 - 1373 K at 1 hour exhibit the layer transparency and p-type conductance. The XPS characteristic shows the peaks at 944 eV and 947 eV attributed for Cu_2O, which is a well-known p-type oxide semiconductor. The very thin Cu_2O layer was formed on the top of thin films. From the electrical measurements in the van der Pauw configuration the layer has a resistance per square of about 211 Ω, holes mobility of 50.5 cm^2/ Vs and carrier density per square of about $5.8 \cdot 10^{14}$/cm^2.

The single particles approach of x-ray miroanalysis for estimation a phase composition of altered ilmenite used in pigments production

poster D-21

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To estimate phase and elemental composition of minerals used in industry, we have applied Electron Probe Microanalysis (EPMA) with standard and single particles approach. The quantitative analysis of the phase and elements content in the minerals used for chemical production is very important for the proper adjustment of chemical reactions. The composition of minerals can change depending on the place where they are mined and their phase and elements content is difficult to evaluate using standard approach. The example of ilmenite and titanium slag which are valuable sources of titanium widely used in industry of pigments production will be presented.
From standard powder diffraction pattern it is difficult to estimate quantitatively the content of phases due to overlapping the diffraction peaks and conventional x-ray fluorescence analysis does not measure of low Z-elements content, therefore quantitative element analysis is also difficult.
The optimal conditions for analysis of low Z-elements starting from carbon were selected to get information using EPMA about possible oxidation state of elements in minerals. Standard ZAF correction and single particles analysis were performed. The spectra measured in single particles mode were evaluated by non-linear squares fitting, using AXIL program. The elemental composition in the particles was calculated with an iterative approximation method based on Monte Carlo simulation. Received data were treated by statistical methods. Applying Hierarchical Clustering Analysis, the particles were divided into different groups, based on their compositional similarity and their relative abundances in the sample. The results of standard and single particles EPMA approaches will be compared and discussed.

Acknowledgments
This work was partially supported by the State Committee for Scientific Research (Republic of Poland) (Grant No72/E-67/SPB/5.PR UE/DZ 27/2003-2005) and by G1MA-CI-2002-4017 (CEPHEUS) of the European Commission.

X-ray fluorescence detection of iron in diaminoacid derivatives of protoporhyrin IX.

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The diaminoacid derivatives of protoporphyrin IX are promising in applications as photosensitizers in diagnosis and photodynamic therapy. Particularly derivatives with good water-solubility generate a lot of interests. It has been shown that due to the presence of selected amino acids residues attached to the porphyrin ring, these novel compounds penetrate more easily into tumor tissues and also clear from healthy tissues faster than others protoporphyrin-based photosensitizers. Nevertheless, the knowledge about chemistry and physical properties of these materials it still not sufficient. The one of not answered question is the role of Fe ions.
Several experimental techniques have been used for investigation of iron in protoporhyrin-like structures, but only few papers present the x-ray absorption approach. This motivated us to apply the XANES and EXAFS analysis to the study of ionic states and distribution of atoms around Fe in different diaminoacid derivatives of protoporphyrin. The content of Fe ions in the studied compounds are low and samples are nonconductive, therefore the only method of spectra detection is the fluorescence detection. Additionally, a set of iron-containing samples having different ionic states of Fe atoms was measured as a reference compounds. Measurements of Fe K-edges were performed at the HASYLAB beamline A1 using five-element Si detector. The samples were cooled down to LN temperature.
The differences in the position and intensity of the peaks of the radial distribution function can already be seen in raw data. To get more quantitative information, a model of the atomic distribution around the iron atom in the investigated samples was designed.

Acknowledgments
This work was supported in part by the Polish State Committee for Scientific Research (Grants No: 2-P03B-106-25, 2-P03B-055-24, and 2-P03B-090-19) and by the IHP-Contract HPRI-CT-2001-00140 and G1MA-CI-2002-4017 (CEPHEUS) of the European Commission.

Pilot study of the utility of diffusion tensor magnetic resonance imaging in lateralising non-lesional temporal lobe epilepsy.

poster D-23

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RATIONALE:
Approximately 40% of patients with medically refractory non-lesional Temporal Lobe Epilepsy (TLE) are not lateralised with current structural MRI techniques including volumetric analysis and T2 mapping. Diffusion tensor (DT) MRI is a relatively new MRI technology that has potential to detect functional abnormalities in patients with normal structural MRI.

Aims:
To perform a pilot study to assess the potential for DT MRI to lateralise non-lesional TLE.

METHODS:
Seven patients with non-lesional TLE (four with hippocampal sclerosis (HS) and four without HS on structural MRI), and well lateralised seizures on ictal-EEG were studied with DT MRI (1.5 Tesla, GE system) performed in 25 directions with b value: 1500 s/mm . The tensor signal was quantitated for voxels placed over the hippocampus and anterior temporal pole bilaterally and the side-to-side ratios correlated with the ictal EEG lateralisation.

RESULTS:
The tensor signal was higher on the epileptogenic side for the hippocampal voxels in 4/7 (71%) of patients, and for the anterior temporal voxels in 4/7 (51%) of patients.

CONCLUSION:
Fractional anisotropy shows a trend to be decreased in the hippocampus ipsilateral to the EEG lateralization. Quantitation of ADC with DT signal in the hippocampal region shows promise for lateralising non-lesional TLE in this pilot study, but further patients and correlation with surgical outcome is required before its role is established.

Quantitative study of Cd atoms distribution in CdTe/ZnTe quantum dots superlattice by HRTEM

poster D-24

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We investigated the CdTe/ZnTe stacked Quantum Dots (QD) superlattice by High Resolution Transmission Electron Microscopy (HRTEM). In the superlattice with 2 ML thick CdTe layer separated by 15 ML thick ZnTe spacer zones of autocorrelation arrangement of QDs was observed on cross-sectional samples . In the plane-view images of single QDs layer taken in <001> zone axis , it can be noticed that the islands have an asymmetric ellipsoid shape along the [100] and [010] directions, the two axis being 6-7nm and 3-4 nm in magnitude respectively and that their heights are below 1.5 nm. The measured strain $\epsilon_[001]$ component suggests the existence of a composition gradient in the lateral as well as in the vertical directions.
Model of super cell containing the cadmium rich QDs with $Cd_0.8Zn_0.2Te$ 1ML wetting layer was "relaxed" by molecular static elastic energy minimization. We have applied the discrete Stillinger-Weber (S-W) potential to Finite Element (FE) solver. For the purpose we have developed novel mesh generator which produced pseudo-elements compatible with S-W energy equations. The supercell with equilibrium x,y,z position of atoms obtained for boundary conditions corresponding to TEM was used to calculate images.The model verification is performed by the comparison of the strain maps measured from simulated images (Figure 2b) strain maps and experimental ones. Although, our approach cannot give unequivocal 3D distribution of cadium atoms in observed zone but the realistic model of anticorrelated CdTe/ZnTe QDs is possible to be obtained after few additional steps of model optimization.

Crystalline structure and surface morphology of Dy_xO_y films grown on Si

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poster D-25

In the last decade a lot of attention was devoted to study the high-k dielectrics (Si_3N_4, Al_2O_3, HfO_2, ZrO_2, La_2O_3) for producing the microelectronic devices and integrated circuits with the equivalent properties to very thin SiO_2. Among the high-k dielectrics being studied, Dy_xO_y appears promising due to its relatively high dielectric constant (k=12) as compared to SiO_2 (k =3.9). The crystalline structure and surface morphology of the Dy_xO_y films grown on Si substrates has been studied using grazing synchrotron radiation diffraction (XRD) and atomic field microscopy. The Dy_xO_y films were obtained by Dy evaporation in the Ar/O_2 (6%) environment followed by annealing in oxygen or argon. The crystalline structure of the Dy_xO_y films becomes better with increasing their thickness and deposition rate in Ar/O_2 environment. The "worth" fine-grained structure closed to amorphous is observed in the Dy_xO_y films with thickness 20.0-30.0 nm deposited at relatively low rates and annealed in oxygen. The thicker Dy_xO_y films deposited at higher rates and annealed in argon have the best polycrystalline structure. The Dy_xO_y roughness is correlated with their crystalline structure. The thinner Dy_xO_y films with the structure closed to amorphous are the smoother. The Dy_xO_y films roughness increases with increasing the drain sizes. There is conformity of the Dy_xO_y surface roughness to the underlying Si surface morphology. The smoother Dy_xO_y surface has the smoother Dy_xO_y-Si interface. The minimum value of the average interface roughness is found to be 0.8 nm in the Dy_xO_y films closed to amorphous. The average interface roughness is measured to be 1.2 nm and 2.0 nm in polycrystalline Dy_xO_y films annealed in O_2 and N_2, respectively. Based on the obtained results it is concluded that studied Dy_xO_y films are suitable for the further investigation as a gate dielectric in the MOS devices.

Image processing of HREM micrograph for determination size distribution of Co nanocrystals in Cu matrix

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poster D-26

Image processing combined with transmission electron microscopy is a powerful tool for investigation of size distribution of nano-objects. The high-resolution, bright- and dark-field images recorded on photo plates were digitalized and used as an input data for image analysis.
The Fourier filtering, autocorrelation, methods were applied for outline determination of Co precipitates. The influence of digitising condition, size and shape of Fourier masks, and parameters of reference regions will be discussed in respect to obtained results.

Modification of the nanostructure of the amorphised Si near-surface layer

Dorota Klinger[1)], **Elżbieta Łusakowska**[1)], **Danuta Żymierska**[1)], **Bolesław Kozankiewicz**[1)], **Lech Nowicki**[2)], **Anna Stonert**[2)], **Julian Auleytner**[1)]

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poster D-27

As a result of the implantation with a respectively high dose, a near-surface layer of highly disordered structure is created in semi-conducting materials. The implantation of Si with Sn^+ ions as well as with the Ge^+ ions is examined and compared due to relatively high mass of ions, sharp boundary between the amorphised layer and the crystal matrix. For crystal lattice reconstruction of the disturbed near-surface layer, ultraviolet laser pulse can be used. Evolution of defect structure is characterised by means of Rutherford back-scattering and atomic force microscopy. Nanosecond laser annealing can lead to the recrystalisation of the amorphised near-surface layer and to formation of misfit dislocations on the surface in the melted regions.

Equilibrium vapor composition in the Pb - I_2 system and mass transport in the PbI_2 - I_2 system

poster D-28

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The wide band gap semiconductor lead iodide (PbI_2) present interest from the practical point of view, since the perspective of their utilization for optical recording of information has been established, they are used in detectors of X-ray and gamma-rays, as well as in some other devices.
Large stoichiometric PbI_2 single crystals with a low dislocation density can be grown from the vapor phase in the presence of excess iodine. This process, however, has not yet been studied in sufficient detail.
The equilibrium vapor composition in the Pb - I_2 system at temperatures from 400 to 2000 K and total pressures from 102 to 105 Pa was assessed by thermodynamic analysis. The results show that the dominant vapor species is PbI_2. PbI_2 dissociation is significant starting at 1000 - 1300 K depending on the total pressure in the system.
PbI_2 transport in the PbI_2 - I_2 system is analyzed using a model of mass transport in a nonisothermal one-dimensional system of constant volume containing one or two vapor species. The derived equations provide a self-consistent solution to the problem of mass transport and pressure distribution in the system. Experimental results confirm that the rate of mass transport is governed by the source and deposition temperatures and iodine vapor pressure. The optimal conditions of PbI_2 crystal growth from the vapor phase are established.

Bolometers on macroporous silicon

poster D-29

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Multi-element IR-detectors of a new type - uncooled bolometric, pyroelectric and thermoelectric matrices have been actively developed during recent years. The important characteristics required of microbolometric matrices are a high temperature coefficient of electrical resistance, low excess noise and good radiation absorption in the working spectral region. The structures based on amorphous or polycrystalline silicon satisfy such requirements. In this work the results of research into macroporous silicon structures made by photoanodic etching are given. The two-dimensional photonic structures on the basis of the macroporous silicon are perspective due to capability of a electromagnetic spectrum transformation by macropores. The light-assisted method of electrochemical etching of n-Si allows the formation of cylindrical macropores with a high ratio of pore depth to pore diameter and with strong periodicity. Such structures are highly promising for modification of the electromagnetic wave spectra in semiconductor devices. Anomalous coefficients of light absorption allow the development of thermal- and photo-sensors on the basis of macroporous silicon.
In this work ohmic structures of the type In-n-Si and In-macroporous n-Si were formed by thermal evaporation of indium in an atmosphere of hydrogen. The bolometric characteristics of macroporous silicon were estimated. The temperature coefficient of resistance ranges from 0.4 - 1% at room temperature to 1.5 - 4% at 77K. Noise level is $(2x5)10^{-9}$ $VHz^{-1/2}$ for frequencies $>$ 10 Hz, and the detectivity of thermal bolometric elements on the base of macroporous silicon might be equaled $5x10^{9}$ $cmHz^{1/2}W^{-1}$. So the investigated macroporous silicon structures are promising for multi-element thermal sensor fabrication due to a high temperature resistance coefficient, low excess noise and good radiation absorption in the working spectral region.

SAXS time-resolved study of monosaccharide-based gel

poster D-30

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Thursday, September 9th

MODERN MATERIALS FOR ADVANCED DETECTORS MODERN DETECTORS FOR ADVANCED MATERIALS

Main Building, room 226

08:55 - 10:30

Recent results on disordered materials from the GEneral Materials Diffractometer, GEM, at ISIS

08:55 - 09:25
invited oral

Alex C. Hannon[1)]

1) Rutherford Appleton Laboratory, Oxon, United Kingdom

The recently constructed GEneral Materials diffractometer, GEM, at the ISIS pulsed neutron source, offers a number of novel features of advantage in the study of the structure of materials. The most important feature is the detector array, which covers a very large area with state-of-the-art scintillator neutron detectors. Eight detector banks cover a range in scattering angle, 2θ, from 1.1 to 169.3 deg., and azimuthal angles from -45 to +45 deg. These allow the neutron diffraction pattern to be measured with a high count rate over a very wide dynamic range.
The 17 metre incident flight path is relatively long, whilst the 5mm detector width is relatively narrow, and these lead to a good resolution which is best for back-scattering with a typical value 0.34% in the 160 deg. detector bank. The high resolution of GEM is well suited to structural studies of crystalline materials. The highest count rate is for the 90 deg. detector bank, which covers a very large solid angle and has a very low background, making it ideal for the study of time-dependent phenomena, such as crystallisation and phase transitions.
The high count rate of the 90 deg. detector bank also provides high quality data up to very high momentum transfers, Q, of about 60 Angstrom^{-1} in favourable cases. For studies of non-crystalline materials this yields an excellent real-space resolution for the correlation function. A novel design has been developed for the lowest angle detector bank which operates inside the sample tank vacuum, extending the minimum Q down to below 0.1 Angstrom^{-1} in favourable cases. An important area of growth for the scientific program on GEM has been in the overlap between crystallography and non-crystalline materials, for example the study of the structure of carbon nanotube materials. Pair correlation function methods, originally developed for the study of glasses and liquids, are now being applied to the study of disorder in crystalline materials.

Digital portable X-ray scanner working in quantum regime based on bulk undoped semi-insulating GaAs radiation detectors

09:25 - 09:45
oral

František Dubecký[1)], **Pavol Ščepko**[2)], **Bohumír Zako**[1)], **Vladimír Sekerka**[2)], **Vladimír Nečas**[3)]

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In the present work developed digital portable X-ray scanner is demonstrated. The scanner operates in "quantum" imaging mode ("single photon counting") with potential improvement of dynamic range in contrast of the observed X-ray images (e.g. [1]). "Heart" of the scanner - detection unit - is based on semi-insulating (SI) GaAs monolithic strip line detectors. Detector chip based on "SAMO" [2] topology is mounted onto flexible PCB support directly connected to the input of readout module through micro-connector. Detectors with pitch 0.25 mm and absorption length of strip 1.25 or 2.5 mm are arranged in the "edge on" irradiation configuration with an active area 0.25x0.22 mm^2. Detection efficiency of the SI GaAs detector reaches a value over 60 % of the theoretical one (75 %) for detection of 60 keV photons at a bias of 200 V. Readout electronics consists of 20 modules with 24 readout channels each fabricated using a progressive SMD technology with automatic assembling of electronic devices. Scanner line is 12 cm long having 480 readout channels and trace length is 15 cm. Position of detection module and position motion controller board are programmable controlled using PC through USB interface. System has the finest step 0.085 mm. Signals from counters included in digital parts of the modules are collected in the PC via USB and evaluated by custom developed software allowing X-ray image reconstruction. Collected data were used for creation of the first X-ray "quantum" images of various test objects using the developed imaging software. General technical properties of the scanner and future work-plan are discussed.

[1] B. Mikulec, Nucl. Instr. And Meth. A 510 (2001) 1.
[2] F. Dubecký, et al. Nucl. Instr. And Meth. A 458 (2001) 152.

09:45 - 10:30
invited oral

GaAs and SiC based position sensitive radiation detectors

Giuseppe Bertuccio[1,2)]

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In the last ten years, several compound semiconductors have been studied for realising X-ray detectors. The research activity is driven by three main guidelines: improving the detection efficiency by taking into account high Z materials, approaching room temperature operation with wide bandgap semiconductors, searching for materials resistant to radiation damage.
Gallium Arsenide has been intensively studied and interesting results have been recently reached demonstrating charge collection efficiencies of almost 100% and equivalent noise charge of 24 electrons r.m.s. (240 eV FWHM for X-rays) at room temperature and 16 electrons r.m.s. (160 eV FWHM) at -30C with pixel detectors. A detailed analysis of the noise sources in these detectors, including trapping phenomena, will be presented in order to highlight the margin of further improvements and the limiting factors of these detectors. In particular a study on the origin of the leakage current in Schottky and pn junction on GaAs will be presented. The relative importance of the front-end electronics for the optimisation of the resolution performance will be addressed as well.
Another material which is giving interesting results in the last few years is Silicon Carbide. SiC radiation detectors has been recently fabricated showing extremely low leakage current densities, down to few pA/cm^2 even above room temperature. SiC pixel detectors with 17 electrons r.m.s. (300 eV FWHM) at 27C and capable to operate at high temperature with adequate resolution have been realised. Equivalent noise charge of 44 electrons r.m.s. (797 eV FWHM) has been measured with the detector/front-end at 100C The present limits and the perspectives for further improvements of SiC detectors and related front-end electronics will be addressed.

10:30 - 11:00

Coffee break

11:00 - 12:30

NEW DEVELOPMENTS IN DETECTOR SCIENCE

Main Building, room 226

11:00 - 11:45
invited oral

Superconducting tunnel junction arrays for high-resolution X-ray spectroscopy

Stephan Friedrich[1)], **Owen B. Drury**[1,2)], **Stephen P. Cramer**[2,3)]

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2) University of California, Davis, Davis, CA, United States

3) Lawrence Berkeley National Laboratory (LBNL), Berkeley, United States

Superconducting tunnel junctions (STJs) can be used as fast high-resolution energy-dispersive X-ray detectors. STJs consist of two superconducting electrodes separated by a thin insulating tunnel barrier. Their operation as detectors is based on measuring the temporary increase in tunneling current after X-ray absorption in one of the electrodes produces excess charge carriers in proportion to the X-ray energy. STJ detectors offer an order of magnitude improvement in energy resolution over conventional Si(Li) or Ge detectors, because the superconducting gap is three orders of magnitude smaller than the energy gap in semiconductors. We have developed a Nb-Al-AlOx-Al-Nb STJ detector arrays and characterized them in synchrotron experiments. They have an energy resolution between 1.7 and 8.9 eV FWHM for photon energies between 50 and 1000 eV, and they can be operated at count rates exceeding 10,000 counts/sec per pixel. For STJ operation in synchrotron-based high-resolution X-ray spectroscopy, we have designed a two-stage adiabatic demagnetization refrigerator (ADR) with a cold finger to hold the STJ inside the UHV sample chamber at a temperature of 0.1 K within 15 mm of a room temperature sample. We will discuss the performance of the spectrometer with special emphasis on its response function and on recent upgrades to improve its efficiency. We will also present different representative applications in material science, such as the characterization of novel semiconductors and superconductors.

3D position sensitive detectors for pattern recognition applications

11:45 - 12:30
invited oral

Rodrigo F. Martins[1], **Hugo Águas**[1], **Daniel Costa, Sónia Pereira, António Marques, Isabel Ferreira, Elvira Fortunato**

1) Centro de Investigacao em Materiais (CENIMAT/ Fac), Campus Caparica, Caparica 2829-516, Portugal

This paper presents results of the spatial and frequency detection limits of an integrated array of 32 one-dimensional amorphous silicon thin film position sensitive detectors with a nip or MIS structure, under continuous and pulsed laser operation conditions. The data obtained show that 0.45×0.06 cm arrays, occupying a total active area of about 1 cm2 have a spatial resolution better than 5 [U+F06D]m (modulation transfer function of about 0.2), with a cut-off frequency of about 6.8 KHz. Besides that, under pulsed laser conditions the device non-linearity has its minimum (about 1.6%), for a frequency of about 200Hz. Up to the limits of the cut-off frequency, the device non-linearity increases to values above 4%. Sensitivities above 50 mV/cm were achieved with linearity near to 99%. Besides that, by using a MIS structure based on ZnO allows an improvement of spectral response towards the UV region, with its maximum response at 540 nm.

Lunch break

12:30 - 14:00

APPLICATIONS OF 1D/2D DETECTORS IN PARTICLE PHYSICS, ASTROPHYSICS AND MEDICINE

Main Building, room 226

14:00 - 15:30

2D detectors for particle physics and for imaging applications

14:00 - 14:30
invited oral

Hans Krüger[1]

1) Univ.Bonn, Bonn, Germany

The demands on detectors for particle detection as well as for medical and astronomical X-ray imaging are continuously pushing the development of novel pixel detectors. The state of art in pixel detector technology to date are hybrid pixel detectors in which sensor and read-out integrated circuits are processed on different substrates and connected via high density interconnect structures. While these detectors are technologically mastered such that large scale particle detectors can be and are being built, the demands for improved performance for the next generation particle detectors ask for the development of monolithic or semi-monolithic approaches. Given the fact that the demands for medical imaging are different in some key aspects, developments for these applications, which started as particle physics spin-off, are becomming rather independent. New approaches are leading to novel signal processing concepts and interconnect technologies to satisfy the need for very high dynamic range and large area detectors. The present state in hybrid and (semi-)monolithic pixel detector development and their different approaches for particle physics and imaging application is reviewed.

Semiconductor detectors for X-ray imaging spectrometry in space

14:30 - 15:00
invited oral

Gerhard Lutz[1]

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X-ray astronomy is a fairly young branch of science. This is due to the necessity of placing the detectors outside of the earth's atmosphere. Imaging was a further problem. Initially coded mask imaging the more sophisticated equivalent of pin hole cameras was used. Making use of the fact that X-rays are totally reflected when impinging with very shallow angle on a extremely smooth mirror surface, allowed the construction of focusing X-ray mirror telescopes, as they are used today. The first of those telescopes launched into orbit used gas proportional chambers as focal plane detectors. These detectors have high enough spatial resolution to match the optical properties of the mirror telescopes. They lack however the energy resolution to do direct spectroscopy. Only a very rough measure for the X-ray energies is available.
The situation changed dramatically with the launch of two X-ray observatories CHANDRA and XMM/Newton in 1999. Both of them use CCD detectors for focal imaging. While CHANDRA with its single telescope uses modified optical MOS CCDs, XMM/Newton has in one of its three telescopes a CCD based on a novel principle. This "pn-CCD" has been developed from scratch specifically for this mission and exceeds the properties of all other CCDs used at present in X-ray astronomy. After nearly five years of continuous operation the detector properties have not deteriorated. An advanced type of pn-CCDs has been developed for the ROSITA and DUO missions. A completely new device, the DEPFET pixel detector is under development for the future European X-ray observatory XEUS.
The function principles and properties of the detectors will be described and illustrated with results obtained in space. Their use in other applications will be discussed.

Medical quantum X-ray imaging with 2D detectors

15:00 - 15:30
invited oral

Jürgen Giersch[1)]

1) Universität Erlangen-Nürnberg, Physikalisches Institut 4, Erwin-Rommel-Straße 1, Erlangen 91052, Germany

After W. C. Roentgen has discoverd his X-rays the benefit for medical diagnostics has been perceived very early. Since then a lot of improvements have been achieved, but modern radiographic systems use still the same principle: the energy of the photons hitting a picture element are integrated over the exposure time. This means that the information about the indiviual photon energy is lost.
In medicine it is important to get as much information as possible by the dose being applied. A so-called quantum imaging system is capable of discerning and processing each single X-ray quantum and is therefore very attractive for medical application. A first step in this direction are photon counting detectors, where each pixel determines the number of the incident photons.
Recent developments have lead to a hybrid pixel detector concept which is a very promising approach for quantum imaging. These detectors are sandwich structures consisting of two flip chiped layers - an X-ray absorbing semiconductor and a read out electronic chip. Both layers are connected by bump bonding technology.
The Medipix2 detector is a very powerful realisation of such a photon counting system. The Medipix2 has an active area of 1.4 by 1.4 cm^2 consisting of 65000 parallel working photon counting pixel cells with a size of 50 μm. The Medipix2 readout chip can be combined with different absorbing materials like Silicon, Gallium Arsenide or Cadmium Telluride.
The challenge in hybrid pixel detectors for medical application is the realisation of large area detectors. But there are already proposals on how to overcome the smallness of a single detector.
Photon counting detectors like Medipix2 might be just the beginnig of a new exciting evolution, the aim could be a spectroscopic pixel detector which is capable of measuring the energy of each single photon. Monte Carlo simulations show that such a detector would lead to a big benefit in X-ray imaging in future.

Coffee break

15:30 - 15:50

RECENT AND FUTURE DEVELOPMENTS IN DETECTOR TECHNOLOGY

15:50 - 17:50

Main Building, room 226

15:50 - 16:20
invited oral

Recent developments in 3D and active edge silicon detectors

John Morse[4], **Sherwood I. Parker**[3], **Cinzia DaVia**[2], **Jasmine Hasi**[2], **Christopher J. Kenney**[1], **Edwin M. Westbrook**[1]

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We are developing pixel sensors with '3D' structures in which columnar electrodes penetrate the entire bulk of high resistivity, silicon substrate. Unlike conventional, planar processed p-n junction diode detectors, which collect deposited electric charge at their surface electrodes, the buried electrodes of the 3D devices create internal electric fields that sweep electric charge laterally within the silicon bulk. This new architecture offers several performance advantages, albeit at the cost of more complex device processing. 3D detector s have now been chosen for large area, pixel detector arrays to replace the phosphor screen-CCD detector systems currently used for protein crystallography, and for HEP applications requiring exceptional radiation hardness. By the use of vertical plasma processing, both 3D and 2D planar detectors have been processed with 'active edges', a technology that ensures charge collection to within a few microns of the physical edge of the device.

We describe the fabrication of these detectors and present some of the test data obtained to date using both synchrotron X-ray microbeams and minimum ionizing particle beams. New data will be presented of energy resolved response maps made using a micron size X-ray beam at the ESRF, that enabled precise measurement of the charge-splitting boundary zones between pixel cells; and the response at the edges of the detectors.

Panel discussion on the future of radiation sensors and detectors in European research and industry

16:20 - 17:50
oral

__Heinz Graafsma__[1], **Erik Heijne**[3], **John Morse**[2]

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With the current developments in micro-electronics and interconnect technologies new and exciting possibilities exists for developing revolutionary new sensors for radiation imaging. The deep sub-micron CMOS technologies (0.13 micron or 0.09 micron) allow one to integrate many signal processing steps into small cells (pixels), resulting in intelligent pixel array sensors. At the same time, new developments in interconnect technologies, driven by the packaging industry (mobile phones for example), allow for the development of stacked modules. The combination of these two developments can provide highly integrated and intelligent sensors. Therefore, the technology is potentially available. Whether, these technologies will also be available for the scientific community is uncertain, simply because of the exponential increase in development costs. Europe has traditionally had a world leading position in "sensor" development, in part due to large scale scientific projects like CERN. To keep this world leading position European research, will have to work together with European industry and European policy makers and funding agencies. The discussion will be introduced by short presentation to set the scene.

Friday, September 10th

POSITION SENSITIVE DETECTORS AT LARGE SCALE FACILITIES

Main Building, room 226

09:00 - 10:30

Towards high-rate and high-resolution time-of-flight area detectors for spallation neutron sources like ESS

09:00 - 09:45
invited oral

B. Gebauer[1]

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Complementary to synchrotron-radiation studies, neutron scattering and diffraction methods are of utmost importance for probing the structure and dynamics of matter at an atomic, molecular and mesoscopic level, however today often suffering from comparatively low source strength. This will change with next generation pulsed spallation neutron sources with MW average proton beam power, which will allow accumulating and analyzing for each neutron pulse a large wavelength band by time of flight. For imaging and diffraction experiments at the strongest projected spallation source ESS in the current EU Joint Research Activity DETNI large-area time-of-flight resolving thermal neutron detectors are being developed with two-dimensional spatial resolution and rate capability down to 50 μm and up to 100 MHz per detector, respectively. In this talk an overview will be given - in comparison with the current state-of-the-art - on novel solutions for thermal neutron detectors, comprising, for instance, silicon micro-strip detectors for neutron radiography applications, hybrid low-pressure micro-strip gas chamber and gas electron multiplier (GEM) detectors with solid neutron converters, and the related front-end ASIC development.

09:45 - 10:30
invited oral

Large area X-ray detectors at the Swiss Light Source

Eric F. Eikenberry[1)], **Ch. Broennimann**[1)], **G. Huelsen**[1)], **H. Toyokawa**[2)], **M. Suzuki**[2)], **R. Horisberger**[1)], **B. Schmitt**[1)], **T Tomizaki**[1)], **A. Wagner**[1)]

1) Paul-Scherrer-Institut, Villingen CH-5232, Switzerland

2) Japan Synchrotron Radiation Research Institute (SPring-8), 1-1-1 Kouto, Mikazuki-cho, Sayo-gun, Hyogo 679-5198, Japan

A large area counting pixel detector for X-rays has been implemented at the Swiss Light Source (SLS). The format is an 1120 x 967 array of 0.217 x 0.217 mm^2 pixels covering an area of 24.3 x 21.0 cm^2. The detector is modular, with each of the 18 modules having an 80 x 34 mm^2 monolithic pixilated silicon sensor bump-bonded to a 2 x 8 array of custom CMOS readout chips. Each pixel in the readout chip contains an amplifier, a single level discriminator and a 15-bit counter. The readout time of the detector is 6.7 ms, after which counting is re-enabled. However, the framing time is limited to 600 ms by the overhead of transferring the image to disk.

This detector has been successfully used to record protein crystallography data at beamline X06 of the SLS. The detector is especially well-suited to recording fine-ϕ-sliced data in which the crystal is rotated continuously and the frames are defined by the detector without the use of a mechanical shutter. In this mode, 9000 frames covering a rotation of 180 deg were recorded at 1 frame/s for crystals of insulin and thaumatin. Analysis of these data is in progress. Traditional 0.5 deg rotation data sets of these specimens were also recorded.

Several single-module detectors have been built from the same modules. These have proved very popular at the Materials Science beamline (X04) of the SLS, and in both diffraction and X-ray diffraction experiments at SPring-8. In applications where traditional practice has been to use a point detector, the speed and greater information content of area detector images is greatly appreciated.

10:30 - 11:00

Coffee break

11:00 - 11:40

POSITION SENSITIVE DETECTORS: APPLICATIONS FOR MODERN MATERIALS

Main Building, room 226

11:00 - 11:20
oral

Confinement effects by means of dielectric methods

Małgorzata M. Śliwińska-Bartkowiak[1)], **Monika Jażdżewska**[1)], **Ravi Radhakrishnan**[3)], **Keith E. Gubbins**[2)]

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3) Massachusetts Institute of Technology, Chemical Engineering Department (MIT), 77 Massachusetts

Avenue, Cambridge, MA 02139, United States

We report experimental and molecular simulation studies that confirm the presence of a hexatic phase in narrow pores. On heating, starting with a solid crystalline phase in the pore, two transitions are observed, the first being crystal to hexatic, and the second occurring at a higher temperature from hexatic phase to liquid. The molecular simulations are for large systems (64,000 molecules) and free energies are determined by the Landau free energy method. These clearly show the two transitions, and the nature of the confined phases are determined by measurement of the spatial and orientational correlation functions. Finite size scaling methods are used to show that these transitions persist in the large system limit. For the narrower pore width studied, only one layer of adsorbate molecules can be accommodated in the pore, and the transitions are second order. With a larger pore two adsorbed layers can be accommodated, and the transitions become first order. The results are consistent with the Kosterlitz-Thouless-Halperin-Nelson-Young theory for melting in two dimensions.
Experimental studies are reported for carbon tetrachloride and aniline adsorbed in activated carbon fibers having slit-shaped pores. Differential scanning calorimetry, dielectric relaxation spectroscopy and nonlinear dielectric effect measurements were made. The measurements show two transitions at temperatures that are in good agreement with those found in the simulations for the crystal/hexatic and hexatic/liquid transitions for both carbon tetrachloride and aniline in activated carbon fibers. Recently a similar effect was found for benzene in ACF.
In conclusion, we find that (a) a hexatic phase can occur in narrow pores, (b) the phase occurs even for simple molecules, and is stabilized by the confinement of the pore; thus it occurs over much broader temperature ranges than has been observed in bulk fluids.

Area detector as a tool to study properties of the magnetic multilayers by the neutron scattering

11:20 - 11:40

Wojciech Szuszkiewicz[2], Krzysztof Fronc[2], Frederic Ott[1], Bernard Hennion[1], Marta Aleszkiewicz[2], Roman Minikayev[2], Wojciech Paszkowicz[2] oral

1) Laboratoire Leon Brillouin, CEA-CNRS, CE Saclay (LLB), Gif sur Yvette 91191, France

2) Polish Academy of Sciences, Institute of Physics, al. Lotnikow 32/46, Warszawa 02-668, Poland

Magnetic quantum structures and magnetic multilayers have been intensively investigated within the last years because they offer unique properties of a large-scale integration devices. Such properties can bo of practical importance (echange interlayer magnetic coupling, giant magnetoresistance etc.) leading to applications in spintronics like, e.g., spin injectors, valves or filters.
The efficiency of given device strongly depends on the crystal quality of layers involved in the structure, on the properties of interfaces, and on the character of magnetic structures at the surface and inside the layers. The chemical quality of the interface (like, e.g., its roughness or a range of diffusion of constituent elements) can be determined by X-ray reflectometry. In the case of magnetic structures, an important point is to characterize the "magnetic" quality of the interface and lateral distribution of magnetization which requires an application of the neutron scattering techniques.
The goal of our work was to present a selected example of application of the area detector in the neutron scattering studies.
The quality of interfaces for Fe/FeN multilayers (deposited in UHV sputtering system and checked by X-ray reflectometry at the Institute of Physics of the Polish Academy of Sciences in Warsaw) was characterized by the spin-polarized neutron reflectometry. Neutron scattering studies were performed at Laboratoire Leon Brillouin in Saclay (France) using two-dimensional neutron detector developed recently in this laboratory. Obtained results are shown and discussed.

Closing address

11:40 - 11:50

Lunch break

12:30 - 14:00

Symposium E

Superconductors - New Developments, New Materials, New Applications and Nanoscale Investigations

Introduction

The scientific aim of this symposium is to provide a forum for the discussion of various newly developed aspects of superconducting materials research. Many topics will be covered: novel perovskite and non-perovskite superconductors, vortices and flux pinning, chemical substitutions and radiation defects, grain boundary engineering, embedded nanoparticles, superconducting nanopowders, superconducting films and heterostructures, nano-engineered structures, pinning arrays and mesoscopic superconductors, nano-characterization techniques, and advanced superconducting detectors and sensors. We would like to thank all the invited speakers and other participants of the symposium for the work required to prepare their presentations and we wish all participants a successful meeting in Warsaw.

Organisers

- Marta Z. Cieplak, Institute of Physics, Polish Acad. Sciences, Warsaw, Poland
- Cornelius J. van der Beek, Laboratoire des Solides Irradis, Ecole Polytechnique, Palaiseau, France;
- Michael R. Koblischka, Universtaet des Saarlandes, Saarbruecken, Germany;
- Katarzyna Karpinska, Institute of Physics, Polish Acad. Sciences, Warsaw, Poland
- Roman Puniak, Institute of Physics, Polish Acad. Sciences, Warsaw, Poland
- Andrzej Winiewski, Institute of Physics, Polish Acad. Sciences, Warsaw, Poland

Scientific Committee

- M. V. Feigel'man (Moscow, Russia),
- L. Forro (Lozanne, Switzerland),
- P. Samuely (Kosice, Slovakia),
- H. Szymczak (Warsaw, Poland),
- H. W. Weber (Vienna, Austria).

Proceedings

Papers will be published in physica status solidi (c).

Monday, September 6th

14:00 - 15:30

Afternoon session

Main Building, room 144

14:00 - 14:45
invited oral

High-current properties of ultrathin YBCO films

Wolfgang Lang[1)], **Ionut Puica**[1)], **Martin Peruzzi**[2)], **Katharina Lemmermann**[2)], **Johannes D. Pedarnig**[2)], **Dieter Bäuerle**[2)]

1) University of Vienna, Institute of Materials Physics, Vienna, Austria

2) Johannes-Kepler-University Linz, Applied Physics, Linz, Austria

The critical current density of a superconductor as a function of temperature and magnetic field is a key quantity for the design of superconductor applications. Some superconducting devices, e.g. fault current limiters, operate into the supercritical current range by design and benefit from the understanding of the superconducting transition in high current densities. Tremendous efforts are currently undertaken to enhance the critical current in technical materials by improving the pinning forces but are limited by the superconducting depairing current that usually cannot be measured directly. Only few experiments have explored the supercritical current region so far. We report on such measurements in extremely high current densities. In order to avoid thermal heating and eventually destruction of our samples that results inevitably from such high dissipation, the measurements are carried out using short-pulse currents with about 50 ns duration. In addition, we use ultrathin films of YBCO, patterned to microbridges to allow for an effective heat transfer into the MgO substrate. The results allow for a direct determination of the depairing current and are in good accordance with the theoretically predicted values. In intense currents the critical temperature is not only shifted to lower temperatures, as seen in conventional measurements, but the shape of the transition changes significantly. The latter effect is attributed to a reduction of the fluctuation paraconductivity with increasing electric field and is compared with our recent theoretical work. Other effects that emerge when supercritical currents are applied to high-temperature superconductors are reviewed, too.

14:45 - 15:30
invited oral

Electric Field Effect Experiments in Thin $Nd_1Ba_2Cu_3O_{7-\delta}$ Films

Daniel Matthey[1)], **Stefano Gariglio**[1)], **J.-M Triscone**[1)]

1) DPMC, University of Geneva, 24 quai Ernest-Ansermet, Geneva 1211, Switzerland

We report on the electrostatic modulation of superconductivity in ultrathin $Nd_1Ba_2Cu_3O_{7-\delta}$ films grown by RF magnetron sputtering using different field effect devices. In epitaxial ferroelectric Pb(Zr,Ti)O_3 / $Nd_1Ba_2Cu_3O_{7-\delta}$ heterostructures, we have used the reversible ferroelectric polarization field to modulate the carrier density of the thin superconducting oxide films. In lithographically patterned structures, reversing the polarization field of the ferroelectric Pb(Zr,Ti)O_3 layer allows large non-volatile modification of the critical temperature of the superconducting films to be obtained without introducing chemical or structural defects. We will also discuss reversible modifications of the superconducting properties in ultrathin $Nd_1Ba_2Cu_3O_{7-\delta}$ films using a novel field effect device based on a single crystal $SrTiO_3$ dielectric gate insulator. With this device, the polarization can be precisely measured allowing the dependence of the superconducting critical temperature on the carrier concentration in the underdoped region of the phase diagram to be determined.

15:30 - 16:00

Coffee break

16:00 - 17:15

Afternoon session - continued

Main Building, room 144

Identification of vortex phases in superconductors from spatially and time resolved magnetic measurements

16:00 - 16:45
invited oral

Marcin Konczykowski[1)], **Cornelis J. van der Beek**[1)], **Vincent Mosser**[3)], **Eli Zeldov**[2)], **Peter H. Kes**[4)]

1) Ecole Polytechnique (X), route de Saclay, Palaiseau 91128, France

2) Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel

3) Schlumberger Utilities Technology Group, Montrouge 92542, France

4) Kamerlingh Onnes Laboratory, Leiden University, Niels Bohrweg 2, Leiden 2333 CA, Netherlands

The understanding of the phase diagram of vortex matter in superconductors is a key issue, both for fundamental physics as well as for applications. The advent of the high temperature superconductors (HTSC) has triggered a big interest in this field, because of the richness of the of vortex matter phase diagram in these compounds. The phase diagram includes a vortex liquid phase and the possibility of a new Brag-glass to vortex-glass transition within the solid phase. Highly anisotropic compounds of the HTSC family exhibit additional phenomena related to the possible decomposition of vortex lines into stacks of point like "pancake" vortices, and the coexistence of crossed lattices of Josephson and Abrikosov type vortices. The dynamic properties represent one of the fundamental properties differentiating these vortex phases. In order to access those properties, we have developed a number of specific measurement techniques based on spatially and time resolved micro Hall probe magnetometry. We will present the experiments carried out on an archetypical layered HTSC, single crystalline BSCCO:2212. We have used heavy ion irradiation in order to introduce well-controlled defects in the form of columnar defects, acting as pinning centres for flux lines and modifying the phase diagram of vortex matter.

Vortex fluctuations in underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystals

16:45 - 17:15
oral

Sylvain Colson[1)], **Marcin Konczykowski**[1)], **Marat B. Gaifullin**[4)], **Yuji Matsuda**[4)], **P. Gierłowski**[2)], **Ming Li**[3)], **Peter H. Kes**[3)], **Cornelis J. van der Beek**[1)]

1) Ecole Polytechnique (X), route de Saclay, Palaiseau 91128, France

2) Polish Academy of Sciences, Institute of Physics, al. Lotnikow 32/46, Warszawa 02-668, Poland

3) Kamerlingh Onnes Laboratory, Leiden University, Niels Bohrweg 2, Leiden 2333 CA, Netherlands

4) Institute for Solid State Physics, University of Tokyo, Chiba 277-8581, Japan

Thermal fluctuations of vortices were studied by microwave measurements of the Josephson Plasma Resonance (JPR) in small single crystals of underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ with a critical temperature T_c = 69.4 K and a zero-field JPR-frequency of approx. 61 GHz. The penetration depth along the c-axis and the anisotropy ratio γ were calculated from zero-field data. The dc magnetic field and temperature dependences of the wandering length of pancake vortices were examined over the entire vortex solid state and explained by the renormalization of the vortex line tension by the fluctuations, finally leading to the dissociation of the vortices at the first order transition.

Poster session

19:00 - 21:00

The effect of film-substrate mismatch on the properties of superconducting $YBa_2Cu_3O_{7-\delta}$ films

Iryna S. Abalosheva[1)], **Zbyszek Adamus**[1)], **Marta Z. Cieplak**[1)], **Marek Berkowski**[1)]

1) Polish Academy of Sciences, Institute of Physics, al. Lotnikow 32/46, Warszawa 02-668, Poland

poster
E-1

The lattice mismatch between the substrate and the film is known to influence strongly the properties of thin films. In superconducting films this may result in the decrease, or, in some cases, in the enhancement of the superconducting transition temperature. It usually affects also the behavior of critical currents which allows accessing the nature of vortex pinning in the films.
In this contribution we study the effect of the in-plane epitaxial mismatch between the substrate and the film on the crystallographic structure and the transport properties of $YBa_2Cu_3O_{7-\delta}$ superconducting films of thicknesses ranging between 600A and 3000A. The films are grown by pulsed laser deposition on the new type of single-crystalline substrates prepared by Czochralski method, with the chemical formula $(SrAl_{0.5}Ta_{0.5}O_3)_{0.7}(CaAl_{0.5}Ta_{0.5}O_3)_{0.1}(LaAlO_3)_{0.2}$, with the in-plane lattice parameter a = 3.8741A. We

find that superconducting properties of the samples are excellent, and generally they improve with increasing of the film thickness as a result of improved structural ordering. We also investigate the influence of the film thickness on the behavior of the critical current densities, and compare the results with the behavior studied previously for other types of substrates [1].

[1] C. J. van der Beek, M. Konczykowski, A. Abaloshev, I. Abalosheva, P. Gierłowski, S. J. Lewandowski, M. V. Indenbom, S. Barbanera, "Strong pinning in high temperature superconducting films", Phys. Rev B. 66, 024523 (2002).

The enhancement of vortex pinning in ferromagnet-superconductor bilayers

poster
E-2

Marta Z. Cieplak[1], Zbyszek Adamus[1], O. Abal'oshev[1], I. Abal'osheva[1], A. Byczuk[1], Marek Berkowski[1], Marcin Kończykowski[2], X.M. Chen[3], Hai Sang[3], C.L Chien[3]

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3) Department of Physics and Astronomy, The Johns Hopkins University, Baltimore 21218, United States

The pinning of vortices in structures consisting of a superconducting layer on the top of magnetic dots or holes, or ferromagnet/superconductor bilayers (FSB) attracts much attention [1-4]. The interest is generated by both the technological promise of devices in which small magnetic field can tune the magnitude of the critical current by adjusting the flux pinning, and by the general scientific interest in properties of "vortex matter". In this study the influence of the magnetic domain reversal on the flux pinning in two different types of FSBs is investigated. The ferromagnetic (FM) layer in both types of FSBs is a cobalt/platinum multilayer with perpendicular magnetic anisotropy, grown by magnetron sputtering. The superconducting layers are either niobium, which is grown on the top of FM layer, or $YBa_2Cu_3O_7$ (YBCO). In this second case the YBCO layer is grown first by the pulsed laser deposition, and the FM layer is grown on the top of it. The global magnetization is measured with the SQUID magnetometer, and the local flux profile in the SC film is probed using an array of Hall sensors. A strong enhancement of the vortex pinning is observed when the magnetic domain reversal of the FM layer is about 80% advanced. Using magnetic force microscopy imaging we demonstrate that the pinning is related to the dendrite-shaped domains left behind during the reversal process which proceeds primarily via the domain-wall motion. The details of the flux profile evolution with the FM domain reversal will be discussed.

[1] M. Baert, et at., Phys. Rev. Lett. 74, 3269 (1995).
[2] M. Lange, et at., Appl. Phys. Lett. 81, 322 (2002).
[3] D. B. Jan, et at., Appl. Phys. Lett. 82, 778 (2003).
[4] L. N. Bulaevskii, et at., Appl. Phys. Lett. 76, 2594 (2000).

Critical Characteristics of Superconducting Thin Films Modified by an Atomic Force Microscope

poster
E-3

Hyeong-Gon Kang[3], Kwang-Yeop Jahng[3], Seokcheol Ko[2], Haeseong Lee[1], Sung-Hun Lim, Byoung-Sung Han[2]

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3) Basic Science Research Institute, Chonbuk National University, 664-14, Duckjin-Dong 1Ga, Jeonju Chonbuk 561-756, Korea, South

An atomic force microscope (AFM) has played a key role in nanotechnology as not only a microscopic tool but also a fabricating tool. In this study the AFM was used in fabricating a superconducting flux flow transistor(SFFT) and characterizing the structure of the fabricated transistor. The SFFT is composed of a control line for producing the magnetic field and a body line with a channel. An applied current in the control line controls the critical current density of the body line and generates a voltage over the critical current density. The surfaces of superconducting thin films were modified in order to control the superconducting flux flow using the AFM lithography. This technique is a mask-less process and an effective method to overcome the difficulties in fabricating a nano size channel when a conventional lithography is applied. Superconducting stripes were patterned on LaAl2O3 substrates by the conventional lithography method. The center of the stripe was selectively oxidized by an AFM probe in the presence of the electric field between the probe and the stripe. Then the oxidized surface was analyzed by the AFM image and the critical current density was measured later on. The roughness increased with the number of scanning and an applied voltage, which means that the critical characteristics of superconducting thin films can be controlled by AFM oxidation process. This study reveals that the AFM technique exhibits its capability to fabricate the superconducting flux flow transistors with nano-channel.

Fluctuations and Dark Count Rates in Superconducting NbN Single-Photon Detectors

Andreas Engel[1,2], **Alexei Semenov**[2], **Heinz-Wilhelm Hübers**[2], **Konstantin S. Ilin**[3], **Michael Siegel**[3]

poster E-4

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3) Universität Karlsruhe, Karlsruhe 76128, Germany

As the size of superconducting structures in one or more dimensions are more and more reduced fluctuations in the superconducting phase become increasingly important. These fluctuations lead to noise in thin-film or nano-structured detectors and ultimately limit their sensitivity. Fluctuating quasi-particle numbers and temporarily created vortex-antivortex pairs are two possible noise-sources near the superconducting phase transition. We considered thermodynamic fluctuations occurring with a probability proportional to exp($-\Delta F/k_B T$), where ΔF is the change in free energy, k_B the Boltzmann constant and T the temperature. ΔF itself is temperature and current dependent in a non-trivial way. We will present model calculations and compare the bias-current and temperature dependence with experimental dark count rates obtained for a NbN single-photon detector. The detector consisted of a thin and narrow meander, which was biased with a direct current slightly less than the temperature dependent critical current. Sufficiently large fluctuations caused voltage transients very similar to those caused by absorbed visible and near-infrared photons and are the major contribution to the measured dark count rates.

Current-Voltage Characteristics of Superconducting Flux Flow Transistor with Multi-Channel Fabricated by Inductively Coupled Plasma

Seokcheol Ko[1], **Byoung-sung Han**[1], **Hyeong-Gon Kang**[2], **Hyo-Sang Choi**[4], **Myoungho Choi**[3]

poster E-5

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3) Department of Medical Information Engineering, Kwangju Health College, 683-3, Sinchang-dong, Gwangsan-gu, Gwangju Chonnam 506-701, Korea, South

4) Department of Electrical Engineering, Chosun University, 375, Seosuk-Dong, Dong-Gu, Gwangju , 501-759, Korea, South

In this paper, we have fabricated superconducting flux flow transistor (SFFT) with two and three channels from epitaxial $YBa_2Cu_3O_{7-\delta}$ thin films with thickness 350 nm and channel width 9 um and length 5 um by an Inductively Coupled Plasma (ICP). We improved the characteristics of the SFFT by forming multi-channels in the body current line. We performed the experiments and simulation of SFFTs controlled by the magnetic field generated by a gate current, which regulates the critical current through the weak link of the body current line and the gate current. We also explained the process to get the I-V characteristic equation and to induce the external and internal magnetic field by Biot-Savart's law. The experimental results are in good agreement with simulation results. It is shown that due to the magnetic coupling between channels, the critical current of a SFFT with three channels is larger than the critical current of two channels in this study.

Nano-Oxidation of Superconducting Flux Flow Transistor using a Conductive Atomic Force Microscope Tip atomic force microscope tip

Seokcheol Ko[1], **Byoung-Sung Han**[1], **Sung-Hun Lim**[3], **Hyeong-Gon Kang**[4], **Haeseong Lee**[2]

poster E-6

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The atomic force microscope (AFM) has exhibited its capbility to fabricate the nano-scale electronic devices. We have fabircated superconducting flux flow transistors (SFFTs) using superconducting thin films. The SFFT, which is composed of two stripe lines is characterized as a transresistance device: one stripe is as a source and drain terminal, the other is as a gate termianl. The important process is to fabricate a channel with sufficient reproducibility and controllability in fabricating SFFT. Generally, the channel of SFFT has been fabricated by the chemical wet etching methods and dry etching method. In this study we present a new fabrication of multi-channels SFFT using the artificial pattern formation method based on the AFM nano-oxidation process. The critical current density in the multi-channels of the fabricated SFFT was decreased by the applied current in a control current line. Comparing the measured with theoretical results, it is shown that the critical current of SFFT with two channels is larger than the critical current of single channel due to the magnetic coupling between channels.

Proposal of DC Dual Reactor Type Superconducting Fault Current Limiter using Switching Operation of YBCO Thin Film

poster
E-7

Sung-Hun Lim[1)], **Han Byoung-Sung**[1)], **Hyo-Sang Choi**[2)], **Chung-Ryul Park**[3)]
1) Research Center of Industrial Technology, Engineering Research Institute, Chonbuk National University, 664-14, Duckjin-Dong 1 Ga, Jeonju 561-756, Korea, South
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In this paper, we proposed dc dual reactor type superconducting fault current limiter (SFCL) using switching operation of YBa2Cu3OX-7(YBCO) thin film. The dc dual reactor type SFCL consisted of a bridge diode, inductively coupled two coils and YBCO thin films. Two coils were wound in parallel with each other, which was connected in series with YBCO thin film. Dc reactor type SFCL using the switching operation of YBCO thin film, which was suggested by us previously, does not require the interrupter and its controller for the detection of the fault current unlike the conventional reactor type SFCL. Dc dual reactor type SFCL, which was developed to increase the short-circuit capacity of dc reactor type SFCL using the switching operation of YBCO thin film, have different fault current limiting characteristics from dc reactor type SFCL using the switching operation of YBCO thin film. Through the experiments, the fault current limiting characteristics of the dc dual reactor type SFCL were investigated and compared with the fault current limiting ones of the single dc reactor type SFCL.

Fault Current Limiting Characteristics of New Resistive Type Superconducting Fault Current Limiter using Flux Linkage

poster
E-8

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The increase in the capacities of power transmission and in fault current of the related machinery in the grid has resulted in the development of various types of superconducting fault current limiters (SFCLs). However, as a solution to increase the ratings of voltage and current of SFCL for the application into real power system, the method to use magnetically coupled coils have been required.
In this paper, we proposed the new resistive type SFCL using flux linkage between coil 1 and coil 2. The proposed SFCL consisted of a YBCO thin film and a reactor, which was wound in parallel with two coils

on a same iron core. The operational characteristics were analyzed based on the equivalent circuit of this SFCL and the fault current limiting characteristics were investigated through the experiments. The limiting fault current and the resistance of HTSC element could be controlled by the adjustment of the inductances of two coils. It was shown through the analysis that this new resistive type SFCL could increase the short-circuit capacity as well as the ratings of voltage.

Transport Properties at Interfaces between Conductive Oxide ReO_3 and Cuprate Superconductors

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poster E-9

As well known superconducting transition temperatures Tc's increase as the number of CuO_2 planes in the unit cell increases up to n=3, for example in a series of Bi-, Tl-, Hg-based cuprate superconductors (CSC's). However, if sufficient carriers are doped in the CSC's including CuO_2 planes above n=4, a higher Tc is expected. It is expected that the higher Tc will be realized at an interface between ReO_3 and CSC's. The ReO_3 reveals the highest conductivity among oxide materials. As conductive oxides are deposited on the CSC's, a carrier doping takes place adequately from the conductive oxides to CSC's deeply around the interface, specifically taking a role like as a charge reservoir block. In this study we attempt to obtain the highest conductive ReO_3 thin film and investigate the transport properties of bi-layer of ReO_3 / CSC's.
The Re oxides thin films are prepared by off-axis RF magnetron sputtering. Target is a metal Re disc and a substrate is quartz. The films are grown at ambient substrate temperature for 60min, and then post-annealing in-situ is carried out in Ar or O_2 atmosphere for 30min. And also ReO_3 thin film is deposited on oxygen-vacant $YBa_2Cu_3O_6$ (YBCO) and $SrCuO_2$, which were already grown with other deposition equipment.
At annealing temperatures above 200 degree C, cubic ReO_3 grew preferentially aligned along the (100) direction. Despite of a large residual resistivity, the resistivity decreased linearly with decreasing temperature. The minimum resistivity was obtained in a film annealed at about 200 degree C and was 4.4×10^{-5} ohm cm at room temperature. Above 280 degee C rhenium oxides was totally sublimated. The resistivity behavior of both bilayers was roughly similar to that of ReO_3 thin film. In this case the interface might be contaminated after exposure to the air. In-situ growth of bilayers will be carried out to develop the resistivity and to show the higher Tc.

Role of self-organisation processes in physico-chemical properties of superconducting cuprates

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poster E-10

The magnetic dilution of superconducting (SC) cuprates was performed to clarify a HTSC mechanism in these oxides. The magnetic properties of the series of complex cuprates based on $La_{1.85}Sr_{0.15}O_4$ with the following substitutions: La - Eu; Sr - Ba, Ca; Cu - Fe, Li, Al and their solid solutions in isomorphous diamagnetic matrix were studied. The examination of temperature and concentration dependencies of magnetic susceptibility points to a very strong tendency of copper atoms to clustering. According to ESR and Mossbauer (with Fe-57 isotope as an atomic probe) study, copper atoms, being in two various oxidation states, are combined in clusters with distorted local oxygen environment. The results of microwave absorption method showed that superconducting properties are registered not only in concentrated oxides but also in extremely diluted Sr and Ba-containing solutions. The introduction of Eu, Li, Ca suppresses superconductivity in a diluted systems. All experimental results can be accounted for by suggesting the existence of nanoclusters of heterovalent Cu (II) and Cu (III) atoms, formed at spontaneous ordering of crystal structure of solid solutions. The electron structure of such clusters depends on a local distortion of nearest oxygen environment, caused by an attitude component of self-organizing process of a substance. The most important point is a temperature-dependent character of local distortions, in this case sharp changes of parameter of exchange interactions between copper atoms and, as a consequence, of superconducting properties of system are probable. By our opinion these nanoclusters are responsible for magnetic and superconducting properties of multicomponent diluted perovskite-like cuprates. The form, size and electron structure of clusters as well as the character of intraclusters interactions will be discussed in details.
The work is supported by RFBR (grant N 03-03-32355).

Normal-state and superconducting properties of Ba1-xKxBiO3 single crystals

poster E-11

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With main goal to study on the character of electron-phonon coupling we measured the magnetic characteristics of single crystals of $Ba_{1-x}K_xBiO_3$ (x=0.34-0.49) for wide temperature range of 4.2K-300K at magnetic fields up to 5T using SQUID magnetometer. The single crystals grown by electrochemical deposition method with the typical size of 2x2x1mm^3 reveal the superconductivity at T_c=26K-31K depending on composition x. The X-ray analysis displays the single-phase structure of the crystals. The volume superconducting fraction of the samples equals to 0.8-0.9. The susceptibility of crystals in the normal state (T=40K-300K) in different fields was studied in order to estimate the density of state N(0) through the term connected with the Pauli paramagnetism. These values of N(0) were compared with the ones obtained from the temperature coefficient of the upper critical field for all crystals. The obtained values of the coupling constants are indicate of moderate-to-strong coupling.

NANOSCALE FLUX PINNING SITES IN HIGH-Tc SUPERCONDUCTORS

poster E-12

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Ideal flux pining centres in high-Tc superconductors should be of nanometre size as the coherence length, ξ, is so small. Therefore, the optimisation of high-T_c superconductor samples concerning high critical current densities and high flux pinning has to take place in the nanometre range. An important goal of the current research is to find specific preparation strategies to create such ideal flux pining sites already during the sample processing. By means of AFM and STM measurements at ambient conditions, we have investigated the topographies of various samples of $YBa_2Cu_3O_x$ (YBCO), $NdBa_2Cu_3O_x$ (NdBCO), (Sm,Eu,Gd)$Ba_2Cu_3O_x$ (SEG) and (Nd,Eu,Gd)$Ba_2Cu_3O_x$ (NEG) high-T_c superconductors. We find that the two systems with the highest critical current densities (NEG, SEG) and hence, the strongest flux pinning [1,2], exhibit microstructures on the nanometre scale which are remarkably different from those obtained in the YBCO system. The stripe-like growth structures observed in our topography measurements may be the key for the considerable improvements concerning the critical current densities especially at high magnetic fields and elevated operating temperature (77 K).

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Influence of Y_2BaCuO_5 particles on the $YBa_2Cu_3O_x$ matrix in melt-textured YBCO superconductors

poster E-13

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By means of automated electron backscatter diffraction (EBSD) analysis, we studied the local orientations of embedded Y_2BaCuO_5 (211) particles within melt-textured $YBa_2Cu_3O_x$ (YBCO) samples. On both components, we obtained high-quality Kikuchi patterns, thus allowing the automated mapping of the crystal orientations and a two-phase analysis of the samples. Investigations were performed on a variety of melt-textured YBCO samples, also including samples prior to the oxygen treatment.
In melt-textured YBCO with (0 0 1) orientation, we find that the embedded 211 particles do not have any preferred orientation, but the maps also reveal that at certain orientations of the 211 particles the YBCO growth is not altered. From the obtained EBSD mappings, we can conclude that the formation of small 211 particles will not disturb the YBCO matrix growth, whereas the presence of large 211 particles causes severe changes in the YBCO growth, leading to the formation of subgrains. The EBSD results are presented in form of local orientation maps and local pole figures.

OIM and X-ray texture analysis of melt-textured YBCO superconductors

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In this contribution, we compare the results of an X-ray based pole figure texture analysis with the local texture analysis by means of Orientation imaging microscopy (OIM) technique. As samples, we employ two different melt-textured YBCO samples; one fully processed and one without oxygen treatment. To enable the direct comparison of the two techniques, we employ the [103] pole figures. The OIM results are presented in form of phase maps, misorientation angle distributions and two-dimensional pole figures. The X-ray texture data are presented in form of two- and three-dimensional [103] pole figures.
We find a clear coincidence between the results obtained by the two measurement techniques on our samples, however, the OIM results are much more detailed, yielding the local grain orientation distribution and quantitative results of the grain or subgrain misorientation angles. Therefore, the OIM measurements give information not accessible to the X-ray pole figure analysis.

The Righi-Leduc effect: an evidence of the competition between holes and electrons in $Nd_{1.86}Ce_{0.14}CuO_{4-\delta}$.

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Measurements of four transport coefficients are reported for a superconducting $Nd_{1.86}Ce_{0.14}CuO_{4-\delta}$ single crystal. Namely the normal state temperature dependencies of the resisitivity (ρ), Hall coefficient (R_H), thermal conductivity (κ) and Righi-Leduc coefficient (S_{RL}) have been investigated. We have noticed that the Hall coefficient changes its sign twice (R_H is positive below 50 K and above 250 K, and negative between these temperatures), whereas S_{RL} remains positive in the whole temperature range. Disagreement between signs of S_{RL} and R_H, strongly suggest that both, n-type and p-type, charge carriers are present in the material. We conclude that hole-like subsystem dominates the heat transport, and seems to obey the Wiedemann-Franz law.

EFFECTS OF DIMENSIONAL QUANTIZATION IN THE SPECTRA OF ELECTRON-POSITRON ANNIHILATION OF NANOLAYER MONOCRYSTAL HIGH-TEMPERATURE SUPERCONDUCTIVE MATERIALS

poster
E-16

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Monocrystal high-temperature superconductors (HTSC) with stratified structure are suitable objects for the investigation of effects of dimensional quantization, because in this case there is no necessity in the preparing of monolayer specimens, homogeneous by thickness, for providing total positron absorption in the HTSC layer. In present paper the possibility of detection of quantum dimensional effects (QDE) in monocrystal HTSC is theoretically shown for the first time. It has been established, that the spectrum of angular distribution of annihilation photons (ADAP) for monocrystal HTSC with stratified structure has strongly anisotropic character, namely, when the axis of the detection system of the installation for ADAP measurements is perpendicular to the projection of total photon pulse on the chosen z-direction in pulse space (R1), the ADAP curve has pronounced step-like character in the range of pulses which corresponds to the positions of occupied electron sub-bands. The charge states of Cu(1) atoms in superconductive chains are considered on the example of Y-Ba-Cu-O oxide and experimental results of the positron probing of core d-electrons at the HTSC is discussed. For this particular case, when the projection of total photons pulse is oriented along the conductive layer, ADAP curve is similar to the inverted parabola(R2). It has been shown, that R2 is significantly shorter than R1.It has been established that the half-width of R2 does not depend on electron characteristics of superconductive layer in HTSC. It is also necessary to take into account the influence of the substrate, as well as the decreasing of anisotropy of ADAP that both are connected with the presence of oxygen bridges in the structure of HTSC monocrystals and with disordering of separate domains.

Microwave complex resistivity in High-T_c Superconductors in the mixed state

poster
E-17

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The microwave response of high-T_c superconductors in the vortex state is determined by superfluid and normal fluid together with the motion of flux lines. The mixing of these contributions makes difficult to isolate the contributions due to the charge carriers. At high enough frequencies, the vortex motion reduces to the simple flux flow. Thus, it can be isolated from the oveall response, allowing for the separate determination of the field dependent superfluid fraction n_s(T,B). We have measured the (a,b) plane complex resistivity at 48 GHz in several highly oriented cuprate superconducting thin films, placed in the end-wall configuration in a resonating cavity, for temperatures from 65 K to T_c and magnetic fields up to 0.8 T (applied along the c axis). By preliminarly identificating the vortex contribution, we obtain the vortex viscosity. We compare our results with data from the literature. Having isolated the vortex motion contribution, we determine the field dependence of the superfluid fraction. We find that it follows a sublinear law ($n_s(T,B)=n_s(T,0)-A\ B^{1/2}$), up to temperatures very close to T_c. This behaviour, which is a common feature of all the ReBCO (Re=Y, Sm) and Bi2212 samples investigated, is in agreement with the predictions for a superconductor with lines of nodes in the gap. Moreover, the extension of this field dependence in nearly the full temperature range explored ($T>65$ K) and up to temperatures close to T_c indicates that such pairing is not smeared out by the high operating temperatures.

We express our thanks to M. Boffa, M. C. Cucolo, A.M. Cucolo (Dip. di Fisica and Unita' INFM, Universita' di Salerno, Italy) and C. Camerlingo (CNR - Istituto di Cibernetica, Napoli, Italy) for samples preparation.

Work on YBCO has been partially supported by Italian MIUR under the FIRB project "Strutture semiconduttore/superconduttore per l'elettronica integrata".

$ZrNi_2In$ - New Superconducting Heusler Alloy

poster
E-18

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Superconductivity was already detected in 18 Heusler alloys, i.e. ternary intermetallics forming a large class of cubic compounds having the composition TX_2Z, where T and X are transition and noble metal atom and Z is sp element. In the paper we present the results of resistivity, dc and ac susceptibility measurements of polycrystalline $ZrNi_2In$. Critical temperature of the compound (defined as the onset of magnetic transition) was equal to $T_c = 9$ K, surprisingly high for this class of compounds (the maximum value of critical temperature was previously obtained for YPd_2Sn and was equal to $T_c = 4.64$ K).
From the dc magnetization measurements lower and upper critical fields were evaluated and their temperature dependence was obtained. From th slope of dHc_2/dT superconducting parameters of the material were calculated from WHH theory.

Electrical properties the oxides $LuBa_2Cu_3O_7$ and $LuBa_2Cu_3O_{0.5}S_{5.5}$

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poster
E-19

One of the important problems in the metallic ceramics investigation is the study of influence of a various type of impurity on them superconductivity property. In work the dependences of resistance from frequency and temperature dependences the conductivity and dielectric permeability of oxides $LuBa_2Cu_3O_7$ and $LuBa_2Cu_3O_{0.5}S_{5.5}$ were investigated.
Researches were carried out on frequency 1592Hz, which, as follows from the impedance diagrams, belongs to high-frequency area, in the field of temperatures 78-400. Temperature dependencies of conductivity the compounds have a Arrenius type. Dielectric permeability is monotonous increase with the temperature increase.
Presumably, in area 310-380 in $LuBa_2Cu_3O_7$ exists the piroelectric phase transition.
The occurrence of three various meanings of energy of activation in $LuBa_2Cu_3O_{0.5}S_{5.5}$ instead of two in $LuBa_2Cu_3O_7$ is probably given by presence at a sample of sulfur.
Increase of a share of oxygen in compound $LuBa_2Cu_3O_7$ and the addition of sulfur results in increase conductivity on the order, dielectric permeability decreases approximately in 5 times.
This work in part was supported by CRDF (grant EK-005-X1) and grant CRDF and Min. of Education of the Russian Federation (Post Doctoral Fellowship, award EK-005-X1, annex 07, No Y1-E-05-09).

Large Fermi surface and nanoscale phase separation in cuprates

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poster
E-20

Assuming that stripes in doped antiferromagnets take a form of two leg ladder-like structures which separate antiferromagnetic domains with opposite direction of the staggered magnetization and assuming that spin Peierls order forms on rungs, we calculate the spectral function of a hole propagating in such a system. In the case of a ladder, longitudinal propagation of a hole may be described in terms of a position exchange between a single hole and a singlet on neighboring rungs. This is a first order process. Propagation of a hole in an antiferromagnetic background, on the contrary, is mediated by a third order process which involves twice the action of the hopping term and once the action of the exchange term in the model Hamiltonian, which is the t-J model. A hopping hole creates linear defects in the antiferromagnetic spin background. Defects are removed if a hole retraces a path along which it has previously moved. Since hopping processes are much faster than processes related to the exchange interaction (t»J) a strong tendency towards confinement by linear defects manifests and the system may be described in terms of quasi-localized spin polarons. Hopping of these objects is mediated by above mentioned high order processes. An effective tight binding Hamiltonian for a quasiparticle propagating in the stripe background is a combination of a model for a bare hole propagating in the ladder-like domain walls and a model for a propagating spin polaron in antiferromagnetic domains. By adding contributions to the spectral function from horizontal and vertical stripes we obtain a pattern which is in qualitative agreement with the Fermi surface identified in a doped LSCO system at 1/8 hole filling by means of ARPES measurements.

Bond-centered spin Peierls ordered stripes in cuprates

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Stripes forming in doped antiferromagnets between domains with opposite direction of staggered magnetization may be considered as domain walls in which filling with holes is enhanced in comparison with magnetic domains. It is not clear, what is the magnetic structure of these domain walls. Recent numerical results suggest that spin Peierls order may appear in doped antiferromagnets. In this work we analyze stability of stripes, or in other words domain walls, that have the shape of two leg ladders in which singlets form on rungs. A hole moving along a dimerized ladder is not confined. On the other hand, a tendency towards confinement may be observed in the motion of a hole in an antiferromagnet. A hopping hole shifts spins and creates linear defects in the magnetic structure on paths along which it has been moving. That confinement is not perfect because a hole may propagate in the antiferromagnetic spin background owing to some high order processes, the contribution of which to the total energy is small and is not decisive to stripe stability. Thus, we analyze motion of a hole along a stripe in terms of two components. The first component is motion of a hole in the domain wall. That component resembles propagation of a hole in the ladder with spin Peierls order on rungs. The second component represents motion of a hole after entering a domain. That motion is governed by the tendency towards confinement and formation of linear defects in the antiferromagnetic structure, so called strings. In order to analyze the stability of a bond-centered stripe we calculate its energy by means of the recurrence method which is suitable to analyze retractable motion of holes along strings. Later we make a comparison with the energy of a site-centered stripe. We deduce that the energy of a bond-centered stripe is lower than the energy of holes in the homogeneous antiferromagnetic background and lower than the energy of site-centered stripe for linear filling higher than 0.7.

Tunneling density of states of MgB_2: evidence for a dominant π-band contribution

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Weakly-transmitting junctions usable for tunneling spectroscopy experiments were fabricated from polycrystalline samples of magnesium diboride with a niobium counter-electrode. A strong nonlinear conductance-versus-voltage behavior for voltages above the values corresponding to the energy gaps of the electrodes was interpreted as a fingerprint of the electron-phonon interaction in superconducting MgB_2. A partial Eliashberg spectral function $\alpha^2(\omega)F(\omega)$ was extracted from the data by the numeric inversion of the standard strong-coupling Eliashberg equations. In a full agreement with recent theoretical simulations for magnesium diboride [O. V. Dolgov et al., PRB 68, 132503 (2003)], we have observed a dominant contribution from the π-band of this two-band superconductor.

Comparison between radiation hardness of $Bi_2Sr_2Ca_2Cu_3O_x$ tapes and MgB_2 tapes and films

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In this work we present a wide spectrum of ac/dc magnetic and magneto-optical characterizations of $Bi_2Sr_2Ca_2Cu_3O_x$ (BSCCO) tapes and MgB_2 tapes, before and after irradiation by means of high energy ions. The fluences were about 10^{11} ions/square centimeter. BSCCO tapes were irradiated up to 15% of their thickness by means of 0.25 GeV gold ions (Tandem facility energy); the penetration depth was evaluated by TRIM simulations. In such tapes there is a decrease of critical temperature of about 0.5 K [1,2,3]; a large sensitivity to the high energy ions is exhibited, showing up in a significant enhancement of critical currents as well as in a large shift of the irreversibility line towards high temperatures (clear signatures of Bose-glass-like transition are present).
MgB_2 tapes were irradiated with 0.25 GeV but the damaging effect was within experimental errors. In order to reach the maximum damaging effect, if present, the gold ions energy was increased up to 4.5 GeV (gold ions, CS-facility energy). TRIM simulations allow to establish that in this case the ions cross about 100% of the sample thickness. No significant changes were found in the useful range of temperatures. Thus MgB_2 bulk exhibits a quite remarkable radiation hardness [4] with respect to high energy ions. The same hardness is exhibited by MgB_2 films under low energy monochromatic protons of 3.5 MeV up to fluences of 10^{16} p/cm^2.
This scenario points towards radiation hardness of MgB_2 as a valuable figure of merit with respect to application of this material in hard ambient.

This work was partially supported by Istituto Nazionale di Fisica Nucleare, Italy (MaBo project)

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Superconducting MgB2 tapes using mechanically alloyed nanocrystalline precursor powder

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poster E-24

It was demonstrated that nanocrystalline MgB_2 samples obtained by mechanical alloying show improved superconducting properties. Monofilamentary and
19 filamentary tapes with Fe sheath have been prepared by the powder-in-tube (PIT) method using mechanically alloyed precursor powders consisting of the constituents Mg, B, and MgB_2. With this precursor the tapes can be annealed at relatively low temperatures of 500...600C. For the 19 filamentary tape Jc values up to 35 kA/cm^2 and 9 kA/cm^2 in fields of 7.5 T and 10 T, respectively, were measured at 4.2 K. Investigation of the microstructure by optical microscopy, SEM/WDX and XRD have shown that the high Jc values may be mainly due to the remarkably small grain size of the MgB_2 phase and defects particularly precipitates of magnesium oxide. The properties of tapes with iron sheath are compared to those with Cu-sheath.

MgB2 thin films fabrication and structuring

Chiara Portesi[1)], **Eugenio Monticone**[1)], **Valeria Dellarocca**[2)], **Renato S. Gonnelli**[2)]

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poster E-25

Since the discovery of its superconducting properties, magnesium diboride has generated a great interest because of its simple structure, relatively high critical temperature and pronounced two-gap nature. These properties make this superconductor good for many potential applications.
In this work, we present the results obtained in the fabrication, characterization and structuring of MgB2 thin film grown by so-called in situ method. This technique consisted in two steps: the first one was the co-deposition of B and Mg by means of e-gun and resistive heater respectively. During the deposition .the substrate was held at temperature of 280C.The second step was the annealing of the as-grown films in the deposition chamber at 500C in inert atmosphere.
Using this method, we obtained MgB2 thin films with rather good electrical properties and smooth and homogeneous surfaces. The analysis of the morphological and structural properties has been performed by means of AFM and XRD respectively. The critical temperature was about 32 -35 degrees and we always observed very sharp transitions; the roughness of the samples was ranging between 10 and 20 nm (if evaluated on 5 mm2 areas), and it was strongly dependent on the films thickness. The films were

polycrystalline, with a columnar growth of the grains and in the best samples we observed a partial orientation along the c-axis.
The samples were structured using standard photolithographic process followed by chemical wet etching or by dry etching. For the chemical etching, we experimented different acid solutions and the best results have been obtained using HCl solution (0.05%),in which the sample was dipped for a few second.. By ion milling, we realized well defined 5 microns wide strips with very sharp edges.

Tuesday, September 7th

Morning session

11:00 - 12:30

Main Building, room 144

Femtosecond Studies of Nonequilibrium Carrier Dynamics in High-Temperature Superconductors

11:00 - 11:45
invited oral

Roman Sobolewski[1,2)]

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We present our studies on nonequilibrium carrier dynamics in high temperature superconductors, using the optical pump-probe spectroscopy method. We have performed our time-resolved measurements of the optical reflectivity change ΔR/R in $HgBa_2Ca_2Cu_3O_{8-x}$ (Hg-1223), Pb- and Gd-doped $Bi_2Sr_2CaCu_2O_{10-x}$ (Bi-2212), and MgB_2 thin-film and single-crystal superconducting samples. The measured optical signals were strongly related to the presence of a superconducting energy gap Δ in the electronic energy spectrum. The superconducting transition at the critical temperature T_c was also clearly observed. In Hg-1223 thin films, the ΔR/R signal measured in the superconducting state was only related to the Cooper pair-breaking and pair-formation dynamics, with no evidence of the phonon bottleneck effect, characteristic for conventional BCS materials. The pair-breaking time in Hg-1223 was measured to be 350 fs and was temperature independent up to T_c. The quasiparticle recombination time was in the 5-10 ps range with the $1/\Delta$ divergence at temperatures close to T_c and the 1/T divergence at low temperatures. In Bi-2212 single crystals, the Cooper pair dynamics below T_c was very similar to that observed in Hg-1223 films. Above T_c, however, we observed the change in the sign and shape of the ΔR/R signal, which we related to the presence of the pseudo-gap state. Finally, in MgB_2 films and crystals, the temperature dependence of the amplitude of the superconducting component of the ΔR/R signal followed the Δ(T) anomalous temperature dependence, which was interpreted for our mixed clean/dirty MgB_2 films as the two Δ's, closing at two different values of T_c's. The same two T_c's were also visible in the double-divergence of the temperature dependence of the electron-phonon relaxation time. The quasiparticle recombination time was on the order of 400 ps and was limited by the phonon escape time.

Elaboration and nanostructuration of very thin superconducting epitaxial films of cuprates (YBaCuO, HgBaCaCuO) and nitrides (MoN, TiN, NbN) on R-plane Sapphire and MgO. Application to ultra-fast and ultra-sensitive devices (single photon detectors, THz mixers, spin-injection and SFQ logics).

11:45 - 12:15
oral

Jean-Claude VILLEGIER[1)], **Bertrand DELAET**[1)], **Laurent FREY**[2)], **Dominique De BARROS**[3)], **Philippe ODIER**[4)]

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Superconducting very thin films (3-8 nm) of cubic B1 nitrides such as TiN, Nb(1-x)TixN or NbN have been achieved in "Hot Electron Bolometer" (HEB) nanostructures or in thin vertical tunnel devices. Very thin layers epitaxially grown, smooth and sharp interfaces are required in order to best benefit from fast ballistic and out of thermal equilibrium effects involving quasi-particles injected or photon generated inside

the superconductor. R-plane Sapphire (up to 3 inch) and (100) MgO substrates have been selected for their large gap and good mechanical, microwave, infrared and surface properties. Films are DC-MAG sputtered from metal targets in a reactive mixture of nitrogen and argon gas, on substrate heated up to 650C. As example, 4.5 nm NbN films covered by a 1.5 nm AlN passivation layer, has a Tc=11 K with a large critical current density at 4.2 K (> 1MA/cm2) and HC2 > 14 Tesla at 1K. Such ultra-thin films undergo a superconducting-insulator transition at low temperature which can be tuned by a magnetic field or by quasi-particle injection (spin polarized or not) opening new physical effects as well applications. Optical transmission and energy gap topography are done by LT-STM, AFM, grazing angle XRD and ellipsometry.
We will describe nanostructuration of fast single photon detectors (SSPD) and THz HEB mixers, by electron beam lithography and reactive ion etching: a 10 μm square pixel has a filling factor > 0.5 with 150 nm wide stripes. IR photon counting at 4 K will be presented at high rates (>10 GHz), with a quantum efficiency suitable for quantum optics and astronomical applications. Spin-injection or Rapid Single Flux Quantum logic circuits can also benefit from LTS and HTS nanostructures: ICM sputter grown 10-30 nm thick YBa2Cu3O7-[U+F064] HEB mixers have been patterned on MgO with Tc > 85K and recently Hg(1-x)Re(x)Ba2Ca(n-1)Cu(n)O(2n+2+[U+F064]) on LAO and MgO with n= 2 and n=3 is showing Tc up to 130 K.

Lunch break

12:30 - 14:00

Afternoon session

Main Building, room 144

14:00 - 15:30

Influence of disorder on H_{c2}-anisotropy and flux pinning in MgB_2

14:00 - 14:45
invited oral

Michael Eisterer[1)]
1) Atomic Institute of the Austrian Universities, Stadionallee, Vienna 1020, Austria

The upper critical field and flux pinning in MgB_2 single crystals were investigated. The implications of these properties for technical applications are discussed and compared with transport properties of polycrystalline bulk samples and iron sheathed wires. In these untextured materials current percolation is important, especially at high magnetic fields. It is shown that the anisotropy of the upper critical field influences the "irreversibility line" and that the application range MgB_2 is limited by the smallest upper critical field (i.e., for the field direction perpendicular to the boron planes).
Disorder, introduced by neutron irradiation with neutrons, enhances the upper critical field, reduces the anisotropy and drastically changes flux pinning. While the enhanced H_{c2} and the reduced anisotropy generally improve the transport properties of the polycrystalline samples, the contribution of the radiation-induced defects to flux pinning is small compared to the as-grown defect structure (grain boundary pinning).

Energy gaps in doped MgB2

14:45 - 15:15
oral

Peter Samuely[1)]
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Point-contact measurements on the carbon and aluminium substituted MgB_2 samples are performed to study a development of the two gap superconductivity [1]. In the carbon substituted MgB_2 the large gap on the σ-band is decreased in an essentially linear fashion with increasing the carbon concentrations. The changes in the small gap Δ_π up to 3.8 % C are proportionally smaller but for the heavily doped sample with 10 % C and $T_c = 22$ K both gaps are still present, and significantly reduced, consistent with a strong essentially linear, reduction of each gap with the transition temperature [2,3]. A comparison with the aluminium doped material is made as well.

[1] P. Szabo et al., Phys. Rev. Lett. 87, 137005 (2001).
[2] P. Samuely et al., Phys. Rev. B 68, 020505(R) (2003).
[3] Z. Holanova et al., Phys. Rev. B accepted

* The work has been done in collaboration with P. Szabo, Z. Holanova, R.H.T. Wilke, S. Bud'ko and P.C. Canfield

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15:30 - 16:00

Coffee break

16:00 - 17:30

Afternoon session - continued

Main Building, room 144

16:00 - 16:30
oral

The superconducting gaps of C-substituted and Al-substituted MgB2 single crystals by point-contact spectroscopy

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We report the results of the first directional point-contact measurements in $Mg(B_{1-x}C_x)_2$ single crystals with 0 <= x <= 0.132 and in $Mg_{1-y}Al_yB_2$ crystals with 0 <= y <= 0.21, obtained at ETH (Zurich) by means of a high-pressure technique in a cubic anvil. We made the point contacts by using the "soft" technique described elsewhere [1]. The Andreev-reflection features of our conductance curves were measured in magnetic fields up to 9 T, applied either parallel to the c axis or to the ab plane of the crystals. By fitting the normalized conductance with the Blonder-Tinkham-Klapwijk (BTK) model generalized to the two-band case we obtained the dependence of the gaps Δ_π and Δ_σ on the C or Al content (x or y). This dependence was confirmed by applying to the junctions a suitable magnetic field B^* able to remove the contribution of the π-band gap to the total conductance, without appreciably affecting the σ-band one [2]. This allowed the separate determination of the gaps via a single-band three-parameter BTK fit.
In C-substituted crystals up to x 0.10, the two-gap nature of superconductivity characteristic of pure MgB_2 is preserved. At x = 0.132 we clearly and reproducibly observed for the first time the theoretically predicted merging of Δ_π and Δ_σ into a single gap Δ 3 meV with a gap ratio $2\Delta/k_BT_c$ close to the standard BCS value [3].
In Al-substituted crystals, we found no evidence of gap merging: Δ_π reaches the value 0.4 meV at y=0.21, where Δ_σ saturates at about 4 meV. The behaviour of $\Delta_\pi(y)$ and $\Delta_\sigma(y)$ cannot be simply explained by the two-band model and can be due to the presence in these crystals of a phase segregation of Al-rich layers.

[1] R.S. Gonnelli et al., Phys. Rev. Lett. 89, 247004 (2002).
[2] R.S. Gonnelli et al., Phys. Rev. B 69, 100504(R) (2004).
[3] R.S. Gonnelli et al., cond-mat/0407265.

16:30 - 17:00
oral

Nano SiC doped MgB_2 bulk superconductor with Tc over 42 K by high gas pressure annealing

Andrzej J. Morawski[1], **Tomasz P. Łada**[1], **Adam Presz**[1], **Tadeusz Mazur**[1], **Ryszard Diduszko**[2,7], **Andrzej J. Zaleski**[3], **Kazimierz Przybylski**[4], **Silvia Bodoardo**[5], **Valeria Dellarocca**[6]

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7) Industrial Institute of Electronics (PIE), Dluga, Warszawa 00-241, Poland

Since affirm that the MgB_2 is a potentially promising material for the large-scale application as superconducting devices, the proper doping substance that can increase the Jc or Tc has been intensively searched. One of the most interesting doping argent is nano-SiC powder.
We investigated the effect of the nano-powder SiC doping of two average grade batches: 6 nm and 18 nm, with the content up to 10 at. % for the commercial MgB_2 powder made by Alfa Aesar.
The syntheses have been made on the cylindrical samples of 3 mm in diameter and 5 to 7 mm in length. Such samples were obtained by uni-axial pressing at 1.5 GPa in three sectors open anvils.
Synthesis were made at an inert gas at pressure of up to 1 GPa at temperature from 1500 K to 1550 K, in the high pressure gas trap system, with the equilibrium magnesium vapor made by the melting of Mg chips inside close vessels, during the experiment lasting for two hours.
As obtained samples thus were superconducting with Tc over 39 K and the highest Tc at 42.6 K was recorded for the sample doped with 1.5 at % of the 6nm SiC. The XRD examinations indicated the MgB_2 phase and a very low addition of Mg, Si and C composites and/or SiC as well as Mg_2Si nano-crystallites. The compositions of the additional phase were strictly dependent of the nano-size grains dimensions (their solubility) and quantity. The lattice parameters for all samples were smaller than for pure MgB_2 initial samples. The SEM, EDX and superconducting properties Hc_2, Tc, Jc, were measured and discussed. The probably effect of tangential strain caused by nano-inclusion of thin amorphous or crystalline layer between the pure or carbon doped MgB_2 larger grain are considered for increasing the Tc of our samples.

MgB_2 THICK FILMS OBTAINED BY ELECTROPHORESIS TECHNIQUE: SYNTHESIS, STRUCTURAL AND SUPERCONDUCTIVE CHARACTERIZATION

17:00 - 17:30
oral

Valeria Dellarocca[1], **Renato S. Gonnelli**[1,4], **Silvia Bodoardo**[2], **Nerino Penazzi**[2], **Gianluca Grenci**[2], **Chiara Portesi**[5], **Mauro Rajteri**[5], **Andrzej J. Morawski**[3], **Tomasz Lada**[3]

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MgB_2 is a material known for several years, but only recently discovered as superconductive at about 40 K. MgB_2 has a simple crystal structure with alternation of boron and magnesium layers, both in hexagonal array. It has mechanical strength and durability higher than superconducting oxides, weak-link-free grain boundaries, high transport critical current density (Jc),coherence length (>5 nm)higher than superconducting cuprates, low-cost starting materials and, above all, a transition temperature accessible to single stage cryocooler. Thanks to these properties, many efforts were done in order to synthesize MgB_2 for large-scale applications, in form of bulk, wires, tapes and films.
In this contribution, we present the results on the preparation and the characterization of MgB_2 thick films supported on Ti/Al_2O_3 and MoBN substrates via electrophoretic deposition technique (EPD).
We prepared superconducting MgB_2 thick films by following two different routes: i) deposition of MgB_2 powder, both pure and SiC doped, followed by a sintering step at high temperature and high Ar pressure in a furnace; ii) deposition of boron films and successive annealing in saturated Mg atmosphere at high Ar pressure.
The EPD deposition occurs at the anode of the electrochemical cell under an electric field of about 180 V/cm. The obtained films are homogeneous and well adhesive to the substrate. The MgB_2 films were then sintered at 1200 K in inert atmosphere, whereas the boron precursors were reacted with Mg at temperature over 1500 K and at high pressure of 1 GPa. X-ray diffraction confirmed the formation of a crystalline MgB_2 phase with hexagonal P6/mmm symmetry in the case of both MgB_2 and B precursors.
The electrical properties of the samples were measured in liquid helium vapour, by using an AC-bridge with the standard four-probes technique and indium contacts. The samples obtained from MgB_2 powder show high Tc of superconducting transition close to 35 K.

20:00 - 22:00

Banquet

Wednesday, September 8th

09:15 - 10:30

Morning session

Main Building, room 144

09:15 - 10:00
invited oral

Superconductivity and Magnetism in Heavy Fermion Systems

Michael Nicklas[3)], **R. Borth**[3)], **E. Lengyel**[3)], **C. F. Miclea**[3)], **G. Sparn**[3)], **John L. Sarrao**[1)], **R. Lackner**[2)], **E. Bauer**[2)], **F. Steglich**[3)]

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Superconductivity is one of the most fascinating phenomenon in solid state physics. In a conventional superconductor Cooper-pairing is mediated by phonons and strongly suppressed by the application of a magnetic field. However, in heavy fermion systems superconductivity develops in close proximity to magnetism or even coexists with magnetism. This opens the intriguing question, which underlying mechanisms mediate superconductivity and/or lead to magnetic order in this class of materials.

Superconductivity in heavy fermion compounds was first discovered 25 years ago in $CeCu_2Si_2$ by Steglich et al.. Until recently, superconductivity in heavy fermion systems appeared only at low temperatures bellow 1 K. $CeCoIn_5$ a member of the $CeMIn_5$ (M=Co,Rh,Ir) family, enters the superconducting state already at T_c=2.3 K, with a maximum T_c=2.6 K at an applied pressure of 1.6 GPa. $CeCoIn_5$ is discussed as a promising candidate of a material where a Fulde-Ferrel-Larkin-Ovchinnikov state is realized in the superconducting phase at high magnetic fields. Another recently discovered system is $CePt_3Si$. $CePt_3Si$ is the first heavy fermion superconductor with a crystal structure without centre of inversion. At ambient pressure $CePt_3Si$ orders antiferromagnetically at T_N=2.2 K and superconductivity develops in the magnetic phase bellow T_c=0.75 K.

We present studies of transport and thermodynamic properties of $CeMIn_5$ (M=Co,Rh,Ir) and $CePt_3Si$ under hydrostatic pressure and in magnetic fields.

10:00 - 10:30
oral

C-axis Magnetotransport in Heavy-Fermion Superconductor $CeCoIn_5$

Artur Malinowski[1,2)], **Michael F. Hundley**[2)], **Cigdem Capan**[2)], **Filip Ronning**[2)], **Nelson O. Moreno**[2)], **Roman Movshovich**[2)], **John L. Sarrao**[2)], **Joe D. Thompson**[2)]

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The recent discovery of a new heavy-fermions (HF) family, $CeMIn_5$ (M=Ir, Rh, Co), raises once again the long-lasting question about the relation between magnetic and superconducting (SC) interactions. $CeCoIn_5$ has T_c=2.3 K and is believed to reside close to a quantum critical point (QCP). Although no long-range magnetic order is present, short-range AF spin fluctuations are observed. In order to understand the interplay between superconductivity and spin fluctuations in $CeCoIn_5$ we have performed c-axis magnetotransport measurements between 40 mK and 300 K and in the fields up to 9 T, applied along c-axis.
Above 20 K the behavior of resistivity along c-axis, ρ_c, and longitudinal magnetoresitivity, LMR, is typical for a HF system. Above T_{ch} 50 K the rho$_c$ is weakly T-dependent while below T_{ch} the ρ_c starts to decrease

rapidly, indicating the development of coherence effects. After subtracting the LMR of the non-magnetic analog, $LaCoIn_5$, LMR caused by the presence of Ce ions scales in the manner characteristic for single-Kondo-impurity regime. All LMR(B) curves between 50 K and 100 K can be superimposed onto a single unique curve when scaling them according to equation LMR(B,T)=f[B/(T+T*)] with T*=2 K.
At lower temperatures resistivity exhibits non-Fermi-liquid (nFL) behavior: ρ_c (ρ_{ab}) below 8 K (12 K) is nearly linear in T. While ρ_{ab} extrapolates to a finite value at 0 K, ρ_c for the same crystal extrapolates nearly to zero. Applying field along c-axis restores the FL behavior: in mK range $\rho_c=\rho_0+AT^2$ for B>=6 T. The coefficient A diverges as $(B-B_{cr})^{-1.4}$. Contrary to ab-plane measurements, however, our results suggest that the critical field B_{cr} lays below B_{c2}. This indicates that the critical behavior observed here is connected with the vicinity to an ordered phase other than the SC state and confirms that $CeCoIn_5$ is close to a magnetic QCP that is masked by the occurrence of superconductivity.

Coffee break

10:30 - 11:00

Morning session - continued

11:00 - 12:15

Main Building, room 144

Magnetism and superconductivity in oxide ferromagnet/superconductor heterostructures

11:00 - 11:45
invited oral

Piotr Przyslupski[1)]

1) Polish Academy of Sciences, Institute of Physics, al. Lotnikow 32/46, Warszawa 02-668, Poland

The studies of superconductor/ferromagnet (S/F) artificial heterostructures attract much attention. Using such structures it is possible to probe in detail the interplay between superconductivity and ferromagnetism. Recent theoretical model [1] predicts the existence of an indirect exchange coupling between ferromagnetic layers across the superconducting layers, similar to the coupling observed in giant magnetoresistance (GMR) systems.

The theory suggests that the most relevant heterostructures to observe such effect are structures built of layers of manganites with colossal magnetoresistance (CMR) and the high temperature superconductors (HTSC). In this talk we describe the experimental studies [2,3] of the structure, transport and magnetic properties of CMR/HTSC heterostructures, based on manganites La0.67Sr0.33MnO3 (LSMO) and superconductor YBa2Cu2O7 (YBCO). Experimental results support the existence of indirect exchange coupling. The interesting effects of interplay of superconductivity and magnetism in LSMO/YBCO will be presented.

[1] C.A.R. Sa de Melo Physica C 387, 17(2003).
[2] P. Przyslupski et al., J. Appl. Phys. 95,2906(2004).
[3] P. Przyslupski et al., Phys. Rev. B 69,134428(2004).

Magneto-optical analysis as a powerful tool to analyse local magnetic field distribution across superconducting and magnetic materials

11:45 - 12:15
oral

Laura Gozzelino[2)], **Danilo Botta**[2)], **Angelica Chiodoni**[2)], **Roberto Gerbaldo**[2)], **Gianluca Ghigo**[2)], **Francesco Laviano**[2)], **Bruno Minetti**[2)], **Enrica Mezzetti**[2)], **Piotr Przyslupski**[1)], **A Tsarev**[1)], **Andrzej Wisniewski**[1)]

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Magneto-optical analysis is a powerful tool to analyse local magnetic field distribution across superconducting and magnetic materials. We present a careful procedure of non-linear calibration for quantitative evaluation of the local magnetic field in superconducting and magnetic materials. In particular the in-plane field distribution must be carefully taken into account to avoid under-estimation of the out of plane component [1,2,3]. The experimental results concern imaging of different superconducting and magnetic materials ranging from low temperature superconductors to magnetic superconducting heterostructures. In particular we present a detailed imaging of a $YBa_2Cu_3O_7/La_{0.7}Sr_{0.3}MnO_3/LaAlO_3$ multilayer. The substrate exhibits a tri-crystal twinned structure. At the tri-crystal centre point substrates twins meet each other in three different directions: the developed magnetic domains exhibit the expected annihilation on twins due to opposite in-plane orientation of the magnetization and form out-of-plane domain-walls. After cooling below YBCO critical temperature, vortices are nucleated over out-of-plane magnetic domain-walls. Following their own stray-field orientation they nicely decorate such magnetic domain-walls.

The italian members of the working group acknowledge the contributions of the Istituto Nazionale per la Fisica della Materia and of the Istituto Nazionale di Fisica Nucleare-Italy. The polish members of the working group acknowledge the contribution of the Polish State Committee for Scientific Research (Contract No. 5 P03B06220).

[1] F. Laviano, E. Mezzetti et al., Supercond. Sci. Technol., 16 (2003), 71
[2] F. Laviano, E. Mezzetti et al., Physical Review B 68 (2003), 014507
[3] F. Laviano, E. Mezzetti et al., Physica C 404 (2004), 220
[4] P. Przyslupski, M. Sawicki et al., J. Appl. Phys. 95 (2004), 2906
[5] P. Przyslupski, M. Sawickiet et al., Phys. Rev. B 69 (2004), in press

12:15 - 14:00

Lunch break

14:00 - 15:30

Afternoon session

Main Building, room 144

14:00 - 14:30
oral

Analysis of high-T_c superconductor compounds on the nanometre scale

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Due to the small coherence lengths of the high-T_c compounds, effective pinning sites are defects or particles of nanometer size according to ξ^3. Integral magnetic measurements of the magnetization as a function of temperature in large applied magnetic fields (up to 7 T) have revealed that practically all high-T_c compounds exhibit spatial inhomogeneities, which can be caused by either oxygen deficiency (YBCO), solid solutions of Nd/Ba (NdBCO and light rare earth 123-type compounds), intergrowths (Bi-based superconductors) or chemical doping by pair-breaking dopants like Zn, Pr, etc. Such local variations of the superconducting properties should be visible in low-temperature scanning tunneling microscopy experiments, and their effects on flux pinning could be studied in a direct way. Various irradiation experiments by neutrons, protons, and heavy-ions have enabled the artificial introduction of effective pinning sites into the high-T_c samples, thus creating many different observations in the integral magnetic data. Furthermore, several sub-structure formations are found in several multi-light rare earth 123-superconductor samples by means of AFM investigations, which may play an important role for the considerably improved critical current densities in these materials. From all these observations, we construct a pinning diagram explaining many features observed in high-T_c samples.

14:30 - 15:00
oral

Effect of preparation conditions on superconducting properties of (Bi,Pb)-Sr-Ca-Cu-O glass-ceramics

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Granular metals and superconductors are very interesting, because of their unique properties and applications. One of the methods of preparing such materials is a glass-ceramics route, that is, by annealing of an amorphous solid in the way leading to partial crystallisation. In this work we present the influence of annealing conditions on superconducting properties of (Bi,Pb)-Sr-Ca-Cu-O high T_c superconductors prepared by a glass-ceramic method.
Superconducting (Bi,Pb)-Sr-Ca-Cu-O glass-ceramic samples were obtained by annealing of amorphous

$(Bi_{0.8}Pb_{0.2})_4Sr_3Ca_3Cu_4O_x$ at temperatures between 750C and 865C for time intervals from 1 minute to 43 hours. The measurements of the temperature dependence of resistivity in annealed samples were carried out between 3 K and 300 K. Critical current densities were determined from magnetic measurements. The electrical and superconducting properties of the material change during annealing because oxide superconductors belonging to the bismuth family $(Bi,Pb)_2Sr_2CuO_x$ (2201), $(Bi,Pb)_2Sr_2CaCu_2O_x$ (2212) and $(Bi,Pb)_2Sr_2Ca_2Cu_3O_x$ (2223) crystallise forming a granular metal and superconductor. Low temperature resistivity and magnetic measurements show that during the growth of crystalline phases superconducting properties develop rapidly. Measurements of magnetisation reveal that isolated grains of superconducting 2212 phase form in the first minute of annealing at 850 C. Further development of superconducting phases leads to subsequent improvement of superconducting properties. Properties of the material (e.g. room temperature resistivity, critical temperature, critical current) and kinetics of changes depend on the temperature and time of annealing. The highest critical current densities (10^6 A/cm^2 at 5 K in 1 T) were obtained for samples annealed at 850 C for 43 h.

Improved Critical Current Properties of $Cu_{1-y}Mo_yBa_{2-x}Sr_xYCu_2O_{7-d}$

15:00 - 15:30
oral

Bogdan Dabrowski[1)]

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By pinning the magnetic field that can penetrate superconducting material in the regions of weaken superconductivity it is possible to enhance critical parameters of HTSC. Theoretical considerations indicate that best regions should have elongated shape with diameter somewhat larger than the superconducting coherence length (10 ? for the ab-plane of HTSC). Usually, extrinsic methods have been applied to produce effective pinning, where the size (100 - 1000 ?) and spacing (overlapping) of pinning regions is far from optimal. We have investigated the substituted bulk and single-crystals of Y123 materials and show that enhanced critical currents jc can be achieved by formation of intrinsic extended defects with the improved size and distribution for Mo- and Sr- substituted Y123. We describe optimization of the superconducting Tc and jc by determining the best compositions, synthesis and annealing conditions. The structural and superconducting properties of the optimized material with Tc 92 K are studied by neutron powder diffraction and M(B) isotherms measured over wide temperature and field ranges to derive the jc(B) and jc(T) that reveal the pronounced peak effect. The extended defects in the CuO chains, the $Mo_2O_{7/2}$ dimers, are identified as effective pinning centers that locally perturb superconductivity in the CuO_2 planes by providing additional weakly interacting pinning centers that increase the pinning force.

Supported by the NSF-DMR-0302617

Coffee break

15:30 - 16:00

Afternoon session - continued

Main Building, room 144

16:00 - 17:30

Scanning tunneling spectroscopic studies of (100) surface of NdBa2Cu3O7-δ single crystals

16:00 - 16:30
oral

Pintu Das[1)], **Michael R. Koblischka**[1)], **Thomas Wolf**[2)], **Uwe Hartmann**[1)]

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2) Forschungzentrum Karlsruhe GmbH, Institute of Solid State Physics, Karlsruhe D-76021, Germany

$NdBa_2Cu_3O_{7-\delta}$ (NdBCO) is an important member of cuprate high-T_c superconductors because of its higher transition temperature as compared to $YBa_2Cu_3O_{7-\delta}$ and critical current density. The similar sizes of the Nd and Ba ions make it possible for Nd ions to replace the Ba ions in the unit cells producing Nd rich phases leading to a spatial T_c variation within the sample. The samples with Nd rich second phase is believed to play an important role in flux pinning [1]. The variation of transition temperature due to the presence of this Nd rich phase is reported to play an important role to explain the increased critical current performance. However, the nature of the basic pinning mechanism needs to be studied in detail. Scanning tunneling spectroscopic studies of these materials are, therefore, necessary to understand the microscopic electronic properties. In this contribution, we report the results of Scanning Tunneling Spectroscopic (STS) measurements performed on the (100) surface of a NdBCO single crystal (T_c = 95.5 K) using a homemade STM at T = 4.2 K. The surface of the crystal was cleaned by chemical etching before doing the measurements [2].

A variety of conductivity (dI/dV) curves were observed in a chosen range of 20 nm × 20 nm. The peak to peak values of the energy gaps ($2\Delta_{pp}$) found from the curves, normalised with respect to the tip to sample distance, to be 59(+/-)8 meV. A position dependent asymmetry in the peak value of dI/dV at the gap edges have been repeatedly observed. At several positions of the sample very low peaks at the gap edges or sometimes no peaks were observed. We observe the second phase electronic properties that are reflected in our conductivity data. Here, we discuss these results and their possible consequences on the pinning mechanism that are accessible by macroscopic measurements.

1. M. R. Koblischka et al., Phys. Rev. B 58 (1998) 2683
2. R. P. Vasquez et al., Appl. Phys. Lett. 53 (1988) 2692

16:30 - 17:00
oral

Influence of line width on critical current of Nb and NbN thin-film bridges

Konstantin S. Ilin[1], **Michael Siegel**[1], **Alexei Semenov**[2], **Andreas Engel**[2], **Heinz-Wilhelm Hübers**[2]

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Sub-micrometer and especially nano-meter sized structures made from thin superconducting films are crucial for development of the modern generation of ultra-sensitive detectors and mixers for a wide spectrum of electro-magnetic radiation [1, 2]. We present results on systematic study of the critical current in superconducting bridges from 50 nm up to 10 micrometers in width. The bridges as well as meander line structures were made from Nb and NbN films thinner than 20 nm and patterned by means of electron-beam lithography and ion milling technique. We have observed three areas in the dependence of the critical current density on the bridge width. For bridges wider than 1 - 2 micrometers the critical current density is almost constant and has a larger value for thicker bridges. The critical current in this range of bridge width is due to de-pinning of magnetic vortices. Narrowing of bridges down to a few hundreds nanometer leads to an increase of the critical current density up to a value, which is about two times smaller than the theoretical value of the de-pairing current. Further reduction of the width results in a drastic decrease of supercurrent density. We consider the bridges as a superconducting core surrounded by a non-superconducting shell [3]. The proximity effect between this normal shell and the central superconducting part of the bridge leads to an effective suppression of superconductivity and as result to a reduction of supercurrent density in nanometer wide bridges. The reasons for formation of the normal shell will be discussed.

[1] A. Semenov et al., Eur. Phys. J. AP 21, 171-178, 2003.
[2] J.J.A. Baselmans et al., Appl. Phys. Lett. 84, 1958-1960, 2004.
[3] K.S. Ilin et al., Proceedings of the 6th European Conference on Applied Superconductivity, 14-18 September 2003, Sorrento Napoli - Italy.

17:00 - 17:30
oral

Experimental evidence of quantum phase slip phenomena in ultra-narrow superconducting channels

Maciek L. Zgirski[1,2], **K.P: Riikonen**[1], **V. Touboltsev**[1], **M. Savolainen**[1], **K. Y. Arutyunov**[1]

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A superconducting wire can be considered as quasi-one dimensional (1D) if its characteristic transverse dimension is smaller than the coherence length ξ. The shape of the bottom part of the resistive transition R(T) of a not too narrow 1D strip is well described by the model of thermally activated phase slips [1,2]. However, if the wire width falls into a 10 nm range, there are predictions that a new phase slip mechanism due to quantum tunneling should be observed [3,4,5]. We have developed a method of progressive reduction the transverse dimensions of e-beam lift-off fabricated nanowires by ion-beam sputtering. Sputtering can be thought as an erosion of the structure due to bombardment of primary ions. The method is very promising, for it lets us directly follow changes in superconductive transition in 1D superconductor along with successive reduction of its cross-section. Aluminum wires with effective diameter < 35 nm did show up a low temperature 'foot' at R(T) dependencies, which can be associated with quantum phase slip mechanism.

References:

[1] J.S. Langer, V . Ambegaokar, Phys. Rev. 164, 498 (1967)
[2] D.E. McCumber, B.I. Halperin, Phys. Rev. B 1, 1054 (1970)
[3] A. Zaikin, D. Golubev, A. van Otterlo, and G. T. Zimanyi, PRL 78, 1552 (1997)
[4] A. Zaikin, D. Golubev, A. van Otterlo, and G. T. Zimanyi, Uspexi Fiz. Nauk 168, 244 (1998)
[5] D. Golubev and A. Zaikin, Phys. Rev. B 64, 014504 (2001)

Poster session 2

Main Building, Main Hall (Duża aula)

19:00 - 21:00

Thursday, September 9th

Morning session

Main Building, room 144

09:15 - 10:30

Superconductivity in carbon nanotubes

09:15 - 10:00
invited oral

helene bouchiat[1)]

1) laboratoire de physique des solides (LPS), Bat 510, Orsay 91405, France

We report low temperature transport measurements on suspended single walled carbon nanotubes (both individual tubes and ropes). The technique we have developed where tubes are soldered on low resistive metallic metallic contacts across a slit enables a good characterization of the samples by transmission electronic microscopy.

It is possible to obtain individual tubes which remain metallic down to very low temperatures with only a small increase of resistance between room temperature and 1K. When the contact pads are superconducting, nanotubes exhibit proximity induced superconductivity with surprising large values of supercurrent. It has also been recently possible to observe intrinsic superconductivity in ropes of single walled carbon nanotubes connected to normal contacts provided that the distance between the normal electrodes is large enough, otherwise superconductivity is destroyed by (inverse) proximity effect. These experiments indicate the presence of attractive interactions in carbon nanotubes which overcome coulomb repulsive interactions at low temperature and opens the investigation of superconductivity in a 1D limit never explored before.

Resistivity Anomaly Observed in Nano-Structured C_{60}-SAM on Ultrathin Au Films

10:00 - 10:30
oral

Nobuyuki Iwata[1)], **Takuto Sakuma**[1)], **Tuo Fanj**[1)], **Hiroshi Yamamoto**[1)]

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Little or Ginzburg have discussed a possibility of room temperature superconductivity (RTS) by an excitonic mechanism in low dimensional system[1-2]. In order to realize the RTS we prepared nano-structured C_{60} derivatives self-assembly monolayer (C_{60}-SAM) on a ultrathin Au film.

Thickness of the Au films must be in the order of nm for the enhancement of interactions between excitons in the C_{60} derivatives and conducting electrons in the Au. Such the Au films are prepared on annealed MgO single crystals, of which surfaces showed flatness in atomic level with a step-terrace structure. The Au films grew along the steps of the MgO. The Au/MgO substrates are soaked in benzene solution of 0.01 mM C_{60} derivatives to obtain C_{60}-SAM. Surface morphology is observed by AFM.

The Au/Mo electrodes and ultrathin Au area are simultaneously obtained on the substrates by RF magnetron sputtering through a metal mask. Behind the mask random kinetic motions of sputtered Au particles resulted in the deposition of ultrathin Au films. The thickness of the ultrathin Au was very sensitive to the gap distance between the mask and the substrate.
When resistivity of the prepared sample is measured, an appearance of the superconductivity will be characterized as an anomalous decrease in the resistivity because of inhomogeneous thickness of the Au films. Several samples revealed such the resistivity anomaly in the high temperature range above 100 K to 200 K. The appearance of the anomaly strongly depended on the Au thickness of the samples. Furthermore such the anomaly vanished as increasing measurement current, which may indicate the break of superconductivity by exceeding Ic. We intend to attempt increase of the anomaly temperature up to room temperature by optimizing the Au film thickness and also to measure magnetic properties to define the superconductivity.

[1]W.A.Little:Phys.Rev.134(1964)A1416
[2]V.L.Ginzburg et al.:Contemp.Phys.9(1968)355

10:30 - 11:00

Coffee break

11:00 - 12:30

Morning session - continued

Main Building, room 144

11:00 - 11:45
invited oral

The interplay of frustration and geometry in Josephson junction arrays on a dice lattice

Piero Martinoli[1], **Mauro Tesei**[1], **Sergey E. Korshunov**[2], **Ricardo Théron**[1]

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2) L.D. Landau Institute for Theoretical Physics, Moscow 119334, Russian Federation

Exposing a Josephson junction array to a magnetic field (B) frustrates the system and results in a wealth of phenomena, which depend on the level of frustration [measured by the magnetic flux (f) per plaquette in units of the flux quantum], the lattice geometry, the underlying symmetries, and the nature of the excitations. A novel localization effect due to the interplay of B with a particular lattice structure, the dice lattice, has been theoretically predicted and observed in experiments exploring the phase boundary of wire networks. In this presentation, we report and discuss the results of sensitive magnetoinductance [L(f)] measurements performed on arrays of proximity-effect coupled junctions on a dice lattice. The inverse magnetoinductance $L^{-1}(f)$ is found to exhibit prominent peaks at f=1/3 and f=1/6 (and weaker maxima also at f=1/9 and f=1/12) reflecting a high degree of superconducting phase coherence in the system. At f=1/2, on the contrary, $L^{-1}(f)$ shows a deep minimum pointing to a strong suppression of phase coherence. Relying on a XY model description of the array, the ground-state vortex configurations for f=1/3 (Abrikosov state) and f=1/6 (rhombic state) are shown to correspond to remarkably compact phase structures, thereby explaining why these states are particularly robust against thermal fluctuations and, consequently, so prominent in $L^{-1}(f)$. In striking contrast, the ground state at f=1/2 is predicted to exhibit a so-called accidental degeneracy allowing for the formation of zero-energy domain walls. Thus, ordering at f=1/2 should be quite vulnerable to thermal fluctuations, in agreement with our experimental observations. Using the star-triangle transformation, the inductance network associated with the frustrated dice lattice can be mapped on an anisotropic triangular lattice, thereby allowing L(f) to be calculated from the ground-state distribution of the gauge invariant phase differences and compared with the experimental data.

11:45 - 12:15
oral

MICROWAVE DETECTION OF JOSEPHSON JUNCTION ARRAYS, INTEGRATED IN THE RESONATOR

Oleksandr M. Ivanyuta[1], **Volodymyr M. Raksha**, **Oleksandr V. Prokopenko**, **Yaroslav I. Kishenko**, **Alexander M. Klushin**[2]

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2) Forschungszentrum Juelich GmbH, Institute of Thin Films and Interfaces (ISG), Leo-Brandt-Str., *Julich D-52425, Germany*

The physics mechanisms of detection of microwave electromagnetic radiation of X- and Ka-band by superconducting nonlinear elements were considered. As the nonlinear elements the high-temperature superconducting (HTS) YBCO bicrystal Josephson junctions were chosen. The array of Josephson junctions was embedded in the surface wave resonator (SWR). This resonator consists of HTS YBCO film with array of junctions on a dielectric substrate with bicrystal grain boundary (yttrium-stabilized zirconium substrate). The junctions were shunted by thin layer of gold in order to achieve a non-hysteresis current-voltage characteristic of the array and to decrease the scattering of junction parameters.
In known similar systems the Josephson junctions are series dc and series ac coupled, so excitation conditions for junctions are unequal. In proposed excitation system on the base of the SWR the junctions are series dc but parallel ac coupled, so the excitation is the same for each junction in the Josephson junction array. Using this excitation method a new class of microwave devices with lower utilized power and greater sensitivity can be designed.
Detecting of a microwave signal by a Josephson junction array embedded in the SWR was experimentally studied. Measurements were carried out starting from critical temperature of the HTS film and down to the hydrogen level using the Gifford-McMohon closed-cycle cryo-cooler. The sensitivity of such type of detectors was measured. It was approximately 10^4 V/W.
So the excitation method by the surface wave resonator allows using the systems with parallel ac biased synchronized HTS Josephson junctions. Such microwave detectors on the basis of Josephson junction arrays embedded in the SWR has higher sensitivity and increased dynamic range.

Key Words: Josephson junction, surface wave resonator, microwave detector.

Lunch break

12:30 - 14:00

Symposium F

Wide Band Gap II-VI Semiconductors: Growth, Characterization and Applications

Introduction

The wide bandgap II-VI semiconductors offer new exciting possibilities for applications in optoelectronics and spintronics. A revolutionary breakthrough in overhead illumination, in picture transmission and in visualization techniques is expected through the introduction of short wavelength emitting LEDs and LDs. Blue/violet color light sources are based on nitrides, but green color is a problem at present. There are some hopes that ZnSe-based structures will be good for such applications. Also ZnO is a promising material for applications in optoelectronics, but also in spintronics, if doped with magnetic impurities.

The application of wide bandgap II-VI materials in these fields requires important breakthroughs in growth techniques, defect control, doping procedures, etc... Knowledge about defect structures in these materials can help to predict their optical properties and solve problems related to degradation, which occurs in ZnSe-based devices under extreme working conditions, such as high current density, high working temperature and high intensity of light fields.

This E-MRS Symposium is aimed to discuss recent progress in these research fields. Material properties, but also applications of new materials in optoelectronic will be discussed. The symposium will provide a forum for presentation and exchange of new ideas and prospects for their future applications.

Organisers

- Prof. Marek Godlewski, Institute of Physics, Polish Academy of Sciences, Warsaw
- Prof. Andrzej Mycielski, Institute of Physics, Polish Academy of Sciences, Warsaw
- Prof. Eugen M. Sheregii, Institute of Physics, Pedagogical University of Rzeszow, Poland
- Prof. Robert Triboulet, CNRS/LPSC, France

Monday, September 6th

Opening / Afternoon session 1

13:50 - 15:30

Main Building, room 134

Coupled II-VI semiconductor quantum dots: manipulation of spin polarization by inter-dot exchange interaction

14:00 - 14:45
invited oral

Jacek K. Furdyna[2], **M. Dobrowolska**[2], **S. Lee**[1]

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2) University of Notre Dame, Department of Physics, 225 Nieuwland Science Hall, Notre Dame, IN 46556, United States

Prospects of employing spin states in quantum dots (QDs) for device applications (e.g., as quantum bits in quantum computing) naturally hinge on the ability to manipulate these states. We will show that exchange interaction makes it possible to change the spin polarization of carriers in one QD by controlling the spin states in an adjacent QD, thus providing a handle for such spin manipulation. We studied self-assembled QDs in the form of double-QD layer systems. For observing interlayer exchange processes, we strategically designed coupled asymmetric structures comprised of QD layers with different QD bandgap energies. The double layers were formed either from CdSe and CdZnSe QDs or from CdSe and CdZnMnSe QDs, separated by ZnSe barriers. We observe well-resolved photoluminescence (PL) peaks originating from the two QD layers, enabling us to identify PL emissions from each QD family, and thus to study the influence of one QD layer on the other. To investigate the spin polarization of carriers in the QDs, we performed polarization-selective magneto-PL experiments by exciting the above structures with unpolarized light, and detecting the PL with the circular polarizations of opposite helicity. When a magnetic field was applied to the CdSe/CdZnSe double-QD layer, intensities of the circularly polarized PL peaks from the CdSe and CdZnSe layers exhibited significant differences, reflecting differences in the degrees of spin polarization of the CdSe and the CdZnSe QDs. This contrasts with single-layer CdSe or CdZnSe QD reference structures, which show nearly identical dependences on the field. The behavior observed on double-layer QD structures is interpreted in terms of anti-parallel spin interaction between carriers localized in pairs of electronically coupled QDs. Such spin interaction is even more pronounced in double-layer QD structures where CdZnSe QDs are replaced by magnetic CdZnMnSe QDs.

Coherent phase transition in CdTe microcavities

14:45 - 15:30
invited oral

Maxime Richard[2], **Jacek Kasprzak**[2], **Regis Andre**[1], **Le Si Dang**[1], **Robert Romestain**[2]

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2) University J.Fourier-Grenoble-I, Lab. Spectrometrie Physique (CEA-CNRS), 17 avenue des Martyrs, Grenoble 38054, France

Exciton-polaritons are bosonic eigenstates of semiconductor microcavities, consisting of a coherent mixing of quantum well excitons and cavity photons. Their density of states is four orders of magnitude smaller than that of excitons, which favors the possibility of reaching high occupancy factor before the breakdown of the exciton bosonic character. Thus polaritons are good candidates for the formation of a Bose condensate, particularly in II-VI microcavities due to the larger binding energy of II-VI excitons. Previous experimental studies of CdTe microcavities have clearly demonstrated that stimulated emission of polaritons can be obtained under non-resonant optical excitation. In this work, we present an experimental study of CdTe polaritons in this high excitation regime.
First, an angle resolved setup allows us to probe the polariton population along the dispersion curve. We observe that the emission dispersion becomes flat. We show that the latter effect can be well explained in terms of coherent collisions between in-phase polaritons. On a second hand, a microphotoluminescence setup allows us to observe a shrinkage and a shape modulation of the emission spot in real space in the stimulated regime. The spatial and transverse coherence of the emission will be discussed.

Coffee break

15:30 - 15:50

Afternoon session 2

Main Building, room 134

15:50 - 17:15

ZnSe-based laser diodes: New approaches for longer lifetimes

15:50 - 16:35
invited oral

Arne Gust[1], **Matthias Klude**[1], **Carsten Kruse**[1], **Elena Roventa**[1], **Detlef Hommel**[1]

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Despite of many potential applications of ZnSe-based green-yellow LDs, their fast degradation is still a problem. But there is no other material including the nitrides which can obtain stimulated emission in the green spectral region. One reason of the degradation is the stability of the QW. The compressive strain of the QW attracts defects, and also Cd outdiffusion takes place into the p-doped area.

First a short review will be given of ZnSe LDs emitting in the full green spectral range. Then the advantages of QDs in those laser structures will be discussed. Finally a green monolithic VCSEL will be presented.

Laser emission in cw-mode around 560 nm from CdZnSSe QWs was reported for the first time by our group in 2001. One approach for suppressing the degradation is the introduction of strain-compensating ZnSSe barrier layers. Conventional LDs and LDs with different arranged barriers were grown by MBE. The achieved enhancement of lifetime was more than an order of magnitude in case of the p-side barrier. Further investigations revealed that a layer of high sulfur amount does not act only as strain compensating layers but also as a blocking layer for the Cd diffusion into the p-layers.

An alternative to achieve longer lifetimes is the usage of CdSe QDs in the active region. LED degradation experiments under constant current have been performed and show a lifetime of 600 h for the QD laser compared to 0.6 h for a QW laser. When processing the QD laser as a ridge waveguide structure the threshold could be reduced from 7 to 1.5 kA/cm^2. This decrement is caused by a large reduction of current spreading. Compared to common ZnSe QW LDs, the discussed QD lasers show an unexpected stability against high current injection.

Furthermore, experimental data from the first monolithic ZnSe-based VCSEL will be presented. The VCSEL exhibits an emission wavelength of 514 nm by optical excitation at RT. The used DBRs can be tuned over the whole visible spectral region.

Optical properties of CdTe quantum dots

16:35 - 16:55
oral

P. Wojnar[1], **Marta Aleszkiewicz**[1], **Jacek Kossut**[1], **Grzegorz Karczewski**[1]

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We investigated electroluminescence (EL), photoluminescence (PL) and micro-photoluminescence (μ-PL) of self assembled CdTe quantum dots (QDs) embedded in different II-VI materials: ZnCdTe, ZnMgTe and CdMgTe. Our structures were grown by Molecular Beam Epitaxy (MBE) employing a new self formation method of the QDs proposed recently by Tinjod et al. [1]. The most important advantage of this method is the possibility of quantum dots formation even when the lattice mismatch between the dot and the barrier material is as small as 2.8%. Another advantage is the possibility of in-situ observation of the 2D-3D transition by RHEED (Reflection of High Energy Electron Diffraction).
The surface of our structures was examined by Atomic Force Microscopy. From these measurements, we obtained the density of dots of the order of 10^{10} cm^{-2}, the average in-plane diameter and the average height being about 30nm and 7nm, respectively.
For EL measurements we have introduced CdTe quantum dots layer into a p-n junction. We have chosen carefully the n-type and p-type materials taking into account their electrical and optical properties. The quality of p-n junctions was characterized by current-voltage measurements. We have studied temperature and voltage dependencies of the luminescence.
The typical PL and EL spectra of a quantum dots layer consist of a very broad line. Its spectral width is determined by inhomogeneity of the sizes and chemical compositions of the quantum dots in the ensemble. In the case of μ-PL, we decrease the diameter of the excitation spot down to 2 μm. The PL line splits into a large number of sharp spikes with the spectral width in range of 100 μeV. The narrow lines are attributed to individual quantum dots. We found that we can significantly shift the position of the luminescence line, when we change the composition of the barrier, from 1.7eV to 2.3eV.

[1] Tinjod F., Gilles B., Moehl S., Kheng K., Mariette H. Appl.Phys.Let.,v 82, 24, p.4340
[

[ABSTRACT TRUNCATED TO 2000 LETTERS]

16:55 - 17:15
oral

Laser stimulated p-n junction formation in CdTe

Aliya Baidullaeva[1)], **Peter Feychuk**[2)], **O. I. Vlasenko**[1)], **P. Mozol**[1)], **P. Pobirovsky**[1)], **P. Siffert**[3)]

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CdTe crystals are promising for their applications in optoelectronic devices, such as solar energy converters, optoelectronic modulators, highly efficient detectors for γ- and X-rays at room temperature.
Usually as-grown undoped CdTe crystals show p-type conductivity. Diffusion and ion implantation of III group elements are commonly used methods for the formation of diode structures. These methods could provide semiconductor doping of high quality, but need high temperature processing. Moreover, the diffusion of impurity on given low depth is difficult. To overcome these disadvantages, we have tested a process of doping p-CdTe with Indium under laser radiation in order to create abrupt In profiles for p-n junctions.
(111) CdTe p-type wafers, grown by the THM method were investigated. Indium was used as a dopant impurity. A thin layer of indium was vapor deposited in vacuum on the Te-side surface of p-CdTe crystal before its irradiation. Samples were irradiated at T=300K with multimode Q-switched ruby laser single pulses with 2x10^{-8} s duration both in air, and in chamber filled with Ar under 2 atmospheres pressure.
It was shown that the use of laser radiation has the potential for doping and producing shallow p-n junction in CdTe crystals. As opposed to doping during the process of growth the formation of p-n junction under laser doping occurs within short time (2x10^{-8} s) with predetermined locality both in depth and on the surface of crystals. The doping deposition thickness and procedure of irradiation necessary for creation of shallow p-n junction were optimized. Current-voltage characteristics of p-n junction in CdTe crystals were investigated. These characteristics of the p-n junction show diode properties with reverse current of 35 nA and 1.8 nA at 100V bias for 10 x 10 mm^2 and for 3 x 3 mm^2 structures respectively.
The mechanisms of shallow p-n junction creation under laser radiation are discussed.

19:00 - 21:00

Poster session 1

Intensity dependence of nanostructure formation on surface of CdTe crystals under pulse laser irradiation and their photoconductivity spectra

poster
F1

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At present the investigations of nanosize clusters formation on crystal surface under laser irradiation is one of the prospective tasks in the semiconductor technology. The sizes and density of these structures ambiguously depend on physical nature of material, power density or irradiation dose, concentration of defects and other factors. Formation of nanostuctures depending on dose of laser irradiation was investigated in CdTe, as the last is promising material for development of advanced optoelectronic devices. It was shown that effect of accumulation plays the basic role in this process.
The question of intensity dependence of nanostructure formation on the surface of CdTe crystals is still open and actual.
The dependence of surface morphology of p-CdTe (111) crystals on power density of laser radiation was investigated by atom-force microscopy method. Photoconductivity (PC) spectra were studied at 300K and 77 K. Crystals were irradiated at T=300K by one pulse of the Q-switched ruby laser radiation with 2•10-8 s duration.
An averaging roughness of surface of inititial sample was about 0.075 nm. It was found, that irradiation of crystals results in formation of the nanostructures with lateral sizes about 19.3-46 nm and heights about 1-5.6 nm. Computer Fast Fourier transformation shows, that nanoclusters are periodic at specific power density of laser irradiation.
After irradiation of sample PC maximum due to band-zoned transition and several additional PC bands of low-intensity at high-energy portion of spectrum were observed in addition to impurity maximum. It was established the correlation between occurrence of additional PC bands and nanoclusters.
Experimental data analysis enabled to ascertain the intensity of laser radiation at which homogeneously distributed nanoclusters with minimum lateral sizes are formed on surface of CdTe crystals. Possible mechanisms of nanosize clusters formation are discussed

Defect redistribution in CdTe after Cd saturated annealing

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poster F2

The effect of Cd saturated annealing at 600^{o}C on electrical and optical properties of undoped CdTe was investigated by Hall effect, conductivity and photoluminescence measurements in the temperature interval of 4.2-300K. We observed that p-to-n conversion occurs in p-CdTe during annealing, where converted n-type layer surrounds the p-type center of the sample (core). The thickness of the converted n-type layer detected by Electron beam induced current method (EBIC) was found close to the forth root of the annealing time and differs from standard diffusion behavior characterized by a square root dependence. High electron mobility 1200 cm^2/Vs and carrier density 2x10^{14} cm^{-3} at room temperature were observed in the n-type layer, which indicates high quality of the sample. Highly compensated donor level with ionization energy E_D 10meV was determined there. Anomalous conversion of the sample back to the p-type was observed after the long time annealing, when the core was annihilated. Electrical properties of as-grown p-type crystal and p-type core were not significantly changed by the annealing contrary to reconverted p-type, where the hole concentration decreased by several orders of magnitude. Purification of the n-type layer due to gettering of fast diffusing impurities into the core region during annealing was observed by photoluminescence, where the intensity of PL lines of the excitons bound to neutral acceptors (A^o,X) in the n-type layer is significantly reduced comparing with that of in as grown crystals.
Observed results are explained by a diffusion of Cd interstitials into the sample together with gettering of foreign rapidly diffusing acceptors in the core region and redistribution of impurity defects to the whole sample and formation of acceptor like defects after core annihilation.

STRUCTURAL DEFECTS IN CdTe CRYSTALS AND NOISE PROPERTIES

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poster F3

The paper presents the results of study of noise charachteristics of cadmium telluride bulk single crystals, both undoped and doped by As and Cl. The noise spectra were measured over a vide range of frequencies, from 1 Hz up to 100 kHz, at 300 and at 80 K. The noise power spectra are of 1/f$^/$gamma , where $\gamma = 0.9$ in the whole frequency range.
At room themperature current noise (Si) is proportional to the square of the dark leakage current trough the sample. Both value and character of spectra depend on the conductivity type of the crystal and on the nature of doped dopand impurity. There are some peaks on the normal-ized curves S_i(f)*f - f which are caused by the presence of local levels inside the bandgap of the crystals under investigation.
At zero biased sample current noise spectra correspond to the white noise spectra and agree well with the calculated results. Analysis of short noise were performed taking into con-sideration the presence of the macrodefects and clusters in the crystalline matrix. It is assumed that these types of inhomogeneities effect the current noise spectra too.

Structural and optical characterization of epitaxial layers of CdTe/PbTe grown on BaF_2 (111) substrates

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poster F4

CdTe and CdTe/PbTe layers were grown on cleaved BaF_2 (111) substrates by molecular beam epitaxy technique employing PbTe, CdTe, and Te_2 effusion cells. The growth of the layers was monitored in-situ by RHEED diffraction technique. Crystal structure was examined by standard X-ray diffraction method. The CdTe/PbTe layers are monocrystalline with (111) crystal orientation and exhibit x-ray rocking curve FWHM parameter of 200-300 arcsec for PbTe and 300-600 arcsec for CdTe. The well defined streaky

RHEED diffraction pattern was observed during the entire process of growth of both layers indicating a two-dimensional mode of growth with a smooth transition between PbTe and CdTe evidenced by a distinct surface reconstruction.
For the optical characterization of CdTe layers, the photoluminescence spectra were studied at T=4.2 K in 750-870 nm (1.40-1.65 eV) spectral range using pulsed excitation at 2.35 eV by YAG laser. In CdTe/BaF_2 (111) layers, the dominant photoluminescence peak is observed at 785 nm and corresponds to the radiative recombination of excitons bound to neutral acceptors. In CdTe/PbTe/BaF_2 (111) heterostructures with thick PbTe buffer, no photoluminescence is observed in the spectral rage studied. It agrees with recent photoluminescence studies of PbTe/CdTe/GaAs (100) epilayers [1], and supports the idea that despite the dramatic differences in electronic structure of CdTe and PbTe these semiconductors form type-I quantum well heterostructures with fundamental optical transitions expected in PbTe well in the mid-infrared.

[1] K. Koike et al, J. Crystal Growth 257 (2003) 212.

$Cd_{1-x}Zn_xTe$ Single Crystals Growth from Vapor Phase

poster F5

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In order to be used as γ-detectors, CdTe single crystals have to be of high resistivity and must possess a high level of perfection and be free of linear as well as volume defects.
The present research presents a new method of CdZnTe single crystals growth with natural faceting by vapor transport using a polycrystal ingot as initial source material. Source polycrystal $Cd_{0,96}Zn_{0,04}Te_{1+-\delta}$ (δ = 0,0001) or $Cd_{0,87}Zn_{0,13}Te_{0,999}$ ingots were synthesized by melting together calculated amounts of elementary components
$Cd_xZn_{1-x}Te$ single crystals were grown in a 35 mm diameter quartz ampoule located in an isothermal medium at 1050-1150 K. The temperature gradient along the ingot was built owing to thermal radiation. By use of a capillary tube the redundant component is removed from the growth zone and deposited in the cold zone. The single crystals growing rate reached as high as 2 cm^3/day. As a result, we obtained single crystals with 2,5x2,5x4 cm^3 dimensions, constrained by natural faces corresponding to the (110), (100) and (111) planes, the dislocation density being 10^3 cm^{-2}.
Measuring of the rocking curves half-height width for reflection planes (CuK_α X-radiation) with Miller indices (111), (220), (311), (422) and (331) gave 25.0 s, 17.5 s, 13.6 s, 20.8 s and 13.6 s values respectively. X-ray patterns obtained in CuK_α radiation do not reveal any volume defects or mechanical stresses.
Crystals of both n- and p-type were obtained, carrier concentration being at 300K n =3x10^{14}/cm^3 or p =1,7x10^{15}/cm^3, with carrier mobility of 326 cm^2/Vs, 69 cm^2/Vs respectively.
Using as source substance a $Cd_{0,96}Zn_{0,04}Te_{1,0001}$ alloy with 0,2 mol% of Ga_2Te_3 single crystals by vapor transport could be grown. They possess a 2x10^6 Ohm cm resistivity at 300 K.

High-temperature behavior of CdTe<Cl> crystals

poster F6

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CdTe crystals, doped by Cl, are widely used for γ-detectors manufacturing due to their high resistivity and atomic number, as well as long carriers lifetime. Up to now, their properties were investigated in details only at rather low temperatures. It is of interest to know the point defect structure of this material at high temperature where it forms, what will allow to govern the type and concentration of point defects. CdTe<Cl> crystals were grown by THM and traditional Bridgman techniques. High temperature Hall effect measurements were carried out under well defined Cd or Te vapor pressure in temperature ranging from 300 to 900^o C in sealed quartz ampoule using graphite contacts.
At room temperature all of them revealed high resistivity (ρ>10^8 Ohm cm) with hole mobility 60 cm^2/Vs. In the investigated samples, the electron mobility decreases from 500 V/cm^2s at 400^{o}C to 170 V/cm^2s at 900^o C. During the first heating up to T=650^{o}C the electron concentration did not depend on temperature or Cd pressure and was 5x10^{18} cm^{-3}; it rises at higher temperatures only. After a quick cooling a rise of [e^-] by 1,5-2 times comparing with initial level is observed. A similar situation is reported during the second and third heating-cooling cycle.
Under Te vapor pressure the samples demonstrated p-type conductivity from 180C(μ = 30 V/cm^2s, [h+]=10^{16} cm^{-3}) up to (μ =5 V/cm^2s, [h+]=3x10^{17} cm^{-3}). Between T=550-800^{o}C the conductivity was bipolar and only for even high values (T>800^{o}C) the mobility becomes really of n-type.
In this paper, the observed phenomena are explained in terms of point defect chemistry by Cl-containing

precipitates dissolution in Cd saturation region and by rising both Te_i^- and V_{Cd}^- concentrations in the Te region.

Detection Efficiency Spectrum of CdTe X- and Gamma-Ray Detectors with a Schottky Diode

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poster F7

CdTe has been regarded as the most suitable semiconductor for X- and gamma-ray detectors operated without cryogenic cooling. Nevertheless, CdTe manufacturers are confronted by severe difficulties caused mainly by the poor transport properties of the material. Takahashi et al. [1,2] reported a significant improvement of the characteristics of the CdTe detectors based on utilizing a Schottky barrier. However, some crucial questions, relevant to the role of the Schottky diode in this type of detectors, remain unanswered.

In this presentation, we focus on spectral distribution of the Schottky detector efficiency, the most comprehensive characteristic of the device. For the first time, in our calculations we take into consideration both the charge loss in the depletion layer with account for nonuniformity of the electric field, and the collection of charges generated in the neutral region of the diode. The detection efficiency spectrum of the stacked detector [3] is also reported.

The preliminary evaluation indicates that the obtained results are conclusive and important. (i) The total charge collection in the depletion region is achieved for the electron lifetime in excess of about 0.01 microseconds rather than several microseconds as in a detector with ohmic con-tacts. (ii) The "diffusion" component of the collected charge can be comparable and even greater in comparison with the commonly considered "drift" component. (iii) For typical parameters of the material, the efficiency of a stacked detector containing more than 8-10 Schottky diodes can be in excess of the "bulk" detector efficiency.

[1] T. Takahashi et al. Proc. SPIE. 3446 29 (1998).
[2] T. Takahashi et al. Nucl. Instr. and Meth. A436 111 (2000).
[3] S. Watanabe et al. IEEE Trans. Nucl. Sci. 49 1292 (2002).

Laser-induced modification of sub-surface region of CdTe:Cl single crystals

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poster F8

Among different II-VI compounds, cadmium telluride attracts much attention owing to a wide spectrum of its technological applications. Irradiation of CdTe with high-absorbed laser pulses may be effectively used to alter parameters of a thin sub-surface layer of the crystal while the characteristics of the bulk remain unchanged. However, correct interpretation of laser irradiation effects is complicated by generation, redistribution and interaction of different types of defects and impurity-defect complexes. These processes are not fully understood up to now.

In this contribution, results on laser irradiation of CdTe:Cl crystals are reported. The samples were irradiated with a single pulse of a ruby laser at power densities of 2.0 - 3.0 J/cm^2.

Selective etching of the irradiated samples revealed a huge increase in dislocation density (up to 10^8 cm^{-2}) in the sub-surface layer with sharp edge between this layer and the bulk. Measurements of photoluminescence (PL) spectra also showed substantial changes in the PL properties of the irradiated samples. First of all, intensities of the so-called W line (around 1.586 eV) connected with excitons localized at the A-centers and the 1.4 eV band are significantly enhanced because of an increase in A-centers concentration. Appearance of new PL lines is assigned to generation of shallow defects whose nature is discussed. Influence of subsequent thermal annealing of the irradiated samples are explored as well.

Inelastic electron-polar optical phonon scattering in wide gap CdHgTe alloys

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poster F9

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In [1,2] the mechanism of electron - polar optical phonon scattering in the narrow gap solid solutions $Cd_xHg_{1-x}Te$ ($0 < x < 0.17$) was considered on the basis of the short-range scattering model within the framework of a precise solution of the stationary Boltzmann equation. It allowed to achieve the coordination between the theory and experiment in the temperature range T >100K i.e. where this scattering mechanism is dominating. The purpose of the present work is to show the possibility of using of a short-range model in a case of wide gap $Cd_xHg_{1-x}Te$ solid solutions.
The short-range interaction potential of an electron with polar optical phonons is finding by the way of solution of a Poisson equation in the limits of one unit cell. Thus the unit cell is substituted by a sphere of effective radius $R=\gamma$ a (a - lattice constant) the magnitude of which lies within the limits of half of the smaller diagonal up to half of the larger diagonal of a unit cell ($0.5 < \gamma < 0.866$).
The calculation of the temperature dependence of electron mobility was made for compositions x = 0.52; 0.59; 1.0 . The magnitude γ for these compositions is equal 0.86 ; 0.866 ; 0.76 respectively. The calculations show that the theoretical curves well agree with the experimental data in the temperature range T > 100 K whereas the curves calculated on the basis of the standard long-range model differ from experiment in 2.5 - 4 times. It testifies that the model, offered us, adequately describe the electron-polar optical phonon scattering in the wide gap $Cd_xHg_{1-x}Te$ solid solutions.

[1]. O.P. Malyk . Inelastic electron scattering on polar optical phonons in mercury telluride. - Accepted for publication in Ukr. Phys. Zhur.
[2]. O.P. Malyk . Inelastic electron-polar optical phonon scattering in the solid solution $Cd_xHg_{1-x}Te$. - Accepted for publication in Journal of Alloys and Compounds.

Folded Acoustic phonons in $(CdTe)_n/(MnTe)_m$ superlattices

poster
F10

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Several short-period, zinc blende (CdTe)n/(MnTe)m superlattices, grown by molecular beam epitaxy, have been studied by Raman spectroscopy. All structures were deposited on (001) oriented GaAs or CdZnTe substrates. The folded longitudinal acoustic phonons (FLA), up to the fourth order, were well observed in the standard backscattering geometry with the incident and scattered polarization parallel to the <010> axis. The frequencies of those FLA correctly followed the usual dispersion law with the superlattice periodicity which allowed us to determine the unknown elastic constant C11 of zinc blende MnTe. The obtained value of C11 was compared to the value obtained by the extrapolation of results corresponding to CdMnTe mixed crystals. From the frequency position of the first order FLA doublet, the index of refraction of zinc blende MnTe was also obtained. Its value was compared with the value determined by a Kramers-Kronig analysis of the reflectivity spectrum, collected on thick MnTe layer.

ELECTROPHYSICAL PROPERTIES OF LIQUID CdTe WITH ARSENIC ADMIXUTES

poster
F11

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A widespread application of CdTe in the γ-ray detector production meets higher requirements imposed on its initial crystal growth conditions and further properties. Electrophysical properties of the CdTe melt especially in the vicinity of a stoichiometric equiatomic composition are essential for solving of a number of technological problems. Investigations of CdTe in the liquid state are few in number due to difficulties of high-temperature measurements and a high pressure of the component saturated streams. Peculiarities of the melting and crystallization were investigated in the course of the viscosity studies [1]. The thorough investigation of electrophysical properties were performed in [2]. Nevertheless, low pressures used in these experiments did not suppress intensive melt evaporation.
In this work the electrical conductivity σ(T) and thermo-emf S(T) of pure liquid CdTe alloys and with admixtures of arsenic (approx. 0.14 at.%) were investigated in a wide temperature range between 1470 K and the crystallization under argon pressure up to 25 MPa.
Admixtures of As do not lead to any peculiarities on the σ(T) curves, but only decrease the absolute values, while S(T) takes the negative values after melting and then regains positive values with heating. Such a behavior suggests that mobility decreasing dominates over the carrier concentration increase during melting. The As admixture forms shallow acceptor levels in the solid CdTe. The pseudogap narrows in the course of cooling and tails the acceptor level. The pure As manifests then itself in the CdTe melt as an

additional scattering center that leads to the electrical conductivity decreasing. The results are analyzed under the assumption that the Fermi level drifts as the sample composition changes.

1. L.Shcherbak, P.Feychuk, Yu.Plevachuk et al., Phys. Stat. Sol. (b), 229(1), 165 (2002).
2. A.Ben Moussa, B.Giordanengo, J.C. Humbert et al., Phys. Rev. B, 62(23), 256 (2000).

The local crystalline structure of ZnCdTe alloys obtained by Far Infrared Synchrotron Radiation measurements

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poster F12

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Far infrared reflectivity spectra of $Zn_xCd_{1-x}Te$ (ZCT) alloys were measured in the expanded (in comparison with previous work [1]) composition range 0.056 to 0.75 using alternatively an infrared synchrotron radiation source and a mercury lamp. Spectra were measured on the FT IR-spectrometer (Bruker Equinox 55) available at the DAFNE-light facility of the INFN-LNF laboratory, with a resolution of 1 cm-1 for samples placed under vacuum in a helium cryostat for temperatures ranging from 20 K to 300 K. The measured spectra were analyzed by a standard Kramers-Kronig procedure to obtain the imaginary part of the dielectric functions. These were unfolded into their component Lorentzian oscillator sets. The unfolding is done using the statistical strained-tetrahedron model with its axioms as proposed by Robouch et al [1] with five-configuration distorted-tetrahedra, and extended to the analysis of far-IR spectra [2]. The unfolding reveals a fine structure with two overlapping bands, structures that had not been previously observed (see [3]). Each of the seven Zn_xCd_{1-x} Te samples upon analysis exhibits the expected eight spectral lines, each defined by its parameter triplet $\{S_k,W_k,G_k\}$. The unfolding yields the three site occupation preference (SOP) parameters {W1, W2, W3 =1}, revealing a distribution close to random {W1=W2=W3ş1}. Hence the real local crystalline structure of $Zn_xCd_{1-x}Te$ is defined. Simultaneously the unfolding yields also deduced from the experiment oscillation strengths for CdTe and ZnTe, with values comparable to those available in literature for binary CdTe and ZnTe compounds. Our results are in good agreement with the proposed model of Ref. [3]. [1] -J. Polit, E.M. Sheregii, E. Ściesińska, J. Ściesiński, E. Burattini J. Konior, A. Kisiel A. Mycielski, Journal of Alloys and Compounds, 371, 172, 2004;[2]- B.V. Robouch, A. Kisiel and J. Konior, J. Alloys Compounds 339, 1 (2002.[3] B.V. Robouch, E.M. Sheregii, J.Polit, J.Cebulski sub to Phys.Rev.B
[ABSTRACT TRUNCATED TO 2000 LETTERS]

Vapour phase growth and characterisation of Cl-doped cadmium telluride single crystals

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poster F13

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A vapour phase method and growth set-up for the pure and Cl-doped CdTe single crystals preparation are described. The optical quality of as-grown crystals was investigated by infrared transmission microscopy over a wide range of wavelengths. It was revealed that their optical and electrical properties depend on the doping level. Undoped and low-doped (Cl concentration $N_{Cl}=10^{17}$ cm^{-3}) materials transmittance is high enough (larger than 60% in the wavelenght range of 2-25 μm) but their resistivity does not exceed 10^6 Ω cm. When the chlorine concentration increases the crystals become semiinsulating ($>10^8$ Ω cm). But the reduction of transmittance was observed for heavily doped ($N_{Cl}>10^{19}$ cm^{-3}) crystals. Their calculated extinction coefficients yield power law dependence on photon energy in the short wavelength range of the spectra. The calculated scattering coefficients correlate well with the concentration and size distribution of the second phase inclusions determined by means of chemical etching technique and by SEM.

Photorefractive CdTe for laser ultrasonics receivers

poster F14

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Semiconductor crystals lacking the symmetry center exhibit photorefractive effect. One of the most promising application of the photorefractive semiconductors is remote detection of ultrasonic waves with adaptive interferometers. Because of the fast response the photorefractive semiconductors exhibit adaptability to a wide range of mechanical and optical disturbances that are encountered in the factory environment. Cadmium telluride (CdTe) possesses the largest electro-optic constant among all semiconductors. It is thus a promising material for use in laser ultrasonic receivers. An important advantage of CdTe is its sensitivity in the near infrared and at 1.5 μm in particular, where many commercial solid-state lasers and laser diodes are available. The latter wavelength is important because it lies in the "eye-safe" spectral range and because this is telecommunication wavelength range.
In present work photorefractive CdTe:Ge crystals are studied as a medium for laser ultrasonic detection at 1.06 μm and 1.55 μm. The complex coupling strength is estimated for the two-beam coupling configuration in the presence of a dc field. Excellent performance of the material is shown at both wavelengths by demonstration of high sensitivity and high cutoff frequency at low intensity.

Study of selfcompensation in CdZnTe:Cl crystals.

poster F15

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The process of self-compensation of conductance in Cd {1-x} Zn$_x$ Te:Cl (x=0,05) crystals was investigated with annealing of the singlecrystal samples in Cd vapors. The samples were stood at temperature 900 under controlled pressure of Cd during the time necessary for setting of diffusion homogeneity of charged lattice defects concentration; then they were slowly cooled up to room temperature. Concentration of Cl in the crystal in this process remains constant and concentration of Cd vacancies is determined by pressure of Cd vapour above the sample.
Concentration of free charge carriers in the samples after annealing (n and p) was defined by measuring of Hall effect. Low n and p values in the obtained samples testify to the deep self-compensation in the crystal in the annealing conditions. The characteristic feature of obtained results is low value of n = 10^7-10^9 cm $^-$3 for wide range of cadmium vapour pressure changes. It considerably differs from analogous dependence of selfcompensation in CdTe:Cl crystals [1]. It is possible to explain this difference by the strong influence of zinc on concentration of the deep center responsible for selfcompensation in a band gap of the semiconductor, i.e. by participation of Zn in creation of the charged lattice defect.

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Peculiarities of relaxation processes in $Cd_{1-x}Mn_xTe$ crystals

poster F16

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Optical and electrophysical properties of $Cd_{1-x}Mn_xTe$ crystals (0,2<x<0,5) grown by Bridgeman method have been studies. It was found that hole conductivity of the crystals is controlled by A_2 (ϵ=0,12 eV) or A_3 (ϵ=0,2 eV) acceptors, and shallow A_1 acceptors are completely compensated. Besides, a tendency to increasing of crystal specific resistance ρ with increasing of manganese content x was detected. The dependence of specific resistance on x is approximately linear so as the dependence of acceptor ionization energies. Solid solution crystals at x<0,06 demonstrated stable and reproducible electric characteristics at heating up to 420 K. But at x>0,06, when A_3 acceptors contribution into conductivity becomes significant, the "hyzteresis" type relaxation processes in the temperature region from 290 K to 420 K were observed. Note, that hole mobilities do not relax and therefore the change of ρ is caused by the change of hole concentration only. Isothermal changes of hole concentration in the limits from half an order to three orders take place in this case depending on solid solution composition over a period of several hours. The relation of specific resistances at points of isothermal change of ρ has the highest values for samples maiden from section of growing ingots with maximal residual impurity concentration. Thus, one can suppose that the relocalization of residual impurities like copper according to "site-interstitial" mechanism can be involved in the relaxation processes.

Compensation mechanisms in CdTe crystals doped with Cr

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poster F17

It is known that Cr ions enter into CdTe crystals in different charge states. Moreover, chromium impurity in CdTe shows a tendency to form in clusters. Thus, properties of cadmium telluride doped with Cr strongly depend on impurity behavior in material and are of much scientific interest. In the work we present the investigation of electrophysical and optical properties of CdTe:Cr samples. Most of the CdTe:Cr samples under study posses p-conductivity type with carrier concentration of $p=10^{11}$-10^{14} cm^{-3}, that is in several orders less then in undoped CdTe. Ionization energies of the acceptors governing the crystals conductivity increase from 0,19 eV to 0,32 eV with hole concentration increasing. High level compensation (k=0,99) of acceptors is observed in this case. An energy model with a number of deep levels in the band gap well explaining electrical and optical properties of CdTe doped with Cr is proposed. Experimental studies allow us to conclude that chromium in p-type CdTe crystals is in a single charged Cr^+ state. n-type conductivity in several CdTe crystals can be explained by the presence of overlapping space charge regions due to the clusters of chromium atoms.

Passivation effect of CdS thin films grown by Chemical Bath Deposition on gallium antimonide surfaces

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poster F18

CdS thin films with different amount of sulphur have been grown by chemical bath deposition method on GaSb single crystal substrates in order to study the passivation of gallium antimonide surface as a function of the nominal ratios concentration c(thiourea)/c (CdCl2) in the solution. The techniques used to investigate the passivation effects include photoacustic (PA) and photoluminescence (PL). Atomic force microscopy (AFM) and x-ray diffractometry were also used to correlate the results obtained from PA and PL measurements.

ZnS THIN FILMS DEPOSITED BY SPRAY PYROLYSIS TECHNIQUE

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poster F19

ZnS thin films were prepared by spray pyrolysis technique using aqueous solutions of zinc chloride and thiourea. The films were characterized by XRD, Raman spectroscopy, SEM, EDX, UV-VIS and FTIR measurements. The phase composition, structural, optical and morphological properties of sprayed films are controlled by Zn/S molar ratio in the solution and the substrate temperature. Highly (001) orientated ZnS films with wurtzite structure and bandgap value of 3.67 eV could be grown at temperatures close to 500^0C using Zn:S molar ratio of 1:2. At Zn:S of 1:1, wurtzite structure of the films is not clearly pronounced and bandgap value decreases to 3.58 eV. The use of Zn-rich (Zn/S>1) solution results in the formation of ZnO phase in addition to ZnS. The grain size in sprayed film decreases by increasing the Zn amount in spray solution.
The amount of residues originated from precursors decreases with increasing the deposition temperature. Chlorine content becomes negligible at growth temperatures of 500^0C, whereas, carbon and nitrogen containing residues are still present in the film according to EDX and FTIR analyses. The type of carrier gas (air or nitrogen) has insignificant effect on the structure and chemical purity of the films.

Properties ZnTe:Cu Thin Films prepared by R.F co-Sputtering

poster F20

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ZnTe-Cu thin films with Cu concentration in the range 3 -9 at % were prepared by co-sputtering using r.f. magnetron sputtering technique. Substrate temperatures between 60 and 320 C and r.f. power of 80 W were used. XRD measurements showed that the films were amorphous below 250 C, while above that temperature a polycrystalline phase with strong preferential orientation of crystallites appears. For undoped films, the XRD spectrum shows the enhancement of the 100 peak of orthorhombic ZnTe polycrystals while for the ZnTe-Cu films evidence was obtained for the presence of $Cu_xZn_{1-x}Te$ phase with x near 0.20. When the films were prepared in presence of a constant number of Cu pieces distributed over the sputtering area, the resistivity was found to decrease sharply with the rise of substrate temperature. This was attributed to the increase in the solubility of Cu in acceptor sites with increasing temperatures. While the resistivity decreases by nearly 6 decades (indicating a corresponding increase in the concentration of Cu dissolved in acceptor sites) the total Cu concentration measured by the X-ray energy dispersive spectroscopy (EDS) increases by a factor of only 2 with substrate temperature between 60 and 320 ^{o}C. This was taken to confirm the presence of the majority of Cu in a $Cu_xZn_{1-x}Te$ phase, thus supporting the results of XRD.
The room temperature transmission and reflectivity were measured in the wavelength range $300 \leq \lambda \leq 3000$ nm. The absorption coefficient was computed using the Swanepoel method. The energy band gap was determined and found to vary significantly with substrate temperature. This was attributed essentially to the appearance of band tails at the principle bands edges produced by perturbation in the local potential associated with the amorphous modification .For Cu-doped samples, further reduction in E_g is brought about through merging of the Cu acceptor with the valence band

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Optical and Electrical Properties of un-doped and Ga-doped $Mg_xZn_{1-x}O$ Films by Sputtering Method

poster F21

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Transparent conducting oxide (TCO) materials have been attracted much attention for flat panel displays and photovoltaic devices. ZnO films are especially attractive since materials they promise lower cost than ITO films and higher conductive and transparence than SnO_2 based TCO films. Recently, wurtzite-type $Mg_xZn_{1-x}O$ (MZO) alloys possess attraction because bandgap energy is larger than that of ZnO. However, there are few reports on MZO films grown by sputtering method.
In this work, un-doped and Ga-doped MZO films were grown by conventional DC and RF sputtering on glass substrate at RT 200 C using $ZnO/MgO/Ga_2O_3$ ceramic target. Sputtered MZO films were performed at constant target doping concentration of MgO 0 20 wt% and Ga_2O_3 0 5 wt%. The films were investigating using X-ray diffraction (XRD), optical transmittance and Hall measurements.
From the XRD results, it was observed that all films exhibited only single-phase of MZO without changing the wurtzite structure of ZnO, and XRD peaks shifted lower angle than ZnO. Values of FWHM also became large with increasing Mg contents. Grain sizes examined by the XRD data using Scherrers equation were in good agreement with those obtained by SEM. Transmittance spectra were exhibited that the absorption edge shifted higher energy range with increasing Mg contents. Furthermore, the resistivity, carrier concentration and moblility decreased with increasing Mg contents.

Composition and properties of ZnS thin films prepared by chemical bath deposition from acidic and basic solutions

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poster F22

The method of chemical bath deposition (CBD) has been successfully employed to deposit films of ZnS. ZnS is a semiconductor material with a wide direct bandgap, which is interesting for application in photovoltaic and optoelectronic devices. The CBD process typically involves decomposition of a suitable precursor in a solution, giving the chalcogenide ions for the reaction with the metal salt. The result of the CBD process preparing ZnS thin films on different substrates depends on the composition of the chemical bath influencing on the aghesion, homogeneity of the films and also the ratio of concurrent deposition rates of ZnS and ZnO. We have performed a comparative study of ZnS growth by CBD on soda lime glass, Si and GaP substrates using an acidic bath (thioacetamide and acetic acid) and a basic bath (ammonia-thiourea) at various temperatures (in the range from 60 to 85C) and deposition times (in the range from 5 to 180 min). The thickness of the films was varied from a few nm to 100 nm. Our observations suggest a homogeneous growth mechanism in the acidic bath. The chemical and crystalline nature of thick (70-100nm) films was investigated and proved by X-ray photoelectron spectroscopy and X-ray diffraction methods. The in-depth composition of the ZnS layers was studied by means of X-ray fluorescence method. The optical band-gap energy was determined to be 3.64 eV from the best fit of the spectroscopic ellipsometry measurements.

Blocking of semiconductor's surfaces by thin graded-gap layers as technique to serious improvement of excess charge carriers excitation efficiency in semiconductor body

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poster F23

Improvement of excitation efficiency of excess mobile electron-hole pairs in semiconductor body during absorption of electro-magnetic radiation is the task under continuous consideration of everybody who does develop and/or manufacture ultimate performance radiation detectors based on semiconductors. We present results of excitation efficiency calculations performed on model structure consists of homogenous absorber layer with fixed energy gap and two graded-gap layers blocking absorber layer from front side and back side. Following assumptions were applied to consideration: interfaces are electrically neutral and density of recombination centers is negligible; value of graded-gap field Eggl is suddenly changed to zero at interfaces. It was shown that excitation efficiency of excess mobile electron-hole pairs in semiconductor body could be sufficiently high even under condition of infinite surface recombination speed on outer surfaces of the structure; it is important to note that big gradient (high intensity field) in graded-gap layers is not required in this case. Specific distribution of excess holes p(z) assists suppression the influx of excess holes from absorber layer to the outer surfaces. Could say that diffusion barrier is built in region of graded-gap layer sided with absorber that prevents excess holes from moving to surface. It is significant to note that strength of surface recombination suppression is almost completely independent on band-gap gradient value in blocking graded-gap layers and could be realized even when standard condition - drift velocity of holes in graded-gap field should prevail over diffusion velocity and surface recombination speed - is not satisfied. Estimation of excitation efficiency is given for different structures used for gamma and X-ray detectors.
[ABSTRACT TRUNCATED TO 2000 LETTERS]

STRAIN EFFECTS ON BAND OFFSETS IN II-VI/III-V HETEROSTRUCTURES

poster F24

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We present a nearest neighbor sp3d5 tight binding study on the external pressure, lattice mismatch and thermal expansion gradient induced interface strain effects on band offsets in II-VI/III-V heterostructures with normal interfaces (e.g., ZnSe/GaAs and HgTe/CdTe) and inverted interfaces (e.g., GaAs/ZnSe and CdTe/HgTe). We screen the valence band energies by the optical dielectric constants of semiconductors at any temperature, pressure, strain„ and alloy composition and then find the band offsets are obtained by matching an average sp3d5 tight binding midgap level, at which the antibonding and bonding states are equal at heterointerface. The sp3 tight binding midgap level is defined at a special point (Baldereschi special point) in the forbidden gaps of constituents. This allows the inclusion of the effects of high symmetry point conduction and valence energy band structure band minimums on defining the thermal equilibrium across the heterointerfaces. Model predictions compare well with the experiment for the band offsets of many lattice matched and mismatched II-VI/II-VI isovalent and II-VI/III-V heterovalent heterostructures. The model predicts that the growth orientation dependence of band offsets for lattice matched heterostructures is due to the change in sign of lattice thermal expansion gradient induced strain across the interface and that in mismatched heterostructures is due to the change in sign of lattice mismatch strain. The electron-phonon interaction has very little effect on the valence band offsets but some effects on conduction band offsets as temperature is increased. Furthermore, the model also predicts that there is a crossover for the band offsets at HgTe/CdTe at pressures about 50 Kbar; becomes smaller than above 50 Kbar.

HIGH PRESSURE ANNEALING-INDUCED REDUCTION IN DEGREE OF COMPENSATION IN (Zn,Mn)Te CRYSTALS

poster F25

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It has been found that bulk ZnTe crystal can be relatively easily doped
to the hole concentration level of 10^{19} cm-3. However, introducing Mn into the ZnTe:P strongly reduces the hole concentration to level of 10^{16} cm^{-3} due to high degree of compensation. In this communication we report the high pressure and high temperature annealing technique, which enabled one to suppress the compensation and to achieve the hole concentration level as high as $5x10^{18}$ cm^{-3}.
The (Zn,Mn)Te crystals ($0<x<0.09$) doped with P to level of $5x10^{19}$ cm^{-3} were grown by high pressure Bridgman technique. Despite of heavy doping, as-grown crystals exhibited hole concentration of only $4x10^{16}$ cm^{-3} and degree of compensation (K) reached 0.9. In order to suppress the compensation, the as-grown crystals were subjected to annealing in nitrogen atmosphere under a pressure of 4 MPa at $T=800^0$ C for a period of one week. After the annealing, K reduced to 0.1 and the hole concentration increased to $5x10^{18}$ cm-3. We suggest that the high K in the as-grown (Zn,Mn)Te:P is connected with interstitial Mn^{2+} ions, which act as double compensating donors. The high pressure annealing transfers the Mn interstitials into random precipitates reducing the concentration of compensating donors. This rearrangement of Mn atom sites is responsible for the reduction in K and an accompanying increase in the hole concentration.

Growth and optical properties of MBE-ZnSe on high-quality ZnTe substrate

poster F26

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II-VI semiconductors with wide-band gap are currently under intense investigation for optoelectronic application in the green-UV range. However, due to the self-compensation effect specific to wide band-gap semiconductors, it is difficult to realize the low resistive p-type ZnSe crystal. The growth of phosphorus-doped p-type conductive ZnTe single crystal has been achieved by the vertical gradient freezing (VGF) method [1]. Using phosphorus-doped ZnTe substrate as a p-type conductor, it is expected the light emitter based on n-ZnSe/p-ZnTe heterojunction. In this paper, we report on the MBE growth of heteroepitaxial ZnSe layer grown on p-ZnTe substrates. While there existed 7.7% lattice mismatch between ZnSe and ZnTe crystal, the ZnSe/ZnTe heteroepitaxial films were successfully achieved on the ZnTe substrate.
The ZnSe layers were grown by MBE using conventional molecular beams on the phosphorus-doped p-type ZnTe(001) substrates grown by the VGF method. The substrate temperatures, Tg, were controlled at the temperature range from 150C to 250C. After thermal treatment of the ZnTe substrates, the ZnSe film was

directly grown on the substrate by MBE method.
After the 3 hrs growth, while the RHEED patterns became spotty at Tg of 150C, the streak patterns are obtained above 200C. These results imply the 2-dimensional growth of the ZnSe on the ZnTe substrate. The I_1^d with LO-phonon, I_v and Y line emissions were dominated in the ZnSe films grown at Tg above 200C. Comparing with these emissions, both E_x and I_2 emission intensities were too weak. Our results suggest that the ZnSe films could be grown on the ZnTe substrate by MBE, and it is expected the hetero p-n junction LEDs based on the p-type ZnTe substrate.
The authors would like to acknowledge Dr. K. Sato, Dr. T. Asahi, A. Arakawa, Nikko Materials Co., Ltd, for the supporting of ZnTe substrates.
[1]K. Sato et. al., J. Crystal. Growth 214/215 (2000) 1080.

Optical Characterization of ZnTe Single Crystal grown by Vertical Gradient Freezing Method

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poster F27

Wide-gap semiconductor, ZnTe, is an ideal material for pure-green light emitting diodes since it has the energy gap of 2.26 eV at room temperature and a band structure is of a direct optical transition type. It is however difficult to realize p-n junctions because of the well-known compensation effect specific to II-VI materials. To attain the conductivity control for ZnTe, it is necessary to understand the behaviors of impurities and defects in ZnTe.
High quality 80 mm diameter ZnTe single crystals were successfully grown by the vertical gradient freezing (VGF) method without seed crystals [1-2]. The 80 mm diameter crystals with 50mm length are largest in bulk-ZnTe single crystals. The grown direction was nearly <111> or <110> direction. The etch pit density measured after HF solution etching was lower than 10000 cm^{-2}, which was lower than that of their solution growth method.
In this paper, photoluminescence (PL) measurement was carried out between liquid helium (4.2K) and room temperatures to study point defects in the Indium (In)-doped, Gallium (Ga)-doped and non-doped ZnTe crystals grown by the VGF method. In the PL spectrum of non-doped ZnTe crystal at 4.2K, three distinct kinds of peaks are present at 522.5nm, 532.0nm and 534.2nm. These emissions are assigned to be the deep acceptor-bound exciton emission (I_1^d), the free-to-acceptor emission (FA) and the donor-acceptor pair (DAP) emission, respectively. On the other hand, both FA and DAP emissions are not detected in In- and Ga-doped ZnTe crystals at 4.2K. The Ga donor- and In donor-bound exciton emissions (I_2) are observed at 522.0nm and 521.6nm, respectively. These results suggest that the high-quality non-doped ZnTe can be grown by VGF method, and both Ga and In atoms behaves donor species in the ZnTe crystals, respectively.
[1] K. Sato et al., J. Crystal Growth 197(1998) 413.
[2] T. Asahi et al., J. Crystal Growth 229(2001) 74.

CdO thin films grown on sapphire substrates

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poster F28

In this communication we report on the structural properties of CdO thin films grown on sapphire bearing in mind their possible applications in optoelectronic devices combined with other II-VI oxides. CdO thin films were deposited onto a-plane, c-plane, r-plane and m-plane sapphire substrates by metalorganic vapor-phase epitaxy, using a two-inlet horizontal reactor in which the oxygen and cadmium precursors are separately introduced into the reaction chamber. The CdO layers, which were grown at 383^oC and atmospheric pressure, have been analyzed by means of X-ray diffraction, including θ-2θ scans, pole figures and rocking curves.
θ-2θ scans have revealed three different CdO orientations namely, (111), (100) and (110), depending on the substrate plane on which the growth has taken place. The orientation relationships between films and substrates have been determined by using the recorded pole figures on several reflections. Finally the crystalline quality of the films has been assessed by measuring the full width at half maximum of the corresponding rocking curves. The results indicate that high quality CdO thin films can be grown on sapphire, stimulating the applications of this material in the field of optoelectronics.

Dynamics of spin interactions in II-Mn-VI semiconductors studied with time-resolved optically detected magnetic resonance

poster F29

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In this communication we analyse dynamics of spin interactions in diluted magnetic semiconductor (DMS) systems of II-Mn-VI. Bulk and low dimensional DMS samples are studied with magneto-photoluminescence and optically detected magnetic resonance, including time-resolved option of the latter experiment. The time-resolved experiment enables a direct observation of dynamics of spin-related interactions, by following photoluminescence response induced by pulse of a microwave radiation at magnetic resonance conditions. Influence of excitation conditions (intensity) on the observed dynamics of the signal response is studied. We demonstrate change of spin relaxation mechanism at high excitation conditions, which is due to very efficient spin-flip interactions between localized spins of Mn ions and spins/magnetic moments of free carriers.

Photoluminescence mapping of p-type to n-type conversion in CdTe

poster F30

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The p-to-n conversion of CdTe single crystals caused by cadmium-saturated annealing atmosphere is investigated by low temperature photoluminescence (PL), electron beam induced current method (EBIC) and galvanomagnetic measurements. Special attention is devoted to the correlation of the possition of p-n junction established by all methods. We show that PL of excitons bound on silver, copper and sodium neutral acceptors in the converted n-type exhibits drastic reduction (about three orders of magnitude) comparing to unconverted p-type or as grown crystal. Simultaneously, we observe that cadmium substitutional acceptors fast diffuse intersticially into remaining p-type, where they recombine with Cd vacancies and accumulate near the p-n junction. This effect has a potential application in the establishment of the position of the p-n junction and by a homogeneity study by PL measurements.

EFFECT of CHEMCALLY ABSORBED ATMOSPHERIC OXYGEN on ELECTRIC and PHOTOLUMINESCENT CHARACTERISTICS of A2B6-MONOCRYSTAL/NATIVE OXIDE STRUCTURES

poster F31

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Development of various technologies (MBE, PLD - pulse laser deposition, laser surface engineering) have made it possible and necessary to study and numerically simulate effect of ambient oxygen chemisorption on operation of the active element prepared by means of the technology. This effect is seemed to be of special importance for electro-optical devices based on A2B6 bulk and thin film materials (CdTe, ZnTe, ZnSe). Native oxide may be considered as a functional part of the structure as a whole. In the abstract we report for the first time experimental data obtained from electric-field measurements performed at the room temperature and photoluminescense at 77 K on the structures A^2B^6- monocrystal/native oxide and CdTe(PLD-thin film)/native oxide present results of numerically modeled chemisorption behavior of oxygen on CdTe. The electric investigations of (ZnTe, CdTe)-monocrystal/native oxide structures have been shown Schottky-like behavior of the field characteristics. Photoluminescence studies of ZnSe-monocrystal/native oxide structures have also demonstrated some special peculiarities of the spectra to be interesting for prospective device preparation.

Fe photoionization transition in ZnSSe:Fe crystals - photo-ESR studies

poster F32

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Charge transfer processes in transition metal ions, which are doped in wide band-gap II-VI semiconductors, are of great interest because of possible application for novel optical and spintronic devices. In this work we study 2+ -> 3+ photoionization transition (PT) of iron ions in ZnSSe:Fe bulk crystals in temperature range of 2 - 100 K. By monitoring changes of the Fe^{3+} ESR (electron spin resonance) signal under external illumination we are able to determine energies of Fe^{2+} -> Fe^{3+} + e_{CB} transition in different ZnSSe host crystals. At low temperature we observe metastable (in part) population of photo-excited Fe^{3+} centers. Free electrons created in the conduction band under the 2+ to 3+ ionization of iron, are efficiently trapped by donor centers. We observe also appropriate photoionization bands in low temperature absorption spectra. Previous studies have shown that the iron PT is an efficient channel for excitation of the Fe^{2+} intra-ion emission in ZnS:Fe at low temperature.

Hetereojunction

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Thin films of Al-doped ZnO (ZnO:Al) are emerging as an alternative candidate to Sn-doped In2O3 (ITO) in solar cells, due to features such as non-toxic, low cost, material abundance, and high stability against a hydrogen plasma and heat cycling. The ITO/Si structure has been extensively studied during the past two decades obtained by various deposition technologies for potential application in solar cell technologies. The conversion efficiencies in solar cells from ITO/c-Si junction achieved were 10-15% using spray pyrolysis. However, little information is available in the literature on n-ZnO:Al/c-Si heterojunction in spite of its interest for the raison of its application in solar cell and other electro optics devices. Spray pyrolysis is an useful alternative to the traditional methods for obtaining thin films of pure and doped ZnO. It is of particular interest because of its simplicity, low cost and minimal waste production. The spray pyrolysis, SP, process allows the coating of large surfaces and it is easy to include in an industrial production line. In this communication, the electrical properties of n-ZnO: Alx(x = 0, 1, 2, 3, 4 %)/c-Si heterojunction prepared by SP on single-crystal n-type and p-type monocrystalline silicon (100) substrates are examined by C-V, I-V methods and admittance spectroscopy at temperature ranges between 150-373 K. The n-ZnO/c-Si heterojunctions shows a height barriers consistent with the difference of energy of the work functions of Si and ZnO; however, the n-ZnO:Al/c-Si heterojunctions present a more complex behaviour due to the defects at or near the n-ZnO:Al/c-Si interface, causing a Fermi energy pinning.

Atomic absorption photometry determination of excess Zn in ZnO

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Zn excess in ZnO is built up automatically at high temperatures. Excess Zn in hydrothermally grown ZnO is investigated by the atomic absorption photometry (AAP) method. To determine the excess zinc in ZnO samples, the AAP of zinc vapour was used in the conditions of solid-vapour equilibrium. Optical absorbance of zinc, proportional to the concentration of zinc atoms in the vapour phase, was registered photoelectrically on the Zn resonance line. Zn AAP allowes to eliminate excess Zn connected differentially in ZnO samples. To fix Zn non-stoichiometry, all the ZnO samples tested were previously heat treated at temperature interval from 850 to 900^0C and at fixed Zn vapour pressures from 0,1 to 0,9 of saturated zinc vapour pressure at given treatment temperature. Our AAP investigations in polycrystalline ZnS and ZnSe showed that the analytically determined concentration of Zn excess appears to be bigger than the concentration of electrically active defects. Zn adsorption on crystallite surfaces must be taken into account in ZnO also. The analysis of temperature dependence of zinc vapour pressure indicated that the value of zinc excess lies in the concentration interval of 10^{18} - 10^{19} cm^{-3} and depends on the sample biography and the conditions of preliminary heat treatment. Impurity metals take active role in the determination of non-stoichiometric zinc. The experimental results were used for preliminary high temperature defect equilibrium calculations for ZnO.

Growth and Optical Properties of Room-Temperature Electrosynthesized ZnO Film with Highly 001 Orientation

poster F35

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ZnO thin film with high 001 orientation was electrosynthesised on ITO-coated glass substrate at room temperature under pulsed voltage. Photoluminescence (PL) shows two obvious peaks: violet band and strong green band. The former is due to the free-excitonic transition and the latter is believed to arise from the single ionized oxygen vacancy (V_o^+). Raman scattering reveals that the 580 cm^{-1} mode and the shoulder peak mode at 550 cm^{-1} originate from the N-related local vibration mode (LVM) and E_1 (LO) mode, respectively.

Preparation and characterization of hexagonal MnTe and ZnO layers

poster F36

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In the first part of this work we present the results of the investigation of high crystalline quality MnTe layers grown epitaxially by MBE. It is known that the bulk MnTe with hexagonal crystalline structure of NiAs is a magnetic semiconductor with a high Neel temperature (310K) [1]. Thin layers of MnTe exhibit also antiferromagnetic properties, and for this reason, they can be used as the pinning layer in semiconductor spin valves. Characterization of our samples by X-ray diffraction revealed a high crystalline quality of hexagonal structure of NiAs-type.With lattice parameters of the unit cell are a=4.166A and c=6.694A. The optical transmission spectra of MnTe measured at low temperature gave a possibility to evaluate the energy gap (1.7 eV). In order to establish the Neel temperature the neutron diffraction measurements were performed. The temperature of the antiferromagnetic transition for our samples was 284.1K

The second part of this work is dedicated to ZnO:N:Mn. Theoretical works predicted that this material can be a ferromagnetic above the room temperature [2].The metallic Zn and ZnTe were grown by MBE. In order p-type conductivity in ZnTe is achieved by nitrogen doping. So, a part of our samples was doped with nitrogen, and some contained few percents of Mn. SIMS measurements help us to evaluate the quantity of N atoms in the ZnTe:N and Zn:N. After growth all samples were oxidized by keeping them in O_2 flow at 600-650^{o}C.The spectra of X-ray diffraction measurements demonstrated only the peaks related to ZnO crystal and substrates. Detailed SQUID measurements of Mn-doped ZnO detected a very weak magnetization persisting up to high temperatures.

[1]N.Kunitomi, Y.Hamaguchi, S.Amzai, J.de Phys.,Vol. 25,p. 568(1964).
[2]T.Dietl, H.Ohno, F.Matsukura, J.Cibert and D.Ferrand,Science,Vol.287, p. 1019(2000).

[ABSTRACT TRUNCATED TO 2000 LETTERS]

THE CONDUCTION MECHANISM OF Al-DOPED ZnO, AZO, FILMS

poster F37

Jose R. Ramos-Barrado[1], **Maria C. Lopez**, **Mercedes Gabás**, **Susana Gota**, **Nicke T. Barrett**, **Jose Avila**

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AZO thin films conductivity increases with the Al content and reaches a maximum at about 3 % doping level; higher doping results in a decrease of conductivity. The density of carrier in the films is determined from the C-V measurements for different Al contents in AZO thin films deposited by chemical spray pyrolysis on p-Si. The carrier concentration is, for all Al concentration, lower than the corresponding theoretical values and, therefore, not all Al+ ions include in the ZnO structure donors electrons. Nevertheless, we have experimental evidence that the gap does not collapse and, thereby, the conductivity increase is not due to a metal-insulator transition. We have measured, using synchrotron radiation in the VUV range, a reduction in the band gap of about 150 meV for the 3% Al doped ZnO film with respect to the undoped and the 1% Al doped ones. This reduction has also been detected in E.E.L.S. measurements which show

a reduction in the band gap of about 200meV for same films. This is due to the hybridization of the Al dopants with the ZnO host lattice. This additional number of electrons is enough to enhance the conductivity by two orders of magnitude in the 3% Al-doped ZnO films because the transport properties in a solid are controlled exclusively by the mafia of electrons at, or, very near to the Fermi surface. Moreover, the electrical conductivity dependence of temperature, measure by the four point method, shows a variable hopping range for the conduction mechanism.

ELECTRICAL AND OPTICAL PROPERTIES OF ZnO AND ZnO:Cr CRYSTALS, GROWN BY CVT METHOD

S. Trushkin[1)], **Krzysztof Grasza**[1)], **Andrzej Mycielski**[1)], **A. Kamińska**[1)], **K. Świątek**[1)], **Pawel Kaczor**[1)], **Adam Barcz**[1,2)], **A. Suchocki**[1)] poster F38

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Pure and chromium doped ZnO crystals were grown in a quartz ampoule with a mixture of H_2+Cl_2 or H_2+C+H_2O, applied as transporting chemical agent. Obtained by this method polycrystals were often red and had monocrystal grains of about 6x7x5 mm^3. The as-grown ZnO crystals were of n-type and had low specific resistivity (about 0.05 cm at 300 K). The content of Cr in the ZnO:Cr crystals was below 10^{18} cm^{-3}, which was proved by SIMS analysis.
The absorption of the as-grown ZnO crystals exhibits a strong near-edge band which is probably due to the oxygen centers, located in the band gap. Absorption edge, caused by the interband transitions is revealed at about 3.2 eV. Oxygen annealing provokes the disappearance of the near-edge band and it proves, that the samples were grown with the oxygen deficiency. The absorption of the ZnO:Cr crystals at T=5 K reveals a band with a peak at about 0,992 eV, which is probably caused by Cr^{2+} center.
The luminescence spectra, excited by the 325 nm He-Cd laser, shows two major luminescence bands with peak energies at 3.2 eV and around 2.5 eV. The first band is assigned to the thermalized bound and free exciton luminescence. The latter one is also observed at the temperature of 10 K and it is probably associated with some defect centers including oxygen vacancy Vo+. Luminescence intensity in this band decreases after the annealing of the samples in the oxygen atmosphere and it confirms its assignment to the oxygen vacancy.
An extra sharp line is also observed in the luminescence spectra of the ZnO crystals at energy of about 2.25 eV. The origine of this line is unknown, since some reports associate it with donor-acceptor pair transitions related to Cu dopant. We shall present the results of high-pressure luminescence experiments in the diamond anvil cell, which provide additional information about the luminescence line origin.

Characterization of Al-doped ZnO thin films deposited by reactive sputtering

Bae-Heng Tseng[1)], **S,H, Hsieh**[1)] poster F39

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Thin films of Al-doped ZnO were prepared by reactive co-sputtering using independently controlled Zn and Al targets. Surface morphology of the films observed in a SEM revealed the nanometer columnar structure. The evolution of columnar structure was closely related to the involvement of Al during the film deposition process. The nanometer columns with a very strong preferred orientation along [002] direction was observed in a film prepared when the RF power ratio of Al and Zn targets was above one. As the power ratio of the targets kept at one, the column size was in the range from 37 to 62 nm when the RF power increased from 20 to 50 W. The refractive index of the film varied from 1.85 to 1.96 (λ = 500 nm) as the column size changed from 37 to 62 nm. All the as-grown films had high resistivity regardless of the amount of Al doping. A considerable reduction of the film resistivity was achieved by rapid thermal annealing at a temperature above 250^{o}C for 15 minutes in a nitrogen gas flow. The lowest sheet resistance obtained in our experiments was 4.78 $\times$ 10^2 Ohm/square. We also found that the sheet resistance of the annealed sample decreased as the Al doping increased. However, too much Al doping might increase the film resistivity because of considerable amount of aluminum oxide existed in the film. ESCA analysis gave the evidence that the amount of aluminum in the form of oxide reduced after annealing. This explains the activation of Al doping found in our experiments.

The Properties of Surface Textured ZnO:Al Films for Thin Film Solar Cells

poster F40

Jinsu Yoo[1)], **Jeongchul Lee**[2)], **Seokki Kim**[2)], **Kyunghoon Yoon**[2)], **I Jun Park**[2)], **Suresh Kumar Dhungel**[1)], **Bojan Karunagaran**[1)], **Devanesan Mangalaraj**[1)], **Junsin Yi**[1)]

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Aluminium doped Zinc Oxide (ZnO:Al) films were deposited by rf magnetron sputtering from a ZnO target mixed with Al_2O_3 of 2.5 % on to glass substrates maintained at different temperatures ranging from 300 to 673 K. Argon gas pressure during the deposition was in the range 0.3-10 mtorr. Structural, optical and electrical properties of the prepared films have been characterized. As the argon gas pressure was increased, the deposition rate was found to decrease and the surface roughness was increased. Furthermore the carrier concentration and the Hall mobility were decreased and thus the electrical resistivity increased. Depending on their structural properties these films develop different surface structures upon post deposition etching in diluted HCl (0.5%). The light scattering properties of suitable film can be controlled over a wide range simply by varying the etching time, substrate temperature and argon pressure. The X-Ray diffraction (XRD) studies showed that the films are highly oriented with their crystallographic c-axis perpendicular to the substrate almost independent of argon pressure and also an improvement in crystallanity for the films deposited at higher temperature was observed. Measurements of transmission spectra reveal that ZnO:Al films have an average transmission of over 85 % in the wavelength range of 400 - 800 nm. Also the films showed an excellent electrical resistivity 1.9 x 10^{-4} ohm-cm, a value comparable to that for indium tin oxide film presently used as a transparent electrode.

Tuesday, September 7th

11:00 - 12:00

Morning session 1

Main Building, room 134

Low-frequency magnons and phonons in hexagonal MnTe

11:00 - 11:20 oral

Wojciech Szuszkiewicz[2)], **Bernard Hennion**[1)], **Barbara Witkowska**[2)], **Andrzej Mycielski**[2)]

1) Laboratoire Leon Brillouin, CEA-CNRS, CE Saclay (LLB), Gif sur Yvette 91191, France

2) Polish Academy of Sciences, Institute of Physics, al. Lotnikow 32/46, Warszawa 02-668, Poland

There is a continuous interest in the properties of II-VI based diluted magnetic semiconductors. The mixed crystals containing Mn and pure MnTe were the object of intensive studies for many years.
The zinc blende modification of MnTe is a metastable phase of this compound and can be grown by the non-equilibrium growth methods only (like, e.g., MBE). Several properties of this compound are now well known. On the contrary, the knowledge about the properties of hexagonal (stable) phase of MnTe is much more limited.
We have started to study the low-frequency collective excitations in hexagonal MnTe by means of inelastic neutron scattering. Single MnTe crystals were grown and characterized at the Institute of Physics of the Polish Academy of Sciences in Warsaw. Neutron scattering measurements were performed at Laboratoire Leon Brillouin in Saclay (France). Low-frequency acoustic phonons as well as magnetic excitations (magnons) have been observed at room temperature and their dispersion along selected high-symmetry directions of the Brillouin zone has been determined. Results of our preliminary measurements were compared with the dispersion of magnons in zinc blende MnTe. The similarities and the differences in the lattice dynamics and in the magnetic properties of both MnTe phases were shown and discussed.

Fabrication and characterization of II-VI diluted magnetic p-n junctions

11:20 - 11:40 oral

Valery Kolkovsky[1)], **Renata Butkute**[1)], **Elżbieta Janik**[1)], **Krzysztof Fronc**[1)], **Grzegorz Karczewski**[1,2)]

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The active control of spins in semiconductors leads to significant advances in technology of digital information storage, magnetic recording and sensing. Recently, Zutic and Fabian have theoretically considered a magnetic p-n junction [1, 2]. One side of the device was made of magnetic material with the giant spin splitting and the other one of a nonmagnetic semiconductor. The presence of external magnetic field could allow spin-polarized current generation, spin amplification, voltage control of spin polarization, and a significant extension of spin diffusion range. They predict new phenomena of exponential and giant magnetoresistance, spin-voltaic effect, spin-valve effect, when a non-equilibrium spin is added into the junction.
The goal of this study is to verify experimentally the predictions of Zutic and Fabian. For this purpose a set of p-n junctions with magnetic n-type (CdMnTe) and nonmagnetic p-type (CdZnTe) regions and a set of p-n junctions with non-magnetic n-type (CdTe) and magnetic p-type (CdZnMnTe) region have been grown by Molecular Beam Epitaxy. The content of Mn in CdMnTe varied from 1 to 5 %. The n-type conductivity was obtained by iodine doping. The nonmagnetic p-type CdZnTe contained from 1.0 to 7.5 % of Zn. p-type conductivity was obtained by nitrogen doping. The quality of grown structures was established from the photoluminescence spectra measured at 4K. The carrier (electrons in the magnetic n region and holes in the non-magnetic p region) concentration was evaluated from Hall measurements. The measurements of current-voltage, resistance-voltage and capacitance-voltage characteristics at different temperatures and different values of magnetic field is discussed from the point of view of spin dependent phenomena and compared to theoretical predictions of Zutic and Fabian.

[1] Zutic I., Fabian J., Das Sarma, Phys. Rev. B, 64, p121201 (2001).
[2] Zutic I., Fabian J., Das Sarma, Phys. Rev. Lett, 88, p066603 (2002).

Search for ferromagnetism in transition metal substituted ZnO

11:40 - 12:00
oral

Bogdan Dabrowski[1], **Stanislaw Kolesnik**[2]

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2) Northern Illinois University, De Kalb IL 60440, United States

The II-VI semiconductor ZnO with both crystal structure (wurtzite) and wide-gap (3.2 eV) similar to GaAs attracted recently considerable attention because of room-temperature ferromagnetism reported in transition metal substituted compounds. If confirmed, these reports, guided by theoretical predictions, would provide practical material for incorporation of spin into semiconductor industry. We have studied structural and magnetic properties of the Mn, Fe, and Co substituted samples synthesized under a wide range of oxygen pressures. No bulk ferromagnetism was observed for any of the single-phase samples obtained over a range of substituted compositions 0 - 20 %. Single-phase compounds demonstrate paramagnetic Curie-Weiss behavior with antiferromagnetic interactions, similar to other diluted semiconductors. Imperfect synthesis conditions could lead to formation of second phases that are responsible for high-temperature ferromagnetic behavior, such as Co-metal and zinc-ferrospinel, or spin-glass behavior observed for $ZnMnO_3$. Absence of ferromagnetism may be caused by our inability to achieve p-type conduction in pure and substituted ZnO.

Supported by the NSF-DMR-0302617 and by the US Department of Education

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Lunch break

12:30 - 14:00

Afternoon session 1

Main Building, room 134

14:00 - 15:20

Identification and recovery of electron irradiation induced point defects in ZnO

14:00 - 14:20
oral

Filip Tuomisto[1], **Kimmo Saarinen**[1], **David C. Look**[2,3]

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3) Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson AFB, Ohio

45433, United States

The electronic properties of zinc oxide (ZnO) seem to be exceptionally resistant to deterioration caused by electron irradiation. The microscopic processes behind the high radiation hardness of ZnO need to be fully understood in order to uncover all the potential applications of the material. The role of vacancies in both self-compensation and the high radiation hardness can be determined by positron annihilation spectroscopy. We have studied both as-grown and 2-MeV electron irradiated single crystal ZnO bulk samples, which were nominally undoped and exhibited n-type conductivity. Recent positron studies have shown that the dominant compensating center in both the as-grown and irradiated material is the zinc vacancy (V_{Zn}), presumably in its doubly negative charge state [1]. The introduction rate of the zinc vacancies in electron irradiation is two orders of magnitude lower than that of gallium vacancies in gallium nitride (GaN), which is a clear manifestation of the radiation hardness. The electron irradiation produces also neutral oxygen vacancies (V_O), and their concentration can be estimated to be significantly higher than that of V_{Zn}. The irradiation-induced defects anneal completely out of the samples in two main stages between 100 ^oC and 300 ^oC, after which the concentration of the compensating centers is the same as in the as-grown material. Shining monochromatic light on the irradiated samples during the positron measurements at 20 K causes an increase of the average positron lifetime at photon energy 2.3 eV, indicating that also negative ion type defects are present, and that they as well as the irradiation-induced zinc vacancies have an ionization level close to 2.3 eV. No such effect was observed after the annealings or in as-grown ZnO.

[1] F. Tuomisto, V. Ranki, K. Saarinen, and D.C. Look, Phys. Rev. Lett. 91, 205502 (2003).

14:20 - 14:40
oral

p-type conducting ZnO: fabrication and characterisation

Eliana Kaminska[1], **Anna Piotrowska**[1], **Jacek Kossut**[2], **Renata Butkute**, **Witold Daniel Dobrowolski**, **Krystyna Golaszewska**[1], **Adam Barcz**[1], **R. Jakieła**, **Elzbieta Dynowska**, **Ewa Przezdziecka**[3], **Dorota Wawer**[1]

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The current high level of research on p-type doping of ZnO is driven by the possibility of important applications such as wide-gap electronics and spintronics, yet high-quality and reproducible p-type ZnO remains a formidable technological challenge.
In this contribution we discuss preparation of p-type ZnO by oxidation of thin films zinc nitride. Nitrogen incorporation is seen as the most prospective way to obtain p-type conductivity. The starting material was grown by rf reactive magnetron sputtering from high purity Zn target, in Ar-N_2 plasma. Crucial point during the deposition was to adjust both the N_2/Ar ratio and the working pressure so as to deposit Zn_3N_2 without any metallic Zn inclusions. For oxidation, samples were furnace annealed in O_2 flow Quartz and sapphire as well as lattice-matched GaN, ZnO and ZrB_2 were used as substrates. The effect of the growth direction - determined by growth conditions - on the structural perfection of the resultant ZnO films as well as on efficiency of nitrogen incorporation was studied. We present results of x-ray diffraction, secondary ion mass spectrometry and optical transmission measurements of the oxidized layers, indicating that formation of ZnO did take place.
We report on the appropriate conditions for the growth of p-type ZnO with Hall effect mobility of 20 cm^2/Vs and carrier concentration of $2x10^{15}$ cm^{-3}. Further increase of p-type conductivity up to $5x10^{17}$ cm^{-3} with mobility of 5 cm^2/Vs was obtained by additional doping the starting material with Cr. We discuss the role of the latter in gettering of hydrogen which, possibly, deactivates the nitrogen acceptors. Finally we address the problem of stability of the films: we found that protection of the surface is necessary in order to prevent p-type conductivity degradation.

Work supported by grants from EC NANOPHOS (contract IST-2001-39112) and from the State Committee for Scientific Research PBZ-KBN-044/P03/2001.

14:40 - 15:00
oral

CVT contactless growth of ZnO crystals

Krzysztof Grasza[1], **Andrzej Mycielski**[1]

1) Polish Academy of Sciences, Institute of Physics, al. Lotnikow 32/46, Warszawa 02-668, Poland

Zinc oxide crystals were grown on the sapphire substrates in silica glass ampoules by Chemical Vapour Transport and Contactless Growth Method. The temperature field configuration and geometrical dimensions which were formerly applied to PVT contactless growth of other zinc and cadmium based II-VI compounds [1] and lead based IV-VI semiconductor compounds appeared to be appropriate for growth of ZnO by CVT. Hydrogen, bromine and chlorine were used as the transport agents, depending on the doping element (As, Cr, Cu) introduced to the crystal. Additional gases (N_2, Ar) and additional Zn were used in order to improve the transport and growth conditions. It appears, that the best growth conditions are obtained in hydrogen atmosphere, keeping the Zn partial pressure close to pressure of hydrogen. Due to changes of the hydrogen pressure during growth, also the partial pressure of the zinc must be changed. Synchronization of these changes remains the main problem in our growth system.

[1] K.Grasza, W.Palosz, Crys.Res.Technol. 34(1999)565

Growth and characterization of thin films of ZnO by Atomic Layer Epitaxy

15:00 - 15:20
oral

A. Wojcik[1,2], **K. Kopalko**[1], **A. Khachapuridze**, **A. Szczerbakow**[1], **Marek Godlewski**[1,2], **Elżbieta Lusakowska**[1], **Wojciech Paszkowicz**[1], **Jaroslaw Domagala**[1]

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2) Cardinal S. Wyszynski University, College of Science, Dept. of Mathematics and Natural Sciences, Warszawa, Poland

We report growth of monocrystalline and polycrystalline thin films of ZnO by atomic layer epitaxy (ALE), often referred to as atomic layer deposition (ALD). ZnO films were grown on several substrates. Monocrystalline films were obtained using GaN/Al2O3 as a substrate, whereas use of sapphire, silicon, GaAs or lime glass resulted in either 3D growth mode or in polycrystalline films showing preferential orientation of the c axis. Crystalline properties of the films are studied with atomic force microscopy and X-ray diffraction techniques. Monocrystalline ZnO films show the structural quality limited by that of the GaN template and very flat surfaces, with roughness below 1 nm RMS. Polycrystalline films are often rougher, showing granular micro-structure. Influence of growth conditions, precursors used and post-growth annealing will be discussed.

This work was partly supported by grant no. PBZ-KBN-044/P03/2001 of KBN. The ALE reactor was bought using SEZAM grant of Foundation for Polish Science.

Coffee break

15:30 - 15:50

Afternoon session 2

Main Building, room 134

15:50 - 17:10

Multiphonon processes in ZnO

15:50 - 16:10
oral

Herbert Willi Kunert[1]

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Utilizing space group theoretical methods we have derived so called "Lattice Modes Representation" (LMR) for the ZnO with the space group C(6v-4). The reduction of the LMR leads to the total number of independent (first order) vibrational modes (species) and their symmetries (irreducible representations (irrps)) originating from the centre as well as from the high symmetry points and lines of the Brillouin zone for ZnO. Considering only long-wavelength modes (k=0) we have derived Raman selection rules for: 1-rst order Raman active modes (1RAMs) meaning all possible overtones and combinations, 2-nd order Raman active modes (2RAMs) (all combinations and overtones) and for the third order Raman active processes (3RAMs) in ZnO as well. We have performed the Raman inelastic light scattering experiment in the frequency regions of 1-rst, 2-nd and the third order Raman active modes. Several multi-phonon processes in ZnO are observed. In addition, the low temperature photoluminescence spectra exhibit some phonon replicas these confirm the presence of multi-phonon processes in ZnO. An external perturbation on the ZnO such as ion-implantation, alpha particle irradiation, thermal annealing, high pressure, and so on, frequently generate, treatment induced, new vibrational modes. These phonons can only be distinguished from the multi-phonon Raman active modes by means of our selection rules.
The derived RAMs can also be useful in the determination of the dynamical matrix for a crystal from which the particular frequencies of modes can be calculated and therefore the phonon density of states can be obtained.

16:10 - 16:30
oral

Growth of single crystal aligned ZnO nanorods on ZnO thin films

Dongxu Zhao[1)], **Caroline Andreazza-Vignolle**[1)], **Pascal Andreazza**[1)]

1) Centre de Recherche sur la Matière Divisée, CNRS - Université d'Orléans (CRMD), 1b rue de la ferollerie, Orléans 45071, France

One-dimensional (1D) wide band-gap nanowhiskers have attracted much interest because their remarkable physical and chemical properties. Fabrication of nanowires of SiC, GaN, ZnSe and ZnO has been reported. Among them 1D ZnO nanostructures attract special attention due to their large excitonic binding energy of 60 meV and high mechanical and thermal stabilities. Recently, ZnO nanostructures including nanowires, nanobelts, and nanotubes, have been fabricated by various methods.Electronic and optical devices based on 1D ZnO nanostructures, such as lasers, sensors, light-emitting diodes, and field emission devices, were studied.
In this report, we present a simple physical vapor-phase transport technique of synthesizing single crystalline ZnO nanorods. These nanorods are supported by different kinds of substrates: Si, Au/Si, ZnO/Si and Au/ZnO/Si. ZnO thin film deposited on Si substrate can be used as a buffer layer and gold can be deposited in order to form nanosized particles. When we only use a thin film of ZnO as a buffer layer or Au as a catalyst the ZnO nanorods grew randomly on the substrate surface. But with using both buffer layer and catalyst, the growth of nanorods was almost vertically aligned perpendicularly to the substrate and the density of rods was higher than other samples with low size distribution. The high resolution transmission electron microscopy, electron diffraction and X-Ray diffraction results show that all the ZnO nanorods are single crystal with preferential orientation. A boundary assistant nucleation mechanism followed by a vapor-solid (VS) process was proposed to explain the nanorod growth. In addition, a strong excitonic emission located at 3.25 eV was observed in room-temperature photoluminescence measurements.

16:30 - 16:50
oral

Characterization of Luminescence in thick MgZnO Layers and MgZnO/ZnO Quantum Wells

Frank Bertram[1)], **Daniel Forster**, **Juergen H. Christen**[1)], **R. Kling**[2)], **Th. Gruber**[2)], **Andreas Waag**[3)]

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3) TU Braunschweig, Institute of Semiconductor Technology (IHT), Hans Sommer Str. 66, Braunschweig 38106, Germany

A series of MOCVD grown MgZnO epitaxial layers (1m thick) with increasing Mg incorporation on ZnO/GaN/sapphire substrate are investigated. No remarkable change of the morphology is found with increasing Mg-content. The laterally integrated cathodoluminescence (CL) spectrum of each sample is dominated by three spectral bands. Two bands at higher energies can be assigned to the MgZnO emission, i.e. for a [Mg] = 6% E1= 3.474eV and E2= 3.442eV at 5K. These two peaks are clearly separated from the ZnO emission (E= 3.356eV). The two MgZnO peaks shift simultaneously to higher energies with increasing Mg-content. Furthermore MgZnO/ZnO/MgZnO single quantum well (SQW) structures on ZnO/GaN/sapphire substrate are investigated and two additional luminescence lines appear clearly assignable to the 2nm thick single quantum well.
Microscopic morphological features of the layers directly correlate with the local spectral CL emission characteristic. While the high energy peak of MgZnO buffer and of the SQW exhibit an almost homogeneous lateral distribution, the emission of the low energy peak of the MgZnO barrier as well as that of the SQW vanishes completely at local surface defects.
The excitation and the temperature dependence is investigated by spatially integrated photoluminescence. No spectral shift with excitation density is found for all samples. However, the intensity ratio of the both MgZnO peaks strongly changes: The intensity of the high energy MgZnO peak exhibits an almost perfectly linear dependency on excitation density whereas the low energy peak increases significantly stronger with excitation. Identical dependencies are found for the SQW structures for both, the MgZnO barriers as well as the two peaks from the ZnO-SQW. Spectral-time-resolved measurements directly evidence the transient competition between the two different recombination channels in the SQW as well as in the MgZnO barriers and the thick MgZnO layers, respectively.

Defects induced by oxygen and hydrogen in CdTe crystals

16:50 - 17:10
oral

A Kisiel[1), Andrzej Mycielski[2), J Polit[3), E Sheregii[3), J Cebulski[3), M Piccinini[4), A Marcelli[4), B V. Robouch[4), M Cestelli Guidi[4,5), A Nucara[5)

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Actually, an important parameter to evaluate the quality of CdTe crystals is the content of residual amount of oxygen in high purity crystals. As a consequence, pure Cd and Te (99,999%) are used to growth CdTe monocrystals and thin films that are then purified by heating in a reduced hydrogen atmosphere. In this purification process is necessary to keep a balance between O and H so that to characterize oxygen and hydrogen contributions we applied both medium infrared (MIR) and far infrared (FIR) reflection spectroscopy. The infrared analysis is a very powerful method to investigate defects and in particular may obtain information on defects created in CdTe monocrystals grown from Cd and Te components purified in a hydrogen atmosphere before crystallization.It is thus interesting to consider the problem of asserting the presence of defects in semiconductor binary compounds, by observing consequences induced by distortions of their elemental tetrahedra due to the presence of vacancies and of insite atoms within the tetrahedra or other intersticial presence.Our model thus considers the system $A(Vz_xZ_{1-x})$ and $(A_{1-y}Va_y)Z$ as composed of five defect tetrahedron configurations: $\{^zT_{-1}, ^zT_{+1}\}, T_0, \{^aT_{-1}, ^aT_{+1}\}$ where $^zT_{-1}$, $^aT_{-1}$ tetrahedron with one vacancy, and $^zT_1$, $^aT_1$, with one interstitial are deformed tetrahedra.Detecting the five frequencies in presence would indicate the presence and amount of the defects being monitored.Reflectivity experiments were performed using a FTIR BRUKER Equinox 55 interferometer using both a standard Hg lamp and IR synchrotron radiation emitted by DAFNE the storage ring working at the INFN-LNF at Frascati.In the mid-infrared (500-3000 cm-1) region of these monocrystalline systems we observed the characteristic vibrational spectra of oxygen and hydrogen bounded to Cd and Te.Also a rich fine structure around the CdTe phonon frequency range in the far IR domain ,has been detected and analyzed.
[ABSTRACT TRUNCATED TO 2
[ABSTRACT TRUNCATED TO 2000 LETTERS]

Wednesday, September 8th

Poster session 2Continuation of the Monday's Poster session 1. The same posters are displayed.

19:00 - 21:00

Thursday, September 9th

Afternoon session 1

Main Building, room 134

14:00 - 15:30

A new approach to the growth of ZnO by vapour transport

14:00 - 14:45
invited oral

<u>Vicente Muńoz-Sanjosé</u>[1), R Tena-Zaera[1), M. C. Martinez-Tomas[1), J. Zúńiga-Pérez[1), S. Hassani[2), R. Triboulet[2)

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The crystal growth of ZnO by vapour transport is classically made with the assistance of additional species that produce a gaseous mixture, the role of which remains often uncertain in the transport and growth processes. We have made a systematic study of the ZnO crystal growth process by vapour transport in presence of different additional species (Zn, C, H_2, Fe, Cu). Transport rates have been measured using an in-situ dynamic technique. The chemical role of each species has been analysed from the thermochemical point of view. It will be shown that, in some cases, additional species in the growth of ZnO by vapour transport promote the generation of an additional Zn pressure. This zinc pressure acts autocatalytically inducing O_2 and Zn partial pressures higher than those corresponding to the stoichiometric and equilibrium conditions at the sublimation interface. In addition we have made a numerical study of the process which shows that partial pressures higher than the equilibrium ones must be present in order to justify the experimental results. The experimental and numerical analysis, here shown, pave the way for new processes to promote the growth of ZnO by vapour transport; using controlled generation of additional Zn vapour as a mechanism to act on the growth and crystal properties.

14:45 - 15:30
invited oral

ZnMgO-ZnO based Heterostructures and Nanopillars grown by MOVPE

Andreas Waag[1)], **Th. Gruber**[2)], **C. Kirchner**[2)], **R. Kling**[2)], **F. Reuss**[2)], **H. Wehmann**[1)], **A. Bakin**[1)]

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Due to its specific optical and magnetic properties - ZnO seems to be a very versatile material platform in the field of optoelectronics, magnetoelectronics, and nanoelectronics. In particular, a self-organized growth mode can be initiated in order to fabricate ZnO nanopillars with a quite homogenous size distribution. ZnO nanostructures offer an unusual adventage: the surface oxidation obviously does not present a problem. Up to now, the work on the ZnO growth by MOVPE (important industrial standard) is relatively limited. Here, we report on the development of MOVPE technology in order to establish a basis for the exploitation of ZnO hetero- and nanostructures. While conventional precursors are available for the metal components (DEZn, Cp_2Mg), the choice of an adequate oxygen precursor for the growth of ZnO and ZnMgO is very important. We have used i-PrOH and t-BuOH for the low temperature growth (300÷500C), and N_2O for the high temperature growth (600÷950C). ZnO or sapphire have been used as substrates. The incorporation of Mg turns out to be difficult due to pronounced prereactions of the Mg precursor. With a careful process control, we were able to fabricate ZnMgO layers with Mg content of up to 9%, and to incorporate these as barriers in ZnMgO/ZnO quantum well structures. Now those barriers allow the fabrication of heterostructures, which include cladding and waveguide layers for optically pumped lasing. In addition, MOVPE can be used to initiate a growth mode resulting in the self-organized growth of ZnO nanopillars with a typical width of only 50 nm and a height of up to 5 μm. Despite small diameter, these free-standing nanopillars show intense PL spectra, with FWHM below 0.5 meV. HRXRD analysis shows that these nanopillars - depending on the growth mode - can be almost completely c-oriented. The fabrication of ZnMgO-ZnO based quantum well structures and nanostructures will be described, including an analysis of their structural and optical properties.

15:30 - 15:50

Coffee break

15:50 - 16:40

Afternoon session 2 / clossing

Main Building, room 134

15:50 - 16:35
invited oral

Cathodoluminescence centres in ZnO

Matthew R. Phillips[4)], **M. Wagner**[4)], **O. Gelhausen**[4)], **V. Coleman**[1)], **J. B. Bradby**[1)], **C. Jagadish**[1)], **E. Malguth**[2)], **A. Hoffmann**[2)], **Ewa M. Goldys**[3)], **J. J. Russell**[5)]

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The chemical origin of the defects responsible for the visible luminescence in ZnO remains controversial. Debate centres on the assignment of these luminescence bands to specific radiative recombination centres, such as oxygen vacancies and zinc interstitials or complexes involving these defects. Of current interest is the role these defects play in the incorporation of high concentrations of transition metals (Fe, Cr, Mn, Ni) in ZnO to produce dilute magnetic semiconductors. In the present work, ZnO films were deposited on Si (100) and glass substrates by RF magnetron sputtering using a high purity ZnO target with different O_2/Ar partial pressure ratios. The cathodoluminescence (CL) and optical properties of these films were investigated as a function of substrate temperature, O_2 concentration, working pressure (1 - 10 mtorr) and post-deposition thermal annealing in N_2 at 500^oC for 1 hour. The position of the optical absorption edge was observed to red shift with increasing O_2 concentration. Post-growth thermal annealing significantly increased the CL intensity of the near band edge CL emission but had virtually no effect on the defect CL emission. The relative intensity of the green, orange and red defect CL bands exhibited a complex dependence on growth conditions. CL measurements from the ZnO films have been compared with monochromatic CL images of defect distributions around indents in high quality single crystal ZnO before and after thermal annealing. Each defect CL emission displayed a distinct spatial distribution around the indent, indicating that each centre has a different chemical origin. Furthermore, the centre responsible for the green CL was observed to have a higher mobility those involved in the orange and red emission. This result suggests that zinc interstitials are involved in the green luminescence as they are the most mobile centres in ZnO. Relationships between the CL emission in ZnO and structural point defects will be discussed.

Symposium G

Functionalisation of Nanoparticles

From letters the small ones I was selecting
And working ants from the meanings.
I wanted to fill cells
With souls of molecules.

(Tudor Arghezi, Romanian poet, 1880-1967)

Introduction

This symposium aimed to present and debate the progress in the theory and applications of functionalised nanoparticles within a multidisciplinary topic covering:

- different methods for obtaining functional nanoparticles by chemical, physical, mechanical or combined methods used to synthesise of ceramic nanoparticles, nanotubes and nanowhiskers,
- Thermodynamic and kinetic modelling of the synthesis processes in order to obtain functional nanoparticles with reproducible surface properties;
- Industrial preparation of compact nanomaterials: sintering, tape casting, injection moulding, innovative processing methods;
- Electronic and atomic structure of aggregates and nanoparticles (point defects, surfaces...), thermodynamic properties of nanoparticles, physical and chemical interactions on nanoparticles surfaces;
- Elaboration of specific characterisation methods to establish fundamental correlations between synthesis/nanostructure/properties and grain size dependent phenomena in different systems obtained from functional nanoparticles;
- Applications of functional nanoparticles based on their catalytic and photocatalytic properties, electronic properties (photoluminescence, cathode-luminescence...), optical and photonic properties, atomic and transport properties, electrical, magnetic and ferroelectric properties, mechanical properties, interactions of nanoparticles with biologic entities;
- Development of smart multifunctional nanomaterials based on functionalised nanoparticles for chemical and biological applications to be used in nano-bio-technologies of tomorrow.

We hope that discussions between participants will bring to life new ideas, new projects and new friendships between participants.

Organisers

- Radu Robert Piticescu, Institute for Non-ferrous and Rare Metals, Bucharest, Romania
- Witold Lojkowski, High Pressure Research Center of the Polish Academy of Science, Warsaw

- Claude Monty, CNRS-Institut de Sceince et de Genie des Materiaux et Procedes, France

Acknowledgements

The symposium was supported by:

- Polish Ministry for Research and Information Technology
- Romanian Government, Ministry of Education and Research, Direction for European Integration
- The European Commission:
  - Contract: No. ICA1-CT-2002-60028
  - Contract: No. G1MA-CT-2002-04055
- High Pressure Research Center "UNIPRESS", Polish Academy of Sciences: SPUB-MSN, SPUB-PRENABIO and other.

Monday, September 6th

Poster session 1

19:00 - 21:00

Nanostructure, nanochemistry and grain boundary conductivity of yttria-doped zirconia

Alin Rizea[1], Jean-Marc Raulot[1], Claude Petot[1], Georgette Petot-Ervas[1], Gianguido Baldinozzi[1]

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poster G-01

This work is aimed to a comprehensive study of the role of the microstructure and of the local chemistry at the grain-boundaries on the ionic grain-boundary conductivity in yttria (9mol%)-stabilized zirconia (YSZ) and in YSZ-alumina composites. Electrical conductivity measurements show that the grain-boundary conductivity (σ_{gb}) increases with the cooling rate at the end of sintering, when the grain size and the amount of Si in the ceramic decreases. Alumina additions lead to a decrease of σ_{gb} in the samples containing 1.0 wt% SiO_2, while σ_{gb} passes through a maximum for heavier silicon contents. These results, coupled to TEM X-ray microanalysis, suggest that alumina nanoparticles interact strongly with SiO_2 at the grain boundaries giving rise to a competitive effect: whereas the alumina nanoparticles increase the insulating character, they also reduce the vitreous phase at the grain boundaries, increasing the conductivity. Moreover, XPS analyses show that Si and Y segregate near the interfaces, on a depth smaller than 600nm. These analyses suggest a kinetic demixing process and they allow to explain the positive effect of a faster cooling rate at the end of sintering, responsible for the smaller amount of Si rejected at the grain-boundaries.

New Nano-Sized Sensing Drug and Its Medical Application

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2) National Institute for Chemical and Petrochemical Research, Bucharest 060021, Romania

poster G-02

Nanomedicine is the application of nanotechnology to the diagnosis and treatment of human disease. This discipline has the potential to change medical science dramatically, as demonstrated, for example, by an innovation in cancer imaging that uses novel diagnostic agents synthesized from nanoparticles. We are conducting research on cluster-based materials for future medical applications. The design of a multifunctional photosensitive particle that is stable and highly efficient will be key to this novel medical application and in the photodynamic treatment (PDT), especially. Three consecutive processes occur during the PDT treatment: initial consumption of oxygen through the photodynamic process; pathophysologic alterations in regional blood supply (hypoxia) and total vascular occlusion (ischemia). The effect of a new drug as TSPP-Sil-TiO_2 was studied in this paper. By coupling with TiO_2, TSPP is loosing the proper absorption bands, due to the chemical bonds SO_2-NH, present in the new synthesized system. The UV-Vis spectrum of the new system indicates J-aggregate form suitable for biomedical applications. The particle size and the morphology of TSPP-Sil-TiO_2 nanoparticles in acrylate matrix were investigated with AFM. The images of TSPP-Sil-TiO_2 nanoparticles in polymer matrix have been compared with TiO_2 nanoparticles alone. We implanted cancer cells under the skin of mice to cause tumors to form. When the size of the tumor grew to about 0.5 cm, it was injected a solution containing fine particles of TSPP-Sil-TiO_2. After 2 or 3 days, were cut open the skin to expose the tumor and irradiated it. The treatment clearly inhibited the tumor growth. A further marked antineoplastic effect was obtained.

Structural and luminescence properties of yttrium-aluminum garnet (YAG) nanoceramics

Dariusz Hreniak[1], Stanisław Gierlotka[2], Wiesław Stręk[1], Witold Lojkowski[2], Bogdan Pałosz[2], Piotr Mazur[1]

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poster G-03

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Preparation of transparent nanoceramics from nanocrystalline YAG ($Y_3Al_5O_{12}$) powders both undoped and activated by RE-ions has been described. The results of structure and morphology investigations have been presented. The decomposition of the nanocrystalline YAG crystals into $YAlO_3$ (YAP) was observed. The temperature and pressure of the transformation was much lower than that reported for bigger crystals. The transformation was connected with grain coarsening. The influence of the preparation method of YAG nanopowders on the transparency of obtained ceramics has been found.

Irradiance measurements of electroluminescence PAQ films

poster G-04

Janusz Jaglarz[1)], **Jerzy Sanetra**[1)]

1) Cracow University of Technology, Institute of Physics (PK), Podchorążych 1, Kraków 30-084, Poland

electroluminescence cells with H[3,4-b]chinoline and 9winylecarbazole [PAQ] layers are promising devices for blue light emitting EL diode. In this work optical reflectance as a function of temperature in copolymers PAQ layers deposited on Si crystalline substrate was measured. Using the Cauchy model of reflectance versus wavelength the refraction coefficient and thickness of the films were determined in temperature ranges from 76 K to 300 K.

Temperature dependencies of optical parameters of 1H[3,4-b]chinoline films used in electroluminescence devices

poster G-05

Janusz Jaglarz[1)], **Jerzy Sanetra**[1)]

1) Cracow University of Technology, Institute of Physics (PK), Podchorążych 1, Kraków 30-084, Poland

electroluminescence cells with H[3,4-b]chinoline and 9winylecarbazole [PAQ] layers are promising devices for blue light emitting EL diode. In this work optical reflectance as a function of temperature in copolymers PAQ layers deposited on Si crystalline substrate was measured. Using the Cauchy model of reflectance versus wavelength the refraction coefficient and thickness of the films were determined in temperature ranges from 76 K to 300 K.

Formation of core-shell nanoparticles under laser ablation of copper and brass in liquids

poster G-06

Pavel V. Kazakevich[1)], **Alexander V. Simakin**[1)], **Valeriy V. Voronov**[1)], **Georgy A. Shafeev**[1)], **David Starikov**[2,3)], **Abdelhak Bensaoula**[3)]

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Experimental results are presented on ablation of either copper or brass targets in a liquid environment (e.g., ethanol, acetone, or water) by irradiation with either a pulsed copper vapor laser (0.51 μm) or a pulsed Nd:YAG laser (1.06 μm). The ablated material is ejected into the surrounding liquid in the form of nanoparticles with an average size of 20 nm. The composition of nanoparticles depends on the nature of the liquid. Ablation of brass (40% Zn and 60% Cu) in ethanol results in formation of core-shell nanoparticles. Brass nanoparticles are characterized by a well-pronounced plasmon wavelength peak at 510-520 nm. Under further laser exposure of the colloidal solution the plasmon resonance of the brass nanoparticles shifts to that of pure Cu nanoparticles at 570-590 nm. Ablation of Cu results in formation of shells only in acetone. In a certain range of laser parameters (fluence and number of laser shots) the surface of the solid target is composed of micro-cones having a regular structure. The distance between neighboring micro-cones in the structure depends on the laser fluence and averages around 30 μm. The composition of micro-cones (Cu/Zn ratio) differs from that of the initial surface.

Forming of hollow spherical ceramic nanoparticles by spray pyrolysis method

poster G-08

Ryszard Gajerski[1], Stanisław Łabuś[1], Andrzej Małecki[1], Barbara Małecka[1], Jan Obłąkowski[1]

1) AGH University of Science and Technology, Faculty of Materials Science and Ceramics (AGH UST), Mickiewicz 30, Kraków 30-059, Poland

Nanoparticles can have different form but predominantly are obtained as solid grains. The properties of many materials based on these nanopowders are relatively well known. Using ultrasonic spray pyrolysis (2,6 MHz) nanopowders composed of hollow ball-shaped grains were obtained. The diameter of grains vary in the range 2 - 400 nm. The obtained nanopowder materials were metallic (Ru, Ag, Pd, Ag-Pd, Ag-Rh), ceramic (Al_2O_3, Al_2O_3-Cr_2O_3, CeO_2, CeO_2-ZrO_2) as well as composite (cermetals: NiO-Au, CeO_2-ZrO_2-Pt and CeO_2-ZrO_2-Au).
As a precursors aqueous solutions of adequate nitrates(V), chlorides, acetates or alkoxides of appropriate metal were used. The total concentration of initial salts solution was in the range 0.1-0.03 mol.dm^{-3}. The concentration of particular solution corresponded to the assumed nanopowder product composition. Aerosols based on such a solution were obtained by ultrasonic nebulization in the stream of adequate carrier gas (i.e. air, Ar+H_2) and introduced into horizontal reactor heated to 500-800^{o}C, depending of the type of solution, carrier gas and its flow rate, were the decomposition of salts occurred. Products of decomposition were caught in electrofilter.
Microstructure of the powders obtained was examined using different methods like TEM, SEM and EDAX. The hollow nanoparticles enable formation of porous ceramic composite membranes of higher permeability than those made of solid particles, which is important for catalytic applications. On the other hand, the dense ceramic membranes can be applied as cathodes in ion transport. The basic advantage of hollow nanoparticles is their low specific weight and presence of metal admixture atoms (Ag, Au, Pt, Ru, Rh) on the surface of nanoparticles. This can give the significant economic effect for many applications e.g. in electronic engineering for conductive path fabrication by screen- or ink-printing techniques.

Magnetic properties of iron-organic nanostructures

<u>Olga M. Osmolowskaia</u>[1], Vladimir M. Smirnov[1], Pavel E. Morozov[1] poster G-09

1) Chemistry Department, Saint Petersburg State University, Saint Petersburg, Russian Federation

The important aspects of nanomagnetism are the magnetic behavior of surface nanostructures containing d-element and the dependence of nano-scale surface interactions on nearest-neighbour environment. Within the program of fabrication surface nanostructures with prearranged properties we have fabricated and studied the metal-oxygen nanostructures on dispersed silica. These structures consisting on mono- and multilayers M-O groups on silica surface were obtained by molecular layering method. It was shown that the magnetic properties are determined by chemical design of nanostrucures (mono, multilayers, periodic and alternating multilayer of 3d and 4f element, for example, from Eu-O and Fe-O groups) as well as the composition of first deposited layer. In the case of iron-oxygen groups the creation of two-dimensional ferromagnetic ordering is possible [1]. In this report the results of experimental study of peculiarities of magnetic properties in periodic nanostructures containing Fe-R groups ($CHCCH_2O$- as R) on silica surfaces are represented. These nanostructures were obtained as a results of a set of alternating irreversible reactions between functional groups of silica, $CHCCH_2OH$ and $FeCl_3$ in gaseous phase at 200C. As a sublayer we used SiO_2 + $CHCCH_2OH$. After deposition $CHCCH_2OH$ on SiO_2 this nanostructure became ferromagnetic and by our opinion it can be useful for spintronic systems. The magnetic properties of surface nanostructures strongly depends on the number of deposited layer Fe^{+3}-R, the effective magnetic moment therewith increase as the number of layer (1-4) from 2.36 to 7.56 MB corresponding at 293 K. The temperature dependence of μ_{eff} points to the antiferromagnetic character of surface interaction. Details on electron structure of these nanostructures will be discussed.
The work is supported by RFBR (grant N 03-02-32748).

[1]. EMRS Fall Meeting 2003, Book of abstr., P. 206

Synthetic methods of nanosized tin dioxide

S A. Papargyri[1], D A. Papargyris[2], A I. Botis[1], A D. Papargyris[1] poster G-10

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Tin dioxide is a wide band semiconductor, with interesting chemical physical and mechanical properties, used in a variety of industrial, domestic, medical and agricultural applications, including gas detectors, transparent conductors, solar cells, anti-static films, nanoelectronic devices etc.
Synthesis of tin dioxide layers can be achieved though a variety of methods including sol-gel, sputtering from a SnO_2 target, tin metal nanoparticles/organometallic precursor oxidation, chemical vapour deposition, physical vapour deposition, solid state reactions.
The main problem with sol-gel, sputtering from a SnO_2 target, and CVD methods especially when they are used in thin layers, are quality problems due to high grain size and production of mixtures of amorphous and crystalline oxide. The high yield and the absence of organic matter involved in the synthesis using solid state reactions are among the advantages of the method. The organometallic precursor routes of SnO_2 production have as a main disadvantage the presence of organometallic precursors and the complex process control.
The main drawbacks with the bulk synthesis of nanowires e.g. using discharge, laser ablation, template, solution, carbon nanotube confined chemical reaction, vapour-liquid-solid (VLS) methods, or the growth of SnO_2 whiskers by VLS, is the requirement of very high temperatures (1110-1300^{o}C), the use of complex apparatus and the formation of large grain size products.
Literature review shows that exist a high interest for the development of new methods e.g. using redox reaction in inverse microemulsion systems, template method using copolymers, solid state process with active carbon and doping of SnO_2 with V_2O_5 and Dy^{3+} and other dopants. Among the main targets are, the use of low production temperature, better control of surface morphology and crystallinity, the simplicity of the process and the use of new dopants.

Polymer matrix composites with nanoparticles of TiC obtained by a sol-gel method

poster G-11

Katarzyna Konopka[1], **Anna Biedunkiewicz**[2], **Anna Boczkowska**[1], **Z. Roslaniec**[2], **Krzysztof J. Kurzydlowski**[1]

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Nanoparticles of carbides, nitrides and carbonitrides can be used to reinforce polymer matrix nanocomposites with desirable strength, hardness, corrosion and wear resistance. To achieve these of desirable properties polymer matrix and nanoparticles need to be optimised.
In the present paper the nanocomposites with polymer matrix were analysed. TiC nanoparticles as reinforcement were produced by sol-gel method. The nanocomposites were obtained in situ, in the reaction mixture and synthesizing copolymers (PEE).
For characterization of TiC nanoparticles, the atomic force microscope (AFM) was used. Microstructure of the composites was observed using a scanning electron microscope. Tensile properties were measured by tensile tests. Moreover, the abrasive wear of nanocomposites was measured. For comparison also samples of polymer were analysed and composites with submicron size of TiC particles.
Results showed that nano-TiC particles in the polymer matrix improve strength, and wear resistance. The results are discussed in terms of size of TiC particles on the properties of bulk composites.

Influence of synthesis conditions on the particles size and the morphology of zinc oxide nanopowders

poster G-12

Tomasz Strachowski[1], **Edward Reszke**[3], **Laura Perchuc**[1], **Ewa Grzanka**[1,4], **Adam Presz**[1], **Tadeusz Chudoba**[1], **Witold Lojkowski**[1], **Larisa Grigorjeva**[2], **Donats Millers**[2]

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Nanocrystalline zinc oxide powder has been successfully prepared by addition of NaOH and urea as the base source via the microwave, resistance heating and conventional hydrothermal process at temperature $<$ 100oC. The effects of synthesis conditions and chemical additives on the particulate properties such as the particle morphology and grain size discussed. The morphology and grain size was monitored by SEM, XRD and BET analysis. Zinc oxide nanopowders was obtained by the decomposition of different zinc saltz in a aqueous solution under alkaline conditions or with addition of urea. The properties of zinc oxide as scintillating material were tested as a function of the technology of production and grain size. The luminescence of zinc oxide nanopowders was studied under three kinds of excitation: pulsed electron beam, nitrogen laser and continuous x-ray excitation.

Preparation and characterization of function localized microspheres

Daisuke Suzuki[1)], **Haruma Kawaguchi**[1)]

1) Science and Engineering, Keio University, Hiyoshi Yokohama, Japan

poster G-13

Unsymmetrical particles were expected to be useful for electrical display or the building block of photonic crystals. We prepared the Au localized polymer particles to use Au unit as activate site for thiol derivative materials. First, we got sub-micron particles by soap-free emulsion polymerization, and arranged onto a polystyrene substrate. Second, Au was sputtered onto the surface of particles, and the particles were removed from the substrate into an aqueous medium. The particles were reacted with functional materials such as ssDNA. These conjugates have potential to create new materials. For this purpose, new snowman-type particles were obtained. The particles are made by DNA hybridization, so they can reversibly be converted from snowman-type to respective spheres and vice versa. In this investigation, we could find it possible to undergo a reaction over the Au on the sub-micron particles, and to build up nano materials by using the novel particles.

An FT-IR Spectroscopic Investigation of Hydroxide Groups in Nano-Crystals of ZrO2.

Agnieszka Opalińska[1)], **Wojtek Dzwolak**[1)], **Tadeusz Chudoba**[1)], **Witold Lojkowski**[1)]

1) Polish Academy of Sciences, High Pressure Research Center (UNIPRESS), Sokolowska 29/37, Warszawa 01-142, Poland

poster G-14

The presence of persistent hydroxide (-OH) groups in nano-crystals of ZrO2 is expected to affect its chemical reactivity, and to increase hydrophilicity of the crystal nano-surfaces. On the other hand, the -OH groups may dump - through the quenching - luminescence of fluorochromes added to the zirconium dioxide. Therefore probing of -OH groups in preparations of ZrO2 is of technological interest.
The strong infrared absorption around 3400 cm-1, corresponding to stretching vibrations of -OH bonds, make FT-IR spectroscopy a very sensitive tool for detection of hydroxyl groups. Yet, focusing on this spectral region is very risky, as a spontaneous absorption of atmospheric water vapor by a hydroscopic powder after heating is likely to give rise to artifacts. That is why the synthetic procedure was modified by a partial isotopic substitution of hydrogen with deuteron. Namely, during the chemical synthesis and precipitation of the ZrO2 roughly 40-50 % of water was replaced with heavy water (D2O). As a consequence, a portion of -OH groups was substituted with -OD groups on the ZrO2 surface being simultaneously trapped within the nano-structure. The -OD stretching vibrations are seen as a separate infrared band at 2600-2400 cm-1. The band is not overlapped by other infrared peaks in ZrO2 and its intensity can be conveniently (without the danger of artifact generated upon handling the sample in the air) treated as a yardstick of the number of hydroxide groups present in the ZrO2.
Nanocrystallie zirconia powders were produced using a microwave driven hydrothermal process under pressure up to 5.5 MPa. For FT-IR spectra, KBr-based pellets containing 1 wt.% of ZrO2 were prepared. All the FTIR spectra were collected in a transmission mode on a Nicolet NEXUS FT-IR spectrometer equipped with a liquid nitrogen-cooled MTC detector.

Hydroxyapatite growth on surfaces modified by CdSe or Si nanoparticles embedded in SiOx thin films

Liliana Pramatarova[1)], **Emilia V. Pecheva**[1)], **Dianka Nesheva**[1)], **Zdravka Aneva**[1)], **Todor Petrov**[1)], **Attila Toth**[2)], **Eniko Horvathe**[2)], **Ferenc Riesz**[2)]

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poster G-23

Surface functionalization of materials by different methods is very often applied to make the surfaces bioactive and biocompatible. In this study the following question is raised: could well established nanotechnology be used to obtain functional nanoparticles and are they able to induce the deposition of

osteoconductive hydroxyapatite (HA) ceramic. It is known that nano dimentions and porous structures influence different biological events and thus they can be utilized in the laboratory to create bilogically integrated multifunctional devices (biomaterials and sensors).
In this paper, subsequent physical vapor deposition of SiOx and CdSe at room temperature or thermal Si nanoparticles growth in SiOx thin film was used to modify glass substrates. To test the ability of the as-nanostructured surfaces to induce the deposition of HA, the samples were immersed in a simulated body fluid (SBF) and simultaneously irradiated with a scanning laser beam for 2 min with a special design. The method of laser-liquid-solid interaction (LLSI) has lead to a synergistic effect due to the nanostructured substrate, aqueous solution and laser irradiation. The grown layers were investigated by light microscopy, SEM, EDX, FTIR and Raman spectroscopy. Light microscopy and SEM revealed a white sponge-like layer covering the surfaces and having nanodimentions, with morphology different from that on initial glass surfaces. Raman and FTIR spectroscopies showed the typical vibrational modes of HA. Results from EDX showed higher Ca and P content in the stripes of the laser-substrate interaction, thus indicating the influence of the laser energy.
This paper showed that the applied nanotechnology could be efficiently used for producing functional nanostructures able to induce HA deposition, and that the proposed novel method of LLSI promotes and enhances the HA nucleation in comparison with the traditional methods of prolonged biomimetic soaking in SBF.

Natural opal as a model system for studying the process of biomineralization

poster G-24

Liliana Pramatarova[1), **Emilia V. Pecheva**[1), **Radina Presker**[2), **Ulrich Schwarz**[3), **Ruediger Kniep**[3)

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Opal is a natural model for a nanostructure due to its nano-sized close packed silica spheres. Its structure is also characterized by the presence of a regular sublattice of voids, filled with a molecular water and accesible to filling by other substances. Using a natural opal as a substrate, no complimentary technique is necessary to produce patterned surface, since it is naturally present in opal. Thus, the property of nano dimentions to efficiently influence different biological events can be utilized in the laboratory and bilogically integrated multifunctional devices (biomaterials, sensors) could be created. Today?s material science is ?learning? from the nature and by approaches resembling the bilogical principles, bio-mimicking and biocompatible materials have been created.
The main purpose of our work is by using nanostructured or other functionalized materials as model systems, to contribute to the study of the biomineralization. Particularly in this study, the ability of a natural opal from Eastern Rhodopes mountain in Bulgaria to induce the deposition of a hydroxyapatite [HA, $Ca_{10}(PO_4)_6(OH)_2$] ceramic layer on its surface from a simulated body fluid (SBF)was reported. Raman, Infrared spectroscopies and X-ray diffraction were used to determine that the opal consists of two main phases: microcrystalline quartz and cristobalite and that the grown from SBF ceramic on both phases is HA with nm grain size.

Radiative electron-hole recombination and degradation processes in thiol-stabilized CdTe nanocrystals

poster G-25

Viktor V. Strelchuk[1), **Peter Feychuk**[2), **Larysa P. Shcherbak**[2), **Maksym Kovalenko**[2), **Vadim P. Bryksa**[1), **Alexander F. Kolomys**[1), **Sergiy G. Krylyuk**[1), **Dmytro V. Korbutyak**[2), **Mikhail Y. Valakh**[1)

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Cadmium telluride nanocrystals (NCs) synthesized by wet chemical routes are very promising objects for various applications including opto- and nanoelectronic devices and biological labeling. However, many of their properties which define the applicability of the NCs, such as radiative recombination pathways, degradation processes, etc., are not fully understood yet.
In this contribution, we report on the synthesis and photoluminescence (PL) investigations of CdTe NCs synthesized in aqueous solution and stabilized with thioglycolic acid. The PL spectra were recorded for the temperature range 5 ? 300 K using different lines of an Ar^+-laser for excitation.
Room temperature PL spectra of the NCs consisted of an intensive line due to near-edge recombination

and a weak low-energy tail connected with the recombination via deep traps. Depending on the synthesis parameters, the maximum position could vary during the solution storage at room temperature in dark. For some samples, freezing of the solution containing NCs resulted in a red-shift of the PL maximum. After that the energy position of the PL line followed the temperature dependence of the CdTe band gap. We suggest that such an unusual behavior is caused by changes in the passivation conditions at solution freezing. Low-temperature PL spectra measured at different excitation energies clearly showed that the main PL line consists of several components. To explain the observed features, a model which accounts for both the near-edge recombination and the recombination via the states created by the cadmium ? thiol and tellurium ? OH complexes at the surface is proposed.

Tuesday, September 7th

Afternoon sessionElectronic and luminescence Properties of nanoparticles

Main Building, room 208

14:00 - 15:30

Molecular impurities in the luminescent ZnO nanocrystals

14:00 - 14:30
invited oral

Larisa Grigorjeva[1)], **Witold Lojkowski**[2)], **Donats Millers**[1)], **Tomasz Strachowski**[2)]

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2) Polish Academy of Sciences, High Pressure Research Center (UNIPRESS), Sokolowska 29/37, Warszawa 01-142, Poland

The luminescence of ZnO nanocrystals produced by different methods was studied and compared with luminescene from bulk single crystal. The luminescence observed is rather different for ZnO nanocrystals produced by different methods, however in all studied sets of nanocrystals the luminescence band at 1.9 - 2.2 eV linked to the intrinsic defects as well as exciton related luminescence (at 3.20 - 3.32 eV) was observed.
The IR absorption spectra shown that all ZnO nanocrystals studied contains besides well known OH groups other molecular impurities also, whereas in single crystal content of other molecular impurities is neglible. Different chemical reactions and processing is used by producers of ZnO nanocrystals. The uncontrolled molecular impurities were incorporated in nanocrystals and/or bound at their surfaces during these chemical processes. Therefore different uncontrolled molecular impurities are responsible for different luminescent properties of ZnO nanocrystals and luminescence could be a simple and powerful tool for ZnO nanocrystals purity checking.
The OH line in IR spectra of ZnO nanocrystals is widened if compared with this line in single crystal. This is an evidence that OH in nanocrystals occupieded a number of different positions, possibly the fraction of these positions are on the nanocrystal surface. The other uncontrolled molecular impurities could be incorporated in different positions also. The luminescence study of ZnO nanocrystals shows that in some cases the intrinsic defects of ZnO were blocked by uncontrolled impurities. This is an promissing tool for nanocrystals engineering.

Assembly of oxide particles in chains in a polymerizing silica sol

14:30 - 14:45
oral

Dinesh C. Agrawal[1)], **Sudip Dasgupta**

1) Indian Institute of Technology Kanpur (IITK), IIT Kanpur India, Kanpur 208016, India

The alkoxide sol-gel process is widely used to form powders, coatings, thin films and fibres. In a silicon alkoxide sol, the reaction conditions can be changed to favour the formation of long chains or three dimensional network structures by adjusting the pH. In the present work the possibility of using the molecules forming during the hydrolysis and condensation reactions in an alkoxide silica sol for the assembly of ZrO_2 particles was investigated. The ZrO_2 particles were suspended in the sol the pH of which was adjusted to 3 to favour the formation of chain like structures. Under suitable conditions it was possible to assemble the ZrO_2 particles in long chains several microns long. It is proposed that the oligomers forming by the hydrolyisis and condensation reactions in the sol act as links between the particles to produce linear assemblies of particles.

14:45 - 15:00
oral

Highly luminescent doped nanoparticles embedded in porous silicon oxide

Nima Taghavinia[1)], **Gilles Lerondel**[2)], **Hisao Makino**[3)], **Takafumi Yao**[4)]

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Yttrium silicate and zinc silicate nanoparticles were formed inside a transparent porous SiO_2 template, by impregnating layers of porous silicon with nitrate solutions of yttrium and zinc, followed by appropriate heat treatment. Yttrium silicate nanoparticles were doped with red emitting Eu^{3+} and blue emitting Ce^{3+} ions, while zinc silicate nanoparticles were doped with blue emitting Eu^{2+} ions. Doping was carried out by adding appropriate impurity ions in the impregnation solution. The product is a dispersion of nanoparticles scattered inside a transparent porous SiO2. The photoluminescence of the samples show strong luminescence of the impurity ions upon UV illumination. The blue luminescence from the Ce^{3+} doped yttrium silicate nanoparticles is stronger than the commercial Y_2SiO_5:Ce^{3+} phosphors. The doped nanoparticles act effectively as "nanophosphors" stabilized inside the SiO_2 porous matrix. The size of the nanoparticles was between 20nm to 200nm. The yttrium silicate nanoparticles show a mixture of Y_2SiO_5 and $Y_2Si_2O_7$ phases, while the zinc silicate nanoparticles look more or less amorphous. Generally we observe an increasing trend in the luminescence intensity, as the extent of doping increases. In case of Eu^{3+}, the luminescence decay time is shorter for higher doping. Detailed structural and optical analysis will be presented.

15:00 - 15:15
oral

Additional Absorption in the Strongly Scattering Absorbing Media

Vasil P. Yashchuk[1)], **Eugen O. Tikhonov**[2)], **Olga A. Prygodjuk**[1)], **Volodymyr I. Bezrodny**[2)], **M. V. Zhuravsky**[1)], **Olga V. Levandovska**[1)], **Yury D. Filatov**[3)]

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The strongly scattering colored and luminescence media are interested as coating with specific color characteristics and as active media of random lasers. Multiple scattering significantly influences the optical properties of the media. This work is devoted to simulation of the process of light propagation through the scattering medium under singular and multiple scattering regimes. The scattering medium is simulated by Monte-Carlo method as randomly located spherical particles dipped into the homogeneous substance. The interaction between light and particles is assumed to accord to geometrical optics that is applicable when particle size is larger than light wavelength.
The beam attenuation coefficient $k_\Sigma$was calculated versus the scattering particle concentration C_p and absorption coefficient of the interparticle substance k_a. The attenuation coefficient k_Σ monotonically grows with the C_p increasing. But it is essentially that k_Σ undergoes sharp change at certain particle concentration range when the absorbing interparticle substance is used. The change is sharpening with k_a increasing and is absent in the case of the non-absorbing substance $k_a=0$.
The sudden change was shown to appear at the particle concentration of single-to- multiple scattering regime transition. Out of the transition region the $k_\Sigma(C_p)$ is a stepless function. The sudden change of the $k_\Sigma(C_p)$ dependence is explained with additional absorption. It appears due to light path lengthening under the multiple scattering regime. The calculated dependencies are in good correlation with experimental results.

15:15 - 15:30
oral

Wavelength Tunable Random Lasers

Vasil P. Yashchuk[1,3)], **Eugen O. Tikhonov**[2)], **Olga A. Prygodjuk**[1)], **Volodymyr I. Bezrodny**[2)]

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Random lasers are principally new sources of stimulated emission where positive feedback realized by multiple light scattering. The laser is active the scattering medium itself without any cavity as well as the other optical elements. Hereupon the lasers distinctions are small gain volume and arbitrary shape.
In this work we investigated lasing parameters of random lasers made of dye polymer solution with embedded scattering particles. The continuous lasing wavelength tuning method was realized in this laser. The method is based on the dye lasing wavelength dependence on the luminescence reabsorption within

active medium [1]. Since the reabsorption is dependent on the active region depth it can be continuously changed by wedge-like sample displacing relatively to the focused pump beam.
We realized the continuous lasing wavelength tune within 8nm spectral range in the R6G random laser with silica scattering particles. The active medium was wedge-like shaped of 0.5cm length with thickness difference Δ d=0.05-0.5mm.
The tune range depends on wedge thickness difference Δ d and light penetration depth into the sample, which could be changed by scattering efficiency varying. The outside tune range is limited by luminescence and absorption spectra overlapping. The accuracy of lasing wavelength tune increases with pump beam cross section σ decreasing. Both lasing threshold and lasing intensity depend on σ and thickness of active medium excited. It is conditioned by two following reasons: effective gain coefficient dependence on the excited region size, and effect of reflection from the sample surfaces on the feedback formation.
[1] E.Tikhonov; Vasil P.Yashchuk, O.Prygodjuk, V.Bezrodny, Yu.Filatov, Functional Materials, v.11,p.142-145,(2003).

[ABSTRACT TRUNCATED TO 2000 LETTERS]

Coffee break

15:30 - 15:50

Afternoon session - continuedBioapplications and catalysis

15:50 - 17:20

Main Building, room 208

Maleic anhydride copolymers as multi-functional materials for advanced applications

15:50 - 16:20
invited oral

Gabrielle C. Chitanu[1), **Gabriela Aldea**[1), **Jean-Michel Nunzi**[2), **Adina G. Anghelescu-Dogaru**[1), **Irina Popescu**[1), **Dana M. Suflet**[1), **Adrian Carpov**[1), **Heikki Tenhu**[3)

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3) Department of Chemistry, University of Helsinki, A. I. Virtasen aukio 1, Helsinki FIN-00014, Finland

The multi-functional materials are one of the most recent topics, which were successfully developed.
Maleic anhydride copolymers are largely used as antiscale agents, phosphate substitutes in detergent compositions, dispersants, flocculants, soil conditioners or in biomedical application as drugs, drug carriers, or biomaterials. The properties of maleic copolymers as multi-functional materials were not yet developed, but it can be easily seen that they are particularly suitable for this purpose. Their chemical structure can be tailored either by the appropriate choice of the comonomer (hydrophilic or hydrophobic) or by the chemical reaction with suitable low molecular compounds bearing different functions: charged groups (which cause them to behave as polyelectrolytes), dyes or chromophores, bioactive molecules, LC moieties, and other. Moreover they can be obtained from easily accessible commercial monomers which are relatively cheap, by radical copolymerization in organic solvents using common initiators. The co-monomer can be N-vinylpyrrolidone (NVP), vinyl acetate (VA), methyl methacrylate (MMA), or styrene (St), given in the order of increasing hydrophobic character. From the results we have already obtained or are in progress it will be presented:
- layer-by-layer deposition from maleic polyelectrolytes and dyes;
- synthesis of new maleic copolymers derivatives containing dyes or chromophores for optical applications;
- systems for controlled delivery of bioactive substances;
- organo-inorganic composites or hybrids based on maleic acid copolymers and phosphates/hydroxyapatite;
- obtaining of microspheres from hydrophobically modified maleic copolymers;
- synthesis of new maleic anhydride copolymers with bulky/hydrophobic comonomers such as vinylnaphthalene, N-vinylcarbazole, N-vinylcaprolactame.

Acknowledgement: This research was partly supported by the Romanian Program MATNANTECH, projects no. C111 and C138.

Hybrid HAp- maleic anhydride copolymer nanocomposites obtained by in situ functionalisation

16:20 - 16:35
oral

Roxana M. Piticescu[1)], **Gabrielle C. Chitanu**[2)], **Mihaela Albulescu**[3)], **Maria Giurginca**[4)], **Madalina L. Popescu**[1)], **Witold Lojkowski**[5)]

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Composite materials offers a good balance between strength and stiffness and exhibit enhanced properties compared to each separately component. In the last decade researchers paid attention to the combination at nanometric scale between inorganic and organic phase due to the expected enhanced properties: hardness, stiffness, mechanical resistance and fatigue resistance. For biomedical composites the most important property is the biocompatibility of the materials. It was demonstrated that synthetic polymers such as: polyethylene (PE), polypropylene (PP), polyurethanes (PU), polytetrafluorethylene (PTFE), vinyl poly-chloride (PVC), polyamide (PA), polymethylmethacrylate (PMMA), polycarbonate (PC), polyethylenetereftalat(PET)are biocompatible and are currently used in medical field.
The aim of the paper is to answer to the question if maleic anhydride copolymer acts as a grain growth modulator or as a biocompatible functionalisation agent for hydroxyapatite.
Experimental work was developed on : nanocomposites synthesis, characterization and citotoxicity tests. Maleic anhydride copolymer - HAp nanocomposites were prepared by in situ functionalisation in hydrothermal conditions and were characterized by chemical quantitative analysis, XRD, FT-IR, SEM, specific surface area and picnometric densities.
Chemical bonding between copolymer carboxyl groups and calcium ions of HAp induced a peak at 1580 cm-1 in the FT-IR analysis. Following the evolution of this characteristic peak with the hydrothermal synthesis conditions (different temperatures and pressures) and corroborating the results with XRD and SEM analysis it was pointed out the copolymer grain growth modulator behavior concomittantly with the functionalization of HAp by the carboxylic groups of the copolymer.
Citotoxicity studies in vitro on mice fibroblast cultures were performed. The results proved the biocompatibility of new hybrid -polymer nanocomposites.

Formation of thalium sulfide layers on polyethilene (PE) sulfured in a solution of higher polythionic acid

16:35 - 16:50
oral

Ingrida Bruzaite[1)], **Vitalijus Janickis**[1)], **Ingrida Ancutiene**[1)], **Valentinas Snitka**[2)]

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TlxS layers of different composition on the surface of polyethylene are formated at first by sulfuration of PE in a solution of higher polythionic acid (H2S33O6) and then by treating it with alkalified up to pH 11,4 thallium(I) sulphate solution. Depending on the conditions of sulfuration and treatment with Tl(I) salt solution, red brownish or grey brown TlxS layers in the surface matrix of PE having different composition were obtained. A kinetic study showed that the amount of thallium in the sulphide layer increased with increasing the duration of PE sulfuration, the temperature of polythionic acid solution, time of sulfured PE treament in the solution of Tl2SO4 and the temperature of this solution. The stoichiometrical composition of layers according the data of chemical analysis varies from Tl0.3S to Tl2.5S. A phase composition of the layers obtained studied by the methods of X-ray photoelectron spectroscopy and X-ray diffraction. The data of Tl 4f7/2, O 1s and S 2p spectra showed that thallium is bonded with sulfur into TlS and Tl2S, but the Tl2SO4 and Tl(OH)3 are adsorbed on the layers surface too. Five thallium sulfide phases, TlS, Tl2S, Tl2S2, Tl4S3 and Tl2S5 were identified in the composition of the layers by X-ray diffraction but the maxima of TlS phase predominates in the diffractograms.The morphology of the TlxS layers during formation and growth was investigated by Atomic Force Microscopy.

Synthesis, characterization and electrocatalytical activity of capped platinum nanoparticles

16:45 - 17:00
oral

Sara Cavaliere[1,2], **Frédéric Raynal**[1], **Arnaud Etcheberry**[1], **Michel Herlem**[1], **Henri Perez**[2]

1) Institut Lavoisier, IREM, UMR 8637 CNRS-Université de Versailles, Versailles 78035, France

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The past decade has seen many improvements in the synthesis and characterization of nanometer-sized metal particles which have interesting potential applications in various fields, such as catalysis, optics and electronics. These nano-objects are almost exclusively stabilized by thiolate molecules, which limit their grown and allow their recovery as powders that can be re-dissolved. When particles are capped by bifunctional molecules, they can react with incoming molecules (over-grafting reactions) in order to modify their crown and then their characteristics. It is of special interest to follow the evolution of nanoparticles properties induced by crown modifications. Whereas most of the papers describing such an approach deal with gold nanoparticles, the present work reports on platinum nanoparticles.
We synthesized 4-mercaptoaniline functionalized platinum particles of 2 nm diameter and we reacted them with 2-thiophenecarbonyl chloride. The derivatized particles were dissolved in DMSO and gave long term stable solutions. The Langmuir-Blodgett technique was then used to build up stable Langmuir films and Langmuir-Blodgett films. The latter were build up on various substrates which allowed characterization by IR, XRD, TEM, XPS.
The electrocatalytical behaviour of the ultra-thin films towards oxygen reduction were investigated in acidic medium. It revealed a direct activity without any previous activation treatment in spite of the presence of the organic shell at the surface of the particles. Furthermore, using XPS we evidenced that the organic crown was not significantly destroyed upon prolonged cycling.
These preliminary results open a way to the study of original and versatile platinum based nanocomposites and suggest interesting potentialities in term of application to fuel cells.

Precipitation of Nickel Hydroxides from Nickel Dodecylsulfate

17:05 - 17:20
oral

Jean-Francois Hochepied[1], **Corinne Coudun**[1]

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Widely used as positive electrode in alkaline rechargeable batteries, nickel hydroxide has received increasing attention during the last decades, and various preparation methods have been developed in order to improve its electrochemical performances. The main features to deal with are particle cristallinity and morphology.
Here we develop classical precipitation techniques applied to nickel dodecylsulfate $Ni(DS)_2$ precursor. This precursor forms direct micelles in water in the studied range of concentrations. Hence it concentrates the reactive cations near a charged surface, which may have significant effect in nucleation (high local supersaturation) and templating effects. Besides, impurities-free hydroxides are rarely obtained with classical counter ions (nitrates or sulfates). As a counterion, dodecylsulfate is too big to be captured in the hydroxide structure, even between the brucite layers. In pH controlled double jet precipitation with soda, the pure phases α, β_{bc} (badly crystallised) and β (well crystallised) may be obtained in basic conditions, whereas morphology is kept similar (platelets). In the same conditions, classical salts never lead to α phase and particle size and morphology are pH dependent.
Now if we consider hydroxide precipitation by ammonia decomplexation via heating, $Ni(DS)_2$ lead to well-calibrated stacks of β-$Ni(OH)_2$ nanopancakes (200nm in diameter and length along the stacking direction) whereas classical salts lead to micrometric macroporous particles constituted by thin interconnected walls.
As a conclusion $Ni(DS)_2$ allows drastic changes if compared to classical salts: depending on the process we may have an effect on crystal structure control (double jet precipitation with soda) or on morphology (ammonia decomplexation). This effects may be explained respectively by the existence of a high local nickel concentration and templating by the surfactant.

Wednesday, September 8th

Morning sessionPiezoelectric applications

09:00 - 10:30

Main Building, room 208

Nanostructuring of Electroceramics: Phase Stabilization Induced by Nanoparticles

09:00 - 09:30
invited oral

PAULA M. VILARINHO[1)]

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Pb(B'1-xB"x)O3 is currently an important family of functional materials. Their value added comes from the excellent dielectric, piezo-, pyro- and ferroelectric properties that they exhibit, being very attractive for multilayer capacitors, piezoelectric transducers, infrared sensors, electrooptic devices, memory applications, to operate under different frequency / temperature conditions. A successful application highly depends on the easiness to adapt the material to the required fabrication technology and to integrate it in a useful and reliable device. Low synthesis temperature that ensure phase purity and minimise interdiffusion is a key aspect for manufacturing Pb(B'1-xB"x)O3 bulk ceramics and films. However it is well known that during synthesis a stable pyrochlore phase (A2B2O7-d) with low dielectric permittivity precedes the formation of the perovskite (Pe) and if it remains degrades the material dielectric response. The crystallization temperature to obtain monophasic Pe materials can then limit their practical application. In this work a new methodology to synthesize Pb(B'1-xB"x)O3 compounds is presented. It combines maximization of crystalo-chemical and thermodynamics requirements for Pe phase stabilization and optimization of the phase formation reaction kinetics by supplying highly reactive nanometric Pe nucleus. It is expected that nanometric Pe particles will act as template for synthesis of Pe at low temperatures, even in those systems in which monophasic materials were reported to be extremely difficult to be obtained. The effect of nanopowders on Pe phase formation is analyzed in two systems: Pb(Zn1/3Ta2/3)O3(PZTa) ceramics and PZT films. For comparison similar materials are prepared by conventional methodologies. XRD, SEM and TEM are used to evidence the role of nanoparticles on Pe phase nucleation and growth. Through a systematic study of the electric response correlation between materials morphology and macroscopic properties is established.
[ABSTRACT TRUNCATED TO 2000 LETTERS]

Pb(Mg1/3Nb 1/3)O3-PbTiO3 Nano-powders by Continuous Attrition Milling for Ceramic Texturing

09:30 - 09:45
oral

Mai PhamThi[1)], **Erling Ringgaard**[2)], **Annette F. Pedersen**[2)]

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Ceramic texturing via Template Grain Growth (TGG) consists in orientating a number of large anisotropic template particles in an ultrafine particle matrix in the green state by tape casting. During sintering, densification of the matrix followed by grain growth consumes the surrounding matrix grains and creates a crystallographically oriented ceramic. Reactivity of the ceramic matrix is the key condition during grain growth. Therefore, large batches of nanopowders are necessary for the textured ceramic process. This work presents the industrial preparation of PMN-PT nano-particles by using the Labstar instrument. PMN-PT powder was synthesized via the columbite precursor method by calcination of oxide precursors at 1050C, mixing and milling with PbO and TiO2 and re-calcining at 800C to form the perovskite powder. Ultrafine and nano-powders were prepared by using attrition milling. Conventional attrition and continuous attrition milling will be performed and compared. Nano-powders will be characterized by TEM, XRD and specific surface area. Influence of grain size on relaxor ceramic properties will be presented

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Microstructural characterization of BaTiO3 ceramic nanoparticles synthesized by hydrothermal technique

09:45 - 10:00
oral

Xin H. ZHU[1,2)], **Jian M. ZHU**[2)], **Shun H. ZHOU**[2)], **Zhi G. LIU**[2)], **Nai B. MING**[2)], **Dietrich Hesse**[1)]

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2) National Laboratory of Solid State Microstructures, Department of Physics, Nanjing University (NJU), Hankou Road 22#, Nanjing 210093, China

In recent years electronic devices such as multilayer ceramic capacitors (MLCs) are urgently required to be miniaturized to meet the high integration demands of microelectronic devices. High dielectric constant materials with ultra-fine grains are highly needed to achieve a thinner dielectric layer. To manufacture reliable MLCs, agglomerate-free, high crystalline and superfine ceramic particles with high purity are required. Barium titanate (BaTiO3) has good dielectric and ferroelectric properties, and is widely used in MLCs. Although the bulk properties of BaTiO3 ceramics have been widely investigated in the past, more

recently, there has been a renewal of interest in nanoscale particles of this material because their electrical properties are strongly dependent upon the grain size and the crystalline structure. Nanocrystalline BaTiO3 particles have been prepared by various wet chemical methods. Among which the hydrothermal method presents some particular advantages such as obtaining high-crystallized powders with narrow grain size distribution and high purity (without heat treatment at high temperature), the yield of a well-defined composition, and a better control of grain size and morphology. In this work, both cubic and tetragonal BaTiO3 nanoparticles (with size of 20 to 100 nm) have been prepared by hydrothermal technique using as-prepared titanium hydroxide and barium hydroxide as starting materials. The microstructure (crystal structure, grain size and distribution, grain morphology, domain structure and microstructural defects) of the tetragonal and cubic phases of nano-sized BaTiO3 particles is examined by XRD, SEM, and (HR)TEM, respectively. The related results will be discussed and presented.
[ABSTRACT TRUNCATED TO 2000 LETTERS]

Spark Plasma Sintering of nano-sized ZrO_2-Al_2O_3-Ti(C,N) composites

10:00 - 10:15
oral

Kim Vanmeensel[1)], **Guy Anné**[1)], **Dongtao Jiang**[1)], **Jef Vleugels**[1)], **Omer Van der Biest**[1)]

1) K.U.Leuven, Department of Materials Science and Engineering (KUL, MTM), Kasteelpark Arenberg 44, Heverlee (Leuven) 3001, Belgium

Spark Plasma Sintering (SPS) permits a very fast densification of ceramic composites, hereby minimising grain growth when the sintering conditions are precisely controlled. This research investigates the possibility to densify ZrO_2-Al_2O_3-Ti(C,N) nanocomposite powder mixtures into fully dense materials using the SPS technique. Mechanical properties as well as electrical conductivity are evaluated as a function of sintering conditions and composite composition.

Coffee break

10:30 - 11:00

Morning session - continued

Main Building, room 208

11:00 - 12:30

NANOSIZED FERROELECTRIC CRYSTALS OBTAINED BY A SELF-PATTERNING METHOD

11:00 - 11:15
oral

Izabela Szafraniak[1,2)], **Ming-Wen Chu**[2,3)], **Marin Alexe**[2)], **Dietrich Hesse**[2)]

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The nature of the ferroelectric size effects has been discussed for decades, however, a unified picture is still missing. It seems that interfacial defects play an important role in size effects of ferroelectrics [1]. To investigate this issue we have prepared epitaxial $Pb(Zr_xTi_{1-x})O_3$ nanocrystals with different Zr/Ti ratio (x between 0 and 0.52), in this way providing a lattice mismatch with the $SrTiO_3$ substrate between 3.4 % and 0.2%.
Epitaxial PZT nanoislands were prepared by chemical solution deposition onto conductive (001) single-crystal STO:Nb substrates. This method allowed us to prepare uniform and good quality structures and to tune the size of the final structures (i.e. their height can be between 5 and 25 nm). A cross-sectional high-resolution transmission electron microscopy (HRTEM) analysis showed that the PZT nanoislands grown on STO have a truncated-pyramid morphology. The islands are single-crystalline and single-c-domain. Using HRTEM the nature of the misfit dislocations has been analyzed. It turns out that they extend into a PZT region with dimensions as large as 4 nm in height and 8 nm in width. Since ferroelectricity is a co-operative phenomenon of a sufficient number of regular noncentrosymmetric unit cells, this significant ratio points to a potential long-range influence on the ferroelectric properties of the PZT nanoislands. Probing the polarization of a large number of bare nanoislands by piezoresponce force microscopy it was found that the PZT (x=0.52) nanoislands with a height of 9 show an apparent polarization instability. By contrast, the same PZT islands with a height of 20 nm show well-developed ferroelectricity, as also do tetragonal, epitaxial $PbTiO_3$ nanoislands 9 nm in height and free from misfit dislocations at the interface.
[1] M.-W. Chu, I. Szafraniak, R. Scholz, C. Harnagea, D. Hesse, M. Alexe, U. Goesele, Nature Materials,

3 (2004) 87.

11:45 - 12:00
oral

Surfactant protective layers on the surface of iron particles

Sofia Mikhailova[1)]

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Finely dispersed iron particles are widely used for magnetic fluids, particulate composites, magnetic microcarriers of biologically active substances etc. The environmental stability of the particles is determined by the peculiarities of the physicochemical structure of self-assembling surfactant layers along with the formation of the surfactant-metal particle interface.
Hence, the surface phase structure and physicochemical structure of the stabilizing layers on the surface of iron particles obtained at different stages of high-temperature reduction in H_2 flow have become the focus of the present investigation performed by means of the XPS, AFM and Mössbauer spectroscopy. Oleic acid was used as a stabilizing agent. For comparison, hexamethylenediamine and acrylamide were also taken as stabilizerz. Particles for Mössbauer spectroscopy study were prepared using an original procedure with the particle "nuclei" from ^{56}Fe and with the particle surface layer, enriched in ^{57}Fe. It follows from Mössbauer spectroscopy data that after partial reduction in H_2 flow disordered or highly distorted $^{57}Fe_3O_4$ phase is seen to be present on the surface of particle "nuclei". The particles are essentially ^{56}Fe with the ^{57}Fe surface layer at the end of reduction. According to the XPS data, all stages of reduction are characterized by the presence of an oxide layer, with its nature dependent on the reduction stage. The peculiarities of the physicochemical structure of the stabilizing layer on the base of oleic acid for the particles obtained on different stages of reduction were clarified using XPS. Also, the structure of the protective layers based on nitrogen-containing organic compounds was studied for the final particles. The corrosion study have shown that it is the structure of stabilizing layers that will determine the iron particle stability in the environment.
[ABST
[ABSTRACT TRUNCATED TO 2000 LETTERS]

12:00 - 12:15
oral

Control of Size in ZnO Nanoparticles Prepared by a Salt-Assisted Spray Pyrolysis Method

Camellia Panatarani[1)], **Wuled Lenggoro**[1)], **Kikuo Okuyama**[1)]

1) Hiroshima University (Hirodai), Kagamiyama 1-4-1, Higashi Hiroshima, Hiroshima 739-8527, Japan

Spray pyrolysis (SP) is an attractive method for preparing uniform size and composition of particles because of its high production rate, continuous unit operation and simple apparatus. However, this method is limited for the production of submicron particles. It is difficult to produce nanosized of particles efficiently because the concept of the SP process deriving one particle from one droplet. The addition of salt-flux such as $LiNO_3$ in the spray pyrolysis for producing smaller (nano) particles has been developed in our laboratory. In this study, $LiNO_3$ was added to a precursor solution of zinc acetate dihydrate prior to its atomization by means of an ultrasonic transducer. The utilization of $LiNO_3$ salt on the preparation of ZnO by spray pyrolysis method is efficient to produce nanosized and enhance the crystallinity of the product. Regarding the influence of $LiNO_3$, at the same processing condition, the mean particles size of $LiNO_3$ assisted product is less than 1/9 times the mean particles size of conventional SP. Solid (dense), non-crinkle single crystalline ZnO particles having nanometer size were successfully obtained after washing the product. In addition, by using the same technique, the particle size can be controlled from 100-26 nm by operating temperature used and the residence time of the particles in the reactor.

12:30 - 14:00

Lunch break

19:00 - 21:00

Poster session 2

Non Oxide Spherical Particle Synthesis by Liquefied Petroleum Gas Firing

poster G-15

Yasumasa TAKAO[1)]

1) National Institute of Advanced Industrial Science and Technology (AIST), Shimoshidami, Nagoya 463-8560, Japan

Synthesis of non-oxide materials includes solid-phase grinding, liquid building-up, plasma, and CVD. The raw powder of the sintered body is commercialized by solid-state synthesis; however, it is non-spherical in shape and its size is below the submicron range. In this synthesis, a prolonged heat treatment at high temperature, under a controlled atmosphere is indispensable. Such a treatment leads to a long grinding process in order to crush the heated aggregate powder. This results in the non-spherical shape of the resultant and leads to difficulties in synthesizing large-sized powder. Since the non-oxide materials have high intrinsic thermal conductivity, they have several potential uses apart from being used as sintered body, such as ceramic fillers. However, spherical powders above submicron levels are indispensable for this application. The ceramic filler powder is commonly produced by liquefied petroleum gas (LPG) firing. The advantages of this direct firing synthesis are high sphericity of product, high controllability of product size, rapid reaction rate (in seconds), productive and inexpensive continuous gas-phase flow reactor (non-batch processing). Despite these advantages, LPG firing has not been utilized in the synthesis of non-oxide materials by reactions in which oxygen has to be included as reactant.

In this study, we found that, conceptually, some Al nitridation syntheses via LPG firing could occur. The LPG firing method can provide a gas diffusion nitridation mechanism, and can therefore produce Al-oxynitride (AlON) and AlN spherical fine particles.

Self-organization and dynamic characteristics study of nanostructured liquid crystal compounds

Natalie V. Kamanina[1)], **Yulia A. Zubtsova**[2)], **Vladimir A. Shulev**[2)], **Mariya M. Mikhailova**[1)], **Andrey I. Denisyuk**[3)], **Igor Y. Denisyuk**[1)] poster G-16

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Self-organization in dispersed liquid crystal compounds based on the charge-transfer complexes between an organic donor (monomer, polymer, nanoparticles) and a fullerene has been investigated. 10 μm nematic liquid crystal cells with the fullerene complexes based on 2-cyclooctylamine-5-nitropyridine, polyaniline, and phthalocyanine nanoparticles have been studied. It was found that the exposure in a few days resulted in the self-arrangement of the nematic liquid crustal system with the fullerene complex. The microscopic study allowed the transition to be revealed from the nematic phase to the smectic one. For all structures the switch-on time close to 50-100 μs has been obtained. It follows from our results that the mechanism of the accelerated rotation of the LC dipoles is likely to be caused by the order parameter change during the transition from the nematic to the smectic induced the fullerene-containing complex introduction. The complex formation was supported by the data of absorption and luminescence spectra, mass-spectroscopy, non-linear measurements of light-induced effects, and a quantum-chemical simulation. Potentials of these systems for laser optics, medicine, and display application have been examined.

Quantum localization on carbon nanoparticles: Activated Carbon Fibers studied by EPR and electric resistivity measurements

Mateusz Kempinski[1)], **Jacek Kaszyński**[2)], **Małgorzata M. Śliwińska-Bartkowiak**[1)], **Wojciech Kempiński**[2)] poster G-17

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2) Polish Academy of Sciences, Institute of Molecular Physics, Mariana Smoluchowskiego 17, Poznań 60-179, Poland

Activated carbon fibers (ACFs) possess nanocrystalllites made up of graphene sheets that create conducting particles, nonuniformly distributed in space. The nanocrystallites are about 2.5 nm. Existence of voids makes ACFs a porous system, with specific surface area of 3000 m^2/g. In such porous material with conductive particles it is necessary that the grains are linked structurally in order to hold sample together. But the linkage is not always electrical.

We report results of the temperature properties of electric resistivity of ACFs, where the model of granular metallic systems [1] is proposed for the electric conductivity of ACFs. For this model, dc electrical

resistivity vs temperature is described as $\rho(T) = \rho_0 \exp[(T_0/T)^{1/p}]$, where p = 2, ρ_0 is a proportionality constant and T_0 varies between 10^2K and 10^4K depending on metallic volume fraction.
EPR measurements of ACFs show localization of paramagnetic centers on nanocrystallites below 100K. It confirms the granular metal model for ACFs.

[1] B. Abeles et al. adv. Phys. 24 (1975) 407

STUDY OF THE SILICON NANOPARTICLES PRODUCED BY LASER ABLATION

poster G-18

Constantin GRIGORIU[1)], **Ionut NICOLAE**[1)], **Victor CIUPINA**[2)], **Gabriel PRODAN**[2)], **Hisayuki SUEMATSU**[3)], **Kiyoshi YATSUI**[3)]

1) National Institute for Lasers, Plasma and Radiation Physics (NILPRP), Atomistilor Str.111, Bucharest R-76900, Romania

2) "OVIDIUS" University, Mamaia 124, Constanta 8700, Romania

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Silicon nanocrystals have raised hopes in applications for Si-based devices. Our interest is synthesis of Si/SiO_2 nanoparticles having dimensions < 10 nm, with the final goal "Quantum Dots" for specific application in biology, micro and nanoelectronics. We present the studies of nanometric silicon powders produced by laser ablation. The effects of laser wavelength, fluence, and gas pressure, on the nanoparticle structure and size distribution have been investigated by transmission electron microscopy.
The nanoparticles have been generated by ablation of a pure silicon target with Nd:YAG laser, second and third harmonic, 532 and 355 nm, pulse duration 5-6 ns, fluence 4-8 J/cm^2. Argon and helium have been used in the pressure range of 250-550 mbar. The nanoparticles have been collected on a filter (pores 100 nm) and analyzed as prepared, without any precaution or special method for deposition on the TEM grids.
The nanoparticles have been in the range of 2-12 nm, 30 percent of them being of 2-4 nm in diameter. The TEM images and SAED patterns reveal spherical silicon nanoparticles with a crystalline silicon core (diamond structure) covered with an amorphous SiO_2 layer (1.2-1.5 nm thick). Some of the clusters are loosely agglomerated, some present chains of welded particles. The size and size distribution of the powders are strong functions of the specific process parameters (laser wavelength, fluence and gas). The experiments showed an optimum at 355 nm, 8 J/cm^2, in helium at 400 mbar, the particles being smallest, with a much narrower distribution.

cBN composites with nanosized binding phase

poster G-19

Wioletta Gorczyńska-Zawiślan[1)], **Ewa Benko**[1,2)], **Piotr Klimczyk**[1)]

1) Institute of Metal Cutting, Wrocławska 37A, Kraków 30-011, Poland

2) University of Bielsko-Biala, Willowa 2, Bielsko-Biała 43-309, Poland

The cubic boron nitride (cBN) is the second hardest material next to diamond. Because of its many excellent physical and chemical properties cBN is even considerably superior to diamond in two areas where diamond‘s performance is poor: its abrasion resistance with ferrous alloys, such as steels and its oxidation resistance. The cBN-ceramics shows high mechanical properties and cutting tools made from it are being widely used for cutting hardened steels, cast iron and nickel-based superalloys. Ti and their compounds are widely used as a binding phase and as a layered phase in the cBN composites. In the present work cBN-TiN composites were investigated. These composites were made using HPHT technique (p=8 GPa, T=1750 ^{0} C). The TiN binding phase was used in two forms: as micro and nanomaterials. From thermodynamical calculations it followed that formation of new phases in the cBN-TiN composites is not possible in the investigated conditions. XRD investigations confirmed that no new phases were formed in the cBN-TiN systems studied. Surface morphology of BN-TiN nanocomposites was observed by scanning electron microscopy. The structure of these composites is compact; TiN phase is uniformly distributed between cBN grains. Hardness was measured by Vickers method using an indentation load of 9.81 N. Hardness of the investigated samples depends on the volume and grain size of the binding phase. Young's modulus of elasticity was measured. It was found that its value depends on the grain size of the TiN phase.

HiPCO single-wall carbon nanotubes under pressures up to 50 GPa: Electrical properties

poster G-20

Olga V. Narygina[1], **Yana Y. Volkova**[1], **Alexey N. Babushkin**[1], **Elena D. Obraztsova**

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Single-wall carbon nanotubes (SWNT) produced by HiPCP method and purified by thermal oxidation in air have been studied by impedance spectroscopy. The purity of nanotubes was estimated as 99% [1]. The dc conductivity measurements were carried out at temperatures 77-450 K. High pressure has been generated in the diamond anvil cell (DAC) with anvils of the "rounded cone-plane" type made of synthetic carbonado-type diamonds. These anvils are good conductors, permitting measurement of the resistance of samples placed between the anvils in the DAC by using the anvils as the electrical contacts to the sample. The activation energy of the SWNT was estimated from the temperature dependences of resistivity.Temperature dependences of HiPCO SWNT resistivity were plotted and analysed. Activation energy dependences of pressure were analysed.

This work was supported in part by grant BRHE EK-005-X1 (Ural research educational center "Advanced materials").

[1] V. Karachevtsev et al, Photoelectric and optic properties of fullerenes, 2002, 179.

Preliminary study on application PE filler modified by radiation

Izabella Legocka[1,2], **Zbigniew Zimek**[1], **Krzysztof Mirkowski**[1], **Andrzej Nowicki**[1] poster G-21

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2) Industrial Chemistry Research Institute (ICRI), Rydygiera 8, Warszawa 01-793, Poland

Mineral filler: magnesium oxide (MgO) has been modified by grafting process initiated by high energy (9 MeV) electron beam treatment. Many vinyl monomers as methyl methacrylate (MMA), maleic anhydride (MA) were used as modifying compounds. The yield of momomers grafting on MgO have been determined as dose depended with optimum at dose 20 - 30 kGy. Fillers have been milled after grafting and its properties have been investigated by FTIR, DSC and TG methods. Modified fillers have been used in compositions with polyethylene (LDPE). SEM was used for investigation of the structure of obtained samples. Mechanical and some thermal properties of selected samples have been measured and discussed. The work present preliminary data of influence of dose level and monomer type on properties of the samples. Generally, the filled polyethylene has been characterized by better dispersibility and betters some mechanical properties. The works will be continued and its results will be useful in similar work on filling of polymers with nanoparticles.

Polyurethane-boehmite nanocomposite

Ewelina A. Zawadzak[1], **Zbigniew Florjanczyk**[2], **Andrzej Wolak**[2], **Bożena Bigos**[2], **Joanna Ryszkowska**[1] poster G-22

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

Polyurethane nanocomposites filled up with boehmite modified by triethylphosphate are the new class of materials. Introduction of organic substituent leads to desintegration of boehmite molecues and results in obtaining nano-filler. Addition of the compatible substituent allows homogenic distribution of nano-filler in polymer matrix and improves properties of origin polymer.
In this study, effect of boehmite and its modification products on structure and properties of polyurethane were investigated. Tensile strenght, Young modulus, grindability and structure analysis of prepared composities were studied. Structure analysis was made by Atomic Force Microscopy. Nanofillers grain dimension analysis was conducted in Transmission Electron Microscopy.

Laser-induced size and shape transformation of silver colloidal nanoparticles

Nikolai V. Tarasenko[1], **Andrei V. Butsen**[1], **Gvidona P. Shevchenko**[2], **Ilona M. Yakutik**[2] poster G-26

1) Institute of Molecular and Atomic Physics (IMAPh), 70 Scaryna Ave., Minsk 220072, Belarus

2) Institute for physical chemical problems of the Belarusian State University, Minsk, Belarus

Spherical silver colloidal nanoparticles 10-30 nm in size prepared in gelatin stabilized ammonia-tartrate electroless deposition solution were exposed to irradiation of a pulsed laser radiation at 532 nm, 400 nm and 266 nm. The unfocused beams of the second (532 nm) and the forth (266 nm) harmonics of Nd: YAG laser operating at 10 Hz (pulse width 15 ns) as well as of a Ti:sapphire laser (its second harmonic output) at 400 nm were used.
The morphological changes of silver nanoparticles caused by the laser irradiation were investigated as a function of incident laser fluence. According to TEM evidence, after laser irradiation at 40 mJ/cm^2 the size and shape of nanoparticles was the same as the initial colloids. However, the morphology of nanoparticles was changed by laser irradiation above 100 mJ/cm^2. TEM investigation showed that the initial small silver particles irradiated at 250 mJ/cm^2 with 3000 pulses (for 5 min) transformed to the right-angled crystals 1400-1500 nm in size probably via fusion of photo-thermally melted nanoparticles. Electron diffraction data evidence that these crystals are not compact, but made up of great many small silver particles. The relative amount of the right-angled particles was estimated to be approximately 20%. At laser fluences higher than 350 mJ/cm^2 spherical particles 70-180 nm in size were formed instead of the right-angled particles. It should be emphasized that the fine 10-30 nm-sized particles were present in the solution in all above-mentioned cases.
The distinct changes in absorption spectra of silver colloids due to morphological changes of nanoparticles were also observed.
Thus, in this paper we show the possibility to change the morphology of silver nanoparticles under laser irradiation of different fluences. The conditions favoring the transformation of nanoparticles shapes and sizes have been determined.

Sensitivity of carrier spectrum in semiconducting nanowire to adsorbed molecules

poster G-27

Victor A. LYKAH[1], **Evgen S. SYRKIN**[2]

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2) Institute for Low Temperature Physics, 47 Lenin ave., Kharkov 61103, Ukraine

Optical and conducting properties of nanoobjects are conditioned with a set of energy quantum levels and filling of these levels with carriers. Tunneling through an individual nanowire is extremely sensitive to the charge state and to the appearance of adsorbed layers.
The present work considers quantum levels of an uncompensated charge carrier inside a perfect semiconductor quantum wire covered by gas of an adsorbed molecules with intrinsic electric dipole moments. The quantum wire may be a usual intrinsic semiconductor or a carbon nanotube with large mean free path. The molecules are redistributed under inhomogeneous carrier's electric field, as a result the stationary Schrodinger equation becomes nonlocal and nonlinear. In the limit of relatively small deviation of the molecules concentration the longitudinal quantization is reduced to the spectral problem for nonlinear Schrodinger equation in the rectangular well. Variables are divided and solution is written in terms of elliptic functions. The selfconsistent system of equations could be reduced to closed set of two transcendent equations for elliptic modulus and the wave number (that gives the energetic spectrum of the carrier) as functions of complete elliptic integrals of the first and second kind.
The main features of solution: 1) the higher the interaction is, the more the nonlinearity is, 2) the strongest effect of the nonlinear interaction does occur for lowest levels while the effect for top levels disappears, 3) the effect should be more pronounced for heavier holes. 4) If the adiabatic approximation is satisfied the carrier's spectrum changes with retard which depends on diffusion time.
For the strong interaction all states of the carrier are localized and could be responsible for the decrease of conductivity in chemisorption wire sensors.

Surfactant-Assisted Low Temperature Synthesis of Shape-Controlled TiO_2 Nanoparticles

poster G-28

Jin Young Kim[1], **Hyun Suk Jung, Sung-Hun Youn, Kug Sun Hong**

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

Anatase phase TiO_2 nanoparticles were synthesized by hydrolysis and peptization of the titanium tetraisopropoxied (TTIP) at a temperature as low as 80^{o}C and the effects of surfactant (cetyltrimethylammonium bromide, CTAB) on the shape of particles were investigated. The addition of surfactant was found to enhance the 1-directional growth of precipitates during the peptization process and increase the aspect ratio of resulting particles. Selected area diffraction (SAED) pattern and high resolution transmission electron microscopy (HRTEM) image revealed that the nanorods are single crystalline in nature and preferentially grown along [110]. X-ray diffraction confirmed that the synthesized powders were pure anatase phase regardless of the addition of surfactants. Bandgap and photocatalytic properties of nanorods were also characterized compared to those of spherical nanoparticles.

Effect of pamlitic acid on carbon nanotubes - epoxy resin composites

Sophie Barrau[2], **Philippe Demont**[2], **Emile Perez**[1], **Alain Peigney**[2], **Christophe Laurent**[2], **Colette Lacabanne**[2]

1) IMRCP, UMR CNRS 5623, Toulouse, France

2) CIRIMAT, UMR CNRS 5085 (L2P-LCMIE), Toulouse, France

poster G-29

As most polymers, epoxy resins are electrical insulators. Air frictions can damage the materials because of charges accumulation. The preparation of composites with conductive fillers allows to solve this problem for a sufficient rate of charge in the matrix. Using carbon nanotubes (CNTs) as a charge offers an attractive way to improve the electrical properties of such composites.
CNTs, mostly single- and double-walled, were synthesized by CCVD [1] and obtained in suspension in HCl after catalytic particles dissolution.
In a first time, an experimental procedure was set up in order to prepare CNTs - epoxy resin composites containing few wt % of CNTs. Scanning electron microscopy pictures (SEM) show an homogeneous dispersion of CNTs bundles. A study of the nanocomposites electrical properties was performed in order to characterize an insulator/conductor transition. The measurements of the complex conductivity were carried out using a broadband dynamic dielectric spectrometer in the frequency range 10^{-2} - 10^{6} Hz and above ambient temperature. The dc conductivity σ_{dc} exhibits a percolation threshold at 0,3 wt % at room temperature with a conductivity about 10^{-4} S.cm^{-1} above 2 wt % of CNTs. The percolation threshold is found to be independent of temperature.
To improve CNTs dispersion, we added, in a second time, an amphiphilic molecule : the palmitic acid. The hydrophobic part is adsorbed onto the nanotube surface. The hydrophilic head induces electrostatic repulsions between nanotubes and then preventing their aggregation [2]. Electrical measurements displays an percolation threshold decrease and SEM pictures show CNTs essentially individuals. This experimental procedure appears promising for future.

[1] E. Flahaut, A. Peigney, Ch. Laurent, A. Rousset, J. Mater. Chem. 2000, 10, 249.
[2] S. Barrau, P. Demont, E. Perez, A. Peigney, Ch. Laurent, C. Lacabanne, Macromolecules 2003, 36, 9678.

Grain Size and Grain Size Distribution of Nanocrystalline Pr-doped Zirconia Powders Obtained in High Pressure Microwave Reactor

Agnieszka Opalińska[1,3], **Roman Pielaszek**[1], **Cristina Leonelli**[2], **Hubert Matysiak**[3], **Witold Lojkowski**[1]

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poster G-30

A novel microwave reactor was used for hydrothermal synthesis of nanocrystalline praseodymium - doped zirconia powdres.
Properties of zirconia and Pr - doped zirconia powders strongly depend on shape, grain size, grain size distribution, phase composition and degree of crystallinity. The microwave driven hydrothermal synthesis permit to precisely control the reaction regime (time, power, pressure) and in consequence provide to expected properties of the resulting nanopowders.
This method is versatile permitting to obtain powders in the range 5 - 100 nm in a few minutes.
In this work we investigated the effect of process parameters on grain size and grain size distribution. It was determined using two methods. The first one was based on analysis of transmission electron microscopy (TEM) images. The second one was based on analysis of the shape of x-ray diffraction (XRD) peaks. The two methods yielded similar results.

Sintering temperature effect on structure and properties of Al2O3/Ni-P composites with interpenetrating phases

poster G-31

Jakub Michalski[1)], **Michal J. Wozniak**[1)], **Katarzyna Konopka**[1)], **Jerzy Bielinski**[2)], **Stanisław Gierlotka**[3)], **Krzysztof J. Kurzydlowski**[1)]

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3) Polish Academy of Sciences, High Pressure Research Center (UNIPRESS), Sokolowska 29/37, Warszawa 01-142, Poland

A ceramic metal composite Al_2O_3/Ni-P was obtained by hot pressing of alumina powder, covered by Ni-P nanoparticles trough chemical plating. Room temperature, 600^{o}C and 1000^{o}C were used in these experiments to consolidate the coated powders. The consolidated and sintered specimens were investigated by SEM, TEM/HRTM, MFM (magnetic force microscope) and hardness test. They revealed that this fabrication method results in a structure of interpenetrating phases with high electric conductivity. It has been also found that samples consolidated at room temperature and sintered at 600^{o}C maintain nanometric grain size of the metallic phase whilst the grains of Ni-P sintered in 1000^{o}C are re-crystallized. The hardness was also investigated, and is discussed in terms of fabrication temperature and structure of obtained composites.

Thursday, September 9th

09:00 - 10:30

Morning sessionTransition metal oxides

Main Building, room 208

Phase stability in nanocrystalline zirconia

09:00 - 09:30 invited oral

Gianguido Baldinozzi[1)], **David Simeone**[1,2)], **Dominique Gosset**[1,2)], **Michael Dutheil**[2)]

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2) CEA Saclay, DMN/SRMA (CEA), CE Saclay, Gif-sur-Yvette 91191, France

Zirconia can be considered one of the most important ceramic materials because of the large range of industrial applications (catalysis, coatings, spacecraft shieldings, paint additives, oxygen sensors, fuel cells, nuclear fuel matrix, alternative high permittivity material to replace silicon oxyde as gate dielectric in MOS devices, ...).
Many of these applications require the use of zirconia in a nanocrystalline form. Several experiments point out that the thermodynamic properties of nanocrystalline solids are particle-size dependent. Size-related effects like lowering of the melting temperature and displacement of the phase boundaries can be predicted. Zirconia can be considered a textbook example for describing these effects. It undergoes several polymorphic transformations with the change of external parameters (T, p, ...). We will discuss in particular the behaviour of the tetragonal to monoclinic martensitic phase transition within the Landau theory framework, pointing out the peculiar effects related to the small grain size of the nanoparticles. Neutron diffraction experiments will illustrate the validity of these arguments and provide some insight to understand the behaviour of zirconia nanocrystals in severe environments as in nuclear reactors or in space applications.

Luminescence of ZrO_2 nanocrystals

09:30 - 09:45 oral

Donats Millers[1)], **Witold Lojkowski**[2)], **Larisa Grigorjeva**[1)], **Agnieszka Opalińska**

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

The time-resolved luminescence have been studied for undoped and doped ZrO_2 nanocrystals. The undoped and Pr doped nanocrystals had dominant tetragonal structure with small admixture of monoclinic fraction. The yttrium stabilized nanocrystals had cubic structure. The comparison of the luminescence from different structure nanocrystals was possible. The luminescence dependence on temperature for undoped ZrO_2 nanocrystals shown that both - nonradiative transitions and luminescence center destroying are responsible for luminescence quenching. ZrO_2:Pr nanocrystal luminescence shown dominant emission from Pr^{3+}, indicating that intrinsic excitation in ZrO_2 are very mobile and efficient energy transfer from matrix to dopand takes place. The luminescence dependence on temperature for ZrO_2:Pr differs from that for undoped nanocrystals. The luminescence from cubic structure ZrO_2 nanocrystal somewhat differs from this of tetragonal structure. The possible reasons are studied. On the one hand the yttrium admixture might be responsible for differencies observed. On the other hand IR absorption spectra indicates that the uncontrolled molecular impurities content in nanocrystals is different. The IR absorption spectra for ZrO_2 and ZrO_2:Pr indicates the same molecular impurities (however amount of them was different) whereas yttrium stabilized nanocrystals IR spectra shown additional groups of absorption lines.

Spectroscopic Ellipsometry and Raman Studies on Sputtered TiO_2 Thin Films

09:45 - 10:00
oral

Bojan Karunagaran[1)], **Kyunghae Kim**[1)], **Suresh Kumar Dhungel**[1)], **Jinsu Yoo**[1)], **Devanesan Mangalaraj**[1)], **Junsin Yi**[1)]

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Titanium dioxide films have been deposited using DC magnetron sputtering onto well-cleaned p-type silicon substrates at the ambient temperature at an oxygen partial pressure of 7x10^{-5} mbar and total sputtering pressure of 1x10^{-3} mbar. The compositions of the films were found to be stoichiometric (O/Ti=2.07) as analyzed by Auger Electron Spectroscopy (AES). The rms roughness of the film is evaluated as 4.8 nm using ex-situ atomic force microscopy.

Optical constants of the films have been determined by spectroscopic ellipsometry (SE) in the photon energy range 1.2 to 5.5 eV at room temperature. The measured dielectric-function spectra reveal that the distinct structures at energies of the E1 (3.53eV), E1+Δ1(3.97eV) and E2 (4.82eV) critical points are due to interband transitions. The dielectric related Optical constants, such as the refractive index, extinction coefficient, absorption coefficient and normal incidence of reflectivity are determined from the SE data and analyzed.

Films of thickness 140 nm are calcinated in air in a muffle oven for 1h at 673 and 773 K. After each calcination, the Raman spectrum was recorded. The frequencies of the Raman bands are identified as 637, 513, 396, 195.1 and 144.3cm^{-1}. Using factor group analysis the 396 cm^{-1} peak is assigned to the B1g mode(ν4), 637cm^{-1} peak to the Eg mode (ν1), 513 cm^{-1} peak to the A1g + B1g modes (ν2 + ν3). It was observed from the factor plane analysis that the A1g (ν3) and B1g (ν2) modes both involve the Ti - O bond stretching normal to the film plane. The peaks at 195.1 and 144.3 cm^{-1}are assigned to the Eg modes represented by ν5 and nu6. In the case of the annealed films, there is no significant change in the peak position and also the intensity of the peaks increases at the same time the FWHM decreases with the increase in the annealing temperature, which can be attributed to the improvement in the crystallanity,which is supported by XRD.

Potential of nano-sized Rare Earth fluorides in optical applications

10:00 - 10:30
invited oral

Ulrich H. Kynast[1)], **Marina M. Lezhnina**[1,2)]

1) University of Applied Sciences Muenster, FB1, Applied Materials Sciences (FHMS), Stegerwaldstrasse 39, Steinfurt 48565, Germany

2) Mari State Technical University, Institute of Physics (MSTUYO), Lenin-pl. 3, Yoshkar-Ola 424 000, Russian Federation

Rare Earth fluorides are a class of materials with high potential in optical applications. On one hand, fluoride lattices allow high coordination numbers for the hosted Rare Earth ions, on the other hand, the high ionicity of the Rare Earth to fluorine bond leads to a wide band gap and very low vibrational energies. These two essential factors in particular contribute to their usability in optical applications based on vacuum ultraviolet (VUV) and near infrared (NIR) excitation. Keywords in this context are 'downconverters' (multiphotonemitters, e.g. YF_3:Pr, $LiGdF_4$:Eu [1]) and 'upconverters' (e.g. YF_3:Yb,Er [2]) as well as NIR-emitters (e.g. LaF_3:Nd [3]). Recent attempts to control the size of such particles down to the nano-scale, at the same time maintaining the performance of their macroscopic counterparts, indicate accessibility of hitherto unrealized optical properties and applications. The preparation and optical characteristics of such nanoparticles and their embedding in polymeric, glassy or porous matrices to enable the manufacture of transparent hybrid materials will be discussed.

[1] R.T. Wegh et al., J. Lum., 82, 93, 1999
[2] L.F. Johnson et al., Appl. Phys. Lett., 15, 48, 1969
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Symposium H

Computational Materials Science

Introduction

One of the most significant accomplishments in computational materials science is the ability to predict materials properties at a level of accuracy and reliability, which is starting to reach - and in some cases surpass - that of experiment. Materials properties, which have become accessible to computations, encompass an impressive range such as the structure of bulk solids, defects, surfaces and interfaces, thermochemistry, mechanical properties, electronic excitations and magnetic behaviour. These remarkable capabilities have attracted the attention of experimental scientists and are now becoming part of industrial research and materials engineering. In this context, this Symposium focuses on ab initio methods, since this type of approach provides deep and unique insight into materials and it has high predictive capabilities for novel systems. A particularly exciting area of computational materials science is the connection between the level of electronic structure and the macroscopic behaviour such as, for example, the ability of a metal to store hydrogen or the shear strength of a material. Driven by the growing interest in nanostructures, the study of systems with reduced dimensionality represents another fascinating field of application. This includes reactions on surfaces as found in heterogeneous catalysts, sensors, and in the environmental degradation of materials. Three critical challenges stand out as major drivers for new theoretical and computational developments, namely (1) the enormous gap between the time scales at the macroscopic and atomic levels; (2) the desire to study larger systems such as dislocations, and (3) the need for higher accuracy, especially in the treatment of excitations. Recent progress in theories such as time-dependent DFT and other treatments of excited states provide promising perspectives and are thus part of this Symposium. The growing importance of molecular systems in materials science such as organic conductors and organic optoelectronic devices requires a broad range of computational capabilities. The Symposium will include this type of highly promising areas, which point towards a connection between solid state science, molecular sciences, and biological sciences.

Organisers

- Erich WIMMER, Materials Design s.a.r.l., France
- Krzysztof Jan KURZYDOWSKI, Warsaw University of Technology, Faculty of Materials Science and Engineering
- Marek NIEZGODKA, Warsaw University, Interdisciplinary Centre for Mathematical and Computational Modelling
- Witold RUDNICKI, Warsaw University, Interdisciplinary Centre for Mathematical and Computational Modelling

Proceedings

Proceedings of the Symposium H of E-MRS Fall Meeting will be published in "Materials Science".

Monday, September 6th

14:00 - 15:30

Afternoon session

Main Building, room 231

Finite Element Analysis of Diffusion Controlled Phase Transformation

14:00 - 14:30
invited oral

GEORGE D. VERROS[1], **Nikolaos A. Malamataris**[2]

1) Technological and Educational Institute of Lamia (TEI, GR), ATHINON STR., LAMIA 35100, Greece

2) Technological and Educational Insitute of West Macedonia (TEI, GR), Kila, Kozani 50100, Greece

Diffusion controlled phase transformations are important in all engineering processes where material science is the main issue, such as alloys manufacture in metallurgical engineering or ceramics, polymeric membrane fabrication etc The main characteristic of diffusion controlled phase transformation is mass exchange between two phases leading to spatial extension of one phase while the other phase shrinks. This results in a moving interface between the two phases. Equilibrium is usually assumed at the moving interface. In this presentation a detailed methodology for modeling diffusion controlled phase transformations in polymeric membrane fabrication and metallurgical engineering with the aid of Galerkin Finite Element Method is presented. So far, the scientific methods that have been used are based on a trial and error procedure both in polymeric and metallurgical phase transformations. Our work alleviates shortcomings of previous approaches, as it results in a complete model, where the governing equations of the problem at hand are solved simultaneously along with appropriate boundary and initial conditions, yielding a complete picture of the physical and chemical phenomena that take place in the processes of interest. [ABSTRACT TRUNCATED TO 2000 LETTERS]

Time multiscale analysis of dynamic delamination

14:30 - 14:45
oral

Stefano Mariani[1], **Anna Pandolfi**[1], **Raffaella Pavani**[2]

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2) Dipartimento di Matematica "Francesco Brioschi", Politecnico di Milano (POLIMI), Piazza L. da Vinci 32, Milano 20133, Italy

We present a numerical procedure to simulate the dynamic debonding of a thin layer from a rigid substrate. The layer is assumed to behave elastically, whereas the process zone -where dissipation occurs- is modelled through a cohesive softening law. Using a simplified approach, in the case of bending dominated delamination the shear deformation can be disregarded. Thus the Euler-Bernoulli kinematics can be adopted to describe the motion of the specimen.
Under such hypotheses, the governing partial differential equation is characterized by two length scales and two time scales (three time scales when rate-dependency is included in the cohesive model). The first length scale is introduced by the size of the specimen, identified by a macroscopic length l_M; the second length scale is introduced by the presence of a process zone in front of the delamination crack tip. As for the time scales, the first one is related to the propagation of a dilatational wave along the free part of the specimen t_g; the second one is a characteristic time t_c, which accounts for the interplay between the debonding layer inertia of and the mechanical properties of the process zone. Length and time scales can differ of several orders of magnitude, conferring to the problem a space-time multiscale nature.
Introducing a spatial discretization (e.g. by central finite differences), the PDE is transformed into an ordinary differential equation system to be integrated in time. Assuming that the spatial discretization is fine enough to capture everywhere the stress distribution, for the numerical solution of the layer dynamics in the process zone an accurate time integration is impelling. In fact, the process zone is characterized by fast changes of the stress distribution. In this work we present the application of a temporal multiscale approach for the analysis of the dynamic delamination, able to capture the essential mechanical features of the process.

3D simulation of deformation and fracture in heterogeneous materials

14:45 - 15:00
oral

Varvara A. Romanova[1], **Ruslan R. Balokhonov**, **Pavel V. Makarov**

1) Institute of Stregth Physics and Materials Science of SB RAS, Tomsk, Russian Federation

In this contribution, a mesomechanical approach [1] to simulate the elasto-plastic behavior and fracture of materials with explicit consideration for their meso-structure has been extended to the three-dimensional case. Deformation and fracture processes in different materials, including a polycrystalline aluminium alloy, a metal matrix composite, steel with coating and coal were numerically studied.
A special procedure we developed in [2] to introduce a three-dimensional heterogeneity in the calculations has been applied to design 3D-structures of the materials above. 3D-calculations of the elasto-plastic deformation and fracture of the materials under loading have been performed in a dynamic formulation of the problem, using the method of a finite-difference approximation. Stress relaxation and strain hardening as well as defect nucleation at the interfaces and cracking were taken into account through model formulations and criteria of yield and fracture. Results of the 3D-calculations have been analysed in details and compared with those obtained from the 2D-approximation. The analysis of material deformation and fracture at different scale levels have been made on the base of the mesomechanical concept [1].

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[2] V. Romanova, R. Balokhonov, P. Makarov, S. Schmauder and E. Soppa, Simulation of elasto-plastic behaviour of an artificial 3D-structure under dynamic loading. Comput. Mater. Sci. 2003. V.28. Issues 3-4. P. 518-528.

A numerical investigation of ductile fracture initiation in ultra high strength low alloy NiSiCrCoMo steel

15:00 - 15:15
oral

Pravin P. Deshpande[1], **Dilip R. Peshwe**, **Shailkumar U. Pathak**

1) Visvesvaraya National Institute of TechnologyE (VNIT), N.Ambazari road, Nagpur 440 011, India

Abstract
In the present wok, a standard specimen subjected to tensile loading is analysed by performing finite element simulations. The deformation at the crack tip is studied . A set of available analytical results and the experimental data on the deformation of ultra high strength low alloy steel NiSiCrCoMo steel are used for the validation .It has been shown that the numerical simulation can be considered as equivalent to performing real experimentation

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Coffee break

15:30 - 15:50

Afternoon session - continued

Main Building, room 231

15:50 - 17:20

COMPUTATIONAL IMAGE ANALYSIS OF MATERIALS MICROSTRUCTURE

15:50 - 16:20
invited oral

Jan Cwajna[1], **Janusz Szala**[1]

1) Silesian University of Technology, Department of Materials Science, Krasińskiego 8, Katowice 40-019, Poland

The paper focuses on the determination of elements of measuring process, whose impact on promptness and precision of a structure‘s quantitative description is the greatest. It also concentrates on the introduction of such changes into the realization of the measuring process elements, that will make it possible to minimize the errors they cause.
Replacement of the classical, i.e. manual and semi-automatic measuring methods with automatic ones has led to significant changes in the measuring process. Measurement of geometric features of analyzed structure elements, which has constituted the greatest problem of the methods applied so far, can be described by universal algorithms, independent from these objects‘ morphologies. The most difficult element of the measuring process is exact detection of objects being measured. It has been shown that detection of all phases existing in a tested material requires a complementary application the different techniques of light as well as of scanning microscopy. In particularly difficult cases, satisfying results are obtained only with the application of the most modern scanning microscopy tools, such as EBSP or mapping. A

disadvantage of these methods is that they are labour- and time-consuming. The solutions presented in the paper enabled considerable acceleration of the latter.
Obtaining a structure's digital image which allows to detect measured objects using solely binarization, is possible, even when preparation procedures were performed correctly, only in sparse cases. Therefore, the initial grey image, before binarization, is to be subjected to additional transformations to remove preparation defects and shadow effect. The new procedures of grain boundaries reconstruction (a controlled segmentation and a conditional reconstruction) and methods of twins boundaries and lamellar precipitation colonies disclosure were also developed.

16:20 - 16:50
invited oral

3-D image analysis in materials science

Leszek Wojnar[1)]

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Statistical characteristics of spatial properties of microstructures (particle density, volume fraction, orientation, etc.) can be obtained by means of stereological methods. Unfortunately, these methods are useless in the case of more advanced analysis, where precise, really 3-dimensional information on particle localization, connectivity, size and shape is required.

The above-described characteristics can be obtained only from 3-D images that can be interpreted as piles of 2-dimensional digital images. Such data sets are currently obtained in most cases from X-ray microtomography. Their subsequent analysis faces several problems that can be divided into three groups:
1. Very high memory and computational power requirements. For example, 2-D gray-scale image of size 512x512 pixels occupies 257 kB, whereas the 3-D image of size 512x512x512 voxels occupies 134 MB of memory.
2. More complicated image processing and lack of theory for some operations, for example skeletonization. Consequently, algorithms prepared and tested for 2-D images cannot be directly adapted for 3-D processing.
3. Difficult visual verification of the results that is routine control tool in the case of 2-D images. Various rendering techniques as well as virtual sections through 3-D images are used to display the results.

The potential and difficulties accompanying 3-D analysis are presented on the basis of several examples:
1. Polymer foam - restoration and characterization of cellular structure.
2. Metallic foam with open porosity - examples of problems with construction of 3-D skeletons
3. Metal matrix porous composites - characterization of 3-D structure of pores
4. Glass fiber epoxy matrix composite - analysis of the spatial distribution of fibers.

16:50 - 17:05
oral

Digital image analysis and visualization of early caries changes in human teeth

Elżbieta Kaczmarek[4)], **Anna Surdacka**[1)], **Teresa Matthews-Brzozowska**[1,3)], **Bogdan Miśkowiak**[2)]

1) Dept. of Conservative Dentistry, Univ. of Medical Sciences in Poznań, Poznań, Poland

2) Dept. of Optometry and Visual System, Univ. of Medical Sciences in Poznań, Poland

3) Dept. of Orthodontics, Wrocław Medical University, Poland

4) Lab. of Morphometry & Medical Image Processing at Chair of Pathology, Univ. of Medical Sciences in Poznań, Poland

Early caries changes are reversible and may heal up. Therefore, our studies first aimed a visualization and analysis of caries after the use of experimental strontium-fluoride toothpastes protecting hard dental tissues. The material consisted of healthy premolars extracted for orthodontic reasons and sectioned into slices. The artificial damage, resembling that of incipient caries, was induced in their enamel. The in situ model was developed by placing the samples on the buccal surfaces of the first molars in healthy subjects, and exposing for 3 or 6 months of the toothpaste activity. SEM topographic analysis of the enamel surface revealed smoothening caused probably by mineral compounds deposition. The quantitative X-ray EDS microanalysis was performed to examine the Ca and Sr content on the enamel surface and layers of 15, 30, 60 and 100 microns deep. The results showed that the toothpaste induces an increased deposition of Ca in sub-superficial layers of the damaged enamel, thus inducing the recovery of its injury. A long term use of the toothpaste significantly promotes remineralization of artificially damaged deeper layers of enamel. Pit and fissure sealing aims a good protection against caries. However, sealant retention depends on the sealant quality and procedures used for fissure preparation. In our in vitro studies, sections of teeth crowns were stained with HE and digitized with a light microscope. The area of enamel demineralization, the width and depth of occlusal fissures and the distance from the bottom of fissures to dentine-enamel junction were measured. Examples are given how the measured parameters differ between caries lesions in fissure sealant and unprotected human premolars. The increasing role of digital imaging need to be defined with the diagnostic problem in mind as the further outcome for the patient in order to plan an effective prophylaxis and treatment of early caries changes.

A micromechanical model of stress-induced martensitic transformations in shape memory alloys

17:05 - 17:20
oral

Henryk Petryk[1)], **Stanisław Stupkiewicz**

1) Polish Academy of Sciences, Institute of Fundamental Technological Research (IPPT PAN), Świętokrzyska 21, Warszawa 00-049, Poland

The paper is concerned with a micro-mechanical model of stress-induced martensitic transformations in single crystals of shape memory alloys. In agreement with numerous experimental observations the transformation is assumed to proceed through the formation and growth of parallel martensitic plates within the austenite matrix. The phase transition takes place when the thermodynamic driving force at a phase transformation front reaches a threshold value. Macroscopic stress-strain relationships that correspond to pseudo-elastic behaviour are derived for evolving laminated microstructures, with full account for different elastic anisotropic properties of the product and parent phases. This difference in elastic properties leads to the redistribution of internal stresses during transformation which can affect the microstructure evolution. The class of analysed microstructures includes higher rank laminates. In particular, formation of internally twinned martensite plates is examined and the effect of detwinning through migration of interfaces between two martensite variants is modelled. In order to study size effects the model is extended by taking into account the interfacial energy. As an application of the model, the evolution of microstructure is studied for cubic-to-orthorhombic and cubic-to-monoclinic transformation in Cu-based shape memory alloys (CuAlNi and CuZnAl). Both the microstructure evolution and stress-strain diagrams are shown to depend on the orientation of the load axis with respect to the crystalline axes of the parent phase as well as on the sense of loading, i.e. tension or compression. Detwinning has been found to reduce significantly the effective tangent stiffness modulus of the twinned martensite. Macroscopically nonuniform transformation is predicted due to the softening behaviour at the material point scale.

Poster session

19:00 - 21:00

FINITE ELEMENT MODELLING OF THE RESIDUAL STRESSES IN THE CERAMIC-ELASTOMER COMPOSITES

poster
H-01

Anna Boczkowska[1)], **Katarzyna Konopka**[1)], **Kamil Babski, Grzegorz Krzesiński, Krzysztof J. Kurzydlowski**[1)]

1) Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland

Ceramic-elastomer composites are obtained via infiltration of porous ceramics by elastomer prior to the curing reaction. The elastomer is synthesized by one-shot method from the diisocyanate, oligodiol and chain extender. The liquid mixture of the substrates is incorporated into ceramics pores using the vacuum pressure in the temperature of 120oC. Next the addition reaction is conducted in this temperature for 14 - 16 h. Since the thermal expansions of the elastomer and ceramics are different upon cooling to ambient temperature, this results in the buildup of residual stresses in the various range of the composite. Moreover, the elastomer shrinks as a consequence of the transformation from the mixture of the substrates in the liquid state to the solid state polymer with the covalently bonded network structure.
Residual stresses are of a significant concern because they can cause a damage in the form of ceramics cracks and delaminations between ceramics and elastomer. They can also effect on the composite mechanical properties.
The aim of the study was the creation of the model describing the residual stresses results in the composites with two different interpenetrating phases in 3D. To calculate the residual stresses the Finite Element Method (FEM) was used.

Modelling the interaction of crack tip with nanostructure, which creating by deformation.

poster H-02

Kateryna M. Borysovska[1)], **Viktor N. Slunyaev**[1)], **Yuriy M. Podrezov**[1)], **Zbigniew Pakiela**[2)], **Krzysztof J. Kurzydlowski**[2)]

1) Institute for Problems of Materials Science, 3, Krzhizhanovsky, Kiev 03142, Ukraine

2) Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland

The fracture of nanocrystalline material was studied. The interaction of dislocation with dislocation wall near the crack tip was analyzed taking into account the image forces as well as their influence on the crack tip. The calculation results allow to estimate the influence of the shield effect of dislocation wall on the fracture toughness and J-integral. It was shown that the wall leads the substantial growth of the dislocation crowd near the crack tip, that in turn leads to increase of fracture toughness and J-integral.

First-principles calculations of beryllium chalcogenide BeS1-xSex properties

poster H-03

Khellil Bouamama[1)], **Khadidja K. Daoud**, **Labgaa N. Noudjoud**, **Kassali K. Kamel**

1) optoelectronics and devices laboratory, Departement of physics, university of Setif, Setif 19000, Algeria

In this present work, we are interesting on the first-principles study of structural, elastic, electronic and dielectric properties of BeSxSe1-x which are potentially good materials for technological applications and are a promising material for blue-green laser diodes and laser-emitting diodes. All calculations were performed within the framework of the density-functional theory DFT [1,2] with the local density approximation LDA for the exchange-correlation energy as implemented in the ABINIT code [3]. We have used the Teter and Pade parameterization [4] for LDA. Only the outermost electrons of each atom were explicitly considered in the calculation, and the effect of the inner electrons and the nucleus (the frozen core) was described within a pseudopotential scheme. We used the Hartwigzen Goedecker Hutter scheme[5] to generate the norm-conserving nonlocal pseudopotentials, which results in highly transferable and optimally smooth pseudopotentials. A plane-wave basis set was used to solve the Kohn-Sham equations in the pseudopotential implementation of the DFT-LDA.

The Brillouin zone integrations were replaced by discrete summations over a special set of k-points using the standard k-point technique of Monkhorst and Pack [6].

For the treatement of the alloy disorder, we have used the virtual crystal approximation VCA [7], in which one studies the crystal with the primitive periodicity, but composed of virtual atoms that interpolate between the behavior of atoms in the parent compounds.

We have calculated the elastic properties of these compounds by computing the components of the stress tensor for small strains using the method developed by Nielsen and Martin [8]. The plane -wave energy cutoff to expand the wave functions is set to be 90 Hartree (1 Hartree = 27.211396 eV). Integrals over the Brillouin zone are performed using Monkhorst-Pack scheme [9] where the k-point mesh used is (8 X 8 X 8).

References:
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[ABSTRACT TRUNCATED TO 2000 LETTERS]

Temperature breakdown phenomenon in zinc monocrystal in strong magnetic fields

poster H-04

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The results of magnetoresistance (MR) measurements of Zn single crystal, with RRR=25000 in temperature range from 4.2K to 50K and in strong magnetic fields (up to 8T) are represented. Angle and temperature dependences of MR were studied on single crystal with orientation [1120]. In the angle interval of 30^0-50^0 degrees thin structure of MR has been detected, which is not observed at 4.2K. In this temperature region a small-angle scattering of electrons on long-wave phonons becomes effective. Such scattering is inelastic, and practically in all interval of rotation angles field has a diffusive character. The thin structure of MR appears as a result of strong intersheet electron-phonon scattering under conditions of the umklapp process. In this case a fundamental modification an electron trajectories is possible. By the analogy with the magnetic breakdown effect, this phenomenon is named the temperature breakdown. In the range of MR, there exist δ and π orbits, connected with orbits round combinations of two horizontal and two diagonal "sleeves" of the "monster". The orbits of monster "sleeves" combinations must pass near the α needle, so presumably the small electron orbit provides a "bridge" for the formation of new

temperature breakdown trajectories. In this case formation of one of two kinds of the orbits is possible: two-sheet or three-sheet orbits.

Interaction induced depolarized light scattering and dipolar absorption spectra of exohedral complexes of rare gases with fullerenes and nanotubes

Zbigniew Dendzik[1], **Marcin Kośmider**[1], **Aleksander Dawid**[1], **Zygmunt Gburski**[1]
1) University of Silesia, Institute of Physics, Uniwersytecka 4, Katowice 40-007, Poland

poster
H-05

We have performed the molecular dynamics study of several exohedral complexes composed of the rare gas ultra-thin atomic films adsorbed on the fullerene or nanotube surface, and calculated the depolarized light [1-2] and dipolar absorption [3] spectra of these systems. The interactions beetween rare gas atoms have been modelled using the HFD-B potentials developed by Aziz and co-workers [4-6], while the intra-molecular interactions beetween the carbon atoms of the fullerenes and nanotubes have been modelled using the potential composed of the components representing the energy of the bonded C atoms (Morse bond, harmonic cosine of the bending angle and a 2-fold torsion potential) and the energy of the van der Waals interaction between the non-bonded C atoms [7-8].

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Dynamics of rare gas ultra thin atomic films covering single-walled carbon nanotubes

Marcin Kośmider[1], **Zbigniew Dendzik**[1], **Zygmunt Gburski**[1]
1) University of Silesia, Institute of Physics, Uniwersytecka 4, Katowice 40-007, Poland

poster
H-06

We have performed the molecular dynamics study of several exohedral complexes [1] composed of the rare gas ultra-thin atomic films adsorbed on single-walled nanotube surface and calculate dynamical properties of these systems. In particular, we identified the vibrational modes of these complexes and analyzed the influence of the structure and phonon modes of the nanotube on the dynamics of the film atoms. The interactions beetween rare gas atoms have been modelled using the HFD-B potentials developed by Aziz and co-workers [2-4], while the intra-molecular interactions beetween the carbon atoms of the fullerenes and nanotubes have been modelled using the potential composed of the components representing the energy of the bonded C atoms (Morse bond, harmonic cosine of the bending angle and a 2-fold torsion potential) and the energy of the van der Waals interaction between the non-bonded C atoms [5-6].

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Structural and dynamical properties of water surrounding a carbon nanotube - computer simulation study

Marcin Kośmider[1], **Mariusz Sokół**[1], **Zbigniew Dendzik**[1], **Aleksander Dawid**[1], **Zygmunt Gburski**[1]
1) University of Silesia, Institute of Physics, Uniwersytecka 4, Katowice 40-007, Poland

poster
H-07

Water exhibits many interesting and anomalous features, such as negative volume of melting, density maximum in the normal liquid range, isothermal compressibility minimum in the normal liquid range, increasing fluidity with the increase of pressure, high-mobility transport for H- and OH- ions, a variety of crystalline polymorphs or significant dielectric constant.

In the present paper, we have studied structural and dynamical properties of water in the vicinity of the single-walled carbon nanotubes of various diameters and chiralities, and compare the results with the results for normal water (without nanotube). The influence of water on the nanotube vibrational modes has also been assessed.

A molecular motor constructed from a double-walled carbon nanotube - computer simulation study

poster H-08

Zbigniew Dendzik[1)], Aleksander Dawid[1)], Marcin Kośmider[1)], Zygmunt Gburski[1)]

1) University of Silesia, Institute of Physics, Uniwersytecka 4, Katowice 40-007, Poland

Recently Tu and Ou-Yang [1] reported a theoretical study suggesting the possibility of constructing a molecular motor constructed from a double-walled carbon nanotube placed in in a thermal bath which exhibits a directional motion with the variation of the bath temperature. In the present paper, we investigate this problem via molecular dynamics simulation and assess the influence of the nanotubes vibrational modes on this system.

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Influence of thickness of PbS thin films on the scattering mechanis

poster H-09

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The thickness dependence of Hall mobility is explored on the films of n-PbS, grown from a vapor phase by the "hot-wall" method of on (111) BaF_2.
Experimental dependence of mobility were approximated by the in a theory expected values, which take into account carriers scattering, characteristic both for massive samples, and thin films. So, in particular, scattering taken into account on deformation potentials of acoustic and optical phonons, polarization potential of optical phonons, on the ionized admixtures and on dislocation of disparity, on a border the film-substrate, border of corns and dispersion, conditioned by surfaces effects.
It is set, that critical thickness of tapes, which the net of distribution, even 12 nm, will appear after, and dispersion on dislocation of disparity prevails to the thickness 0,4 nm, carrier scattering on border of corns characteristically for 1,5-2 nm. At films thickness anymore than 2 nm basic contribution in mobility gives scattering on the films surface. A value of free length was taken on at computations 50 nm, and as by a volume mobility the expected 400 $cm^2\ V^{-1}\ s^{-1}$.

Ceramic hydration with expansion: The structure and reaction of water layers on magnesium oxide. A cyclic cluster study.

poster H-10

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The search for novel materials, the reduction of dimensions and the need for optimization are challenges which frequently have to consider the surfaces or interfaces of ceramics. Among these the alkaline earth oxides MgO and CaO are model substrates. They find widespread applications as insulators, cements, catalysts, sensors, supports for metals or semiconductors. An important reaction is their hydration, proceeding with large expansion. Its first step is the adsorption of water.
The adsorption of water on the magnesium oxide surface has been studied using the semiempirical SCF MO method MSINDO. The cyclic cluster model including long range Madelung potentials is implemented. Both molecular adsorption and dissociative adsorption was found to occur. The latter was stabilized by hydrogen bonding from neighboring water molecules and surface oxygen. Whereas a single water molecule does not dissociate on MgO (100) surface, several energy minima exist for the experimentally observed low temperature (3 x 2) monolayer consisting of a mixture of dissociated and molecular water. The energy and structure of the fully hydroxylated (1 x 1) MgO (100) surface experimentally observed at 300 K, has

been studied theoretically for the first time. It is shown that this structure is favorable for the naturally occuring reaction of MgO with water, which leads to the thermodynamically stable brucite $Mg(OH)_2$. The reaction proceeds with appreciable volume increase, which, in a rigid matrix can generate large pressure inducing phase transitions and harmful cracking.

TECHNIQUES FOR EVALUATING STRESSES AND STRAINS IN MICRO-SYSTEMS

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Well-known finite element method is an excellent tool for the assessment of the integrity of micro packages because it is often impossible or very difficult to measure temperature distributions and plastic zones on such tiny components. However this method employs mostly the classical continuum mechanics, which is based on the fundamental idea that laws of motion and the axioms of constitution are valid for every element of the body no matter how small it may be. When the spatial discretisation grid is refined, the finite element approximation becomes more accurate in the sense that the displacement gradients become stronger but this assumption is not longer applicable as the characteristic dimension of a structure becomes comparable to or smaller than the periodic atomic scale domain. It is accepted that many effects on the continuum start developing at the atomic level. Therefore, a computational mechanics method is necessary that can couple different in kind scales, one scale in which the boundary conditions are applied and the other in which atoms reside. The results of atomistic calculations depend upon two factors: the interatomic potential used to model the interactions between the atoms in the inner region and the boundary conditions used to model the effect of outer region. The aim of investigations is to provide a non-local description of nano-materials versus discrete formulations based on mechanics of nano-structures. These studies on the non-local description of nano-materials are motivated by homogenisation of the atomic theory of Bravais lattices, aimed at a better description of phenomena taking place in crystals on a scale comparable to the range of interatomic forces. The evaluation of stresses in micro-systems, which lead to damage is also the centre of attention.

Modelling electronic structure of unusual metallic fluorides of Ag(II)

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We investigate computationally two representative examples of higher fluorides of Ag(II), namely $KAgF_3$ and $AgFBF_4$. Both compounds formally contain linear $(Ag\text{-}F)^+$ chains in which divalent silver is coordinated additionally by four fluoride anions. For $AgFBF_4$, the equatorial coordination is weak, and leads to metallic conductivity in 1D, as comes out from our band structure calculations. For $KAgF_3$, however, the axial coordination is very strong, and the compound is virtually a 2D metal (i.e. mainly the x^2-y^2 orbitals of Ag participate in electronic transport in this interesting material). The fluoroargentates are thus unique examples of conducting fluorides, as first predicted by theory (W.Grochala, R.Hoffmann, Angew. Chem. Int. Ed. Engl. 40(15): 2743-2781 2001).

First-principles study of phonon-based properties of magnetic $CuFeS_2$

Jan Łażewski[1)], **Hans Neumann**[2)], **Krzysztof K. Parlinski**[1)] poster H-14

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Chalcopyrite, $CuFeS_2$, has very interesting history and has been known and used for very long time. About 2500 years ago it was used as a material for ancient statuettes. Its structure was the first determined structure in USA (in 1917). The first steps in semiconductor electronics were also connected with the $CuFeS_2$. It was used as a material for detecting radio waves. In spite of so reach history even basic properties of this material are not well known. Some of published data should be considered with care. Specially experimental acoustic phonon dispersion relations measured with inelastic neutron scattering and elastic constants seem to be inaccurate. A comparison of them with heat capacity as well as compressibility

factors show that they should be revised. We present ab initio structural parameters as well as dynamical and thermodynamical properties of chalcopyrite. The first principles plane-wave pseudopotential calculations based on density functional theory (DFT) were used to determine structural parameters. The Born effective charges were obtained using Berry phase method. Phonon dispersion relations were evaluated from Hellmann-Feynman forces with the direct method. The thermodynamical properties were derived from phonon density of states with quasi-harmonic approximation.
This work was partially supported by the Polish State Committee of Scientific Research (KBN), grant no 1 P03B 104 26.

Ablated Particle Movement in a Pulsed Laser Deposition System

poster H-15

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Pulsed Laser Deposition (PLD) technique is a quite common laboratory technique, known to have many advantages for the thin films depositions. Several ways for the improvement of the film surface quality have been investigated in literature. However, it still has a several drawbacks (e.g. droplet formation) which makes it unusable for some industrial applications. Work presented in this paper is aimed to provide a more comprehensive understanding of PLD techniques and ways to improve the control of the deposited thin film parameters.
A novel three-dimensional model has been proposed for simulating plume behavior and 'micron-sized particles' movement and interaction. It describes the plume expansion in vacuum or into an environmental gas and particles interaction with various obstacles. The model simulates 'standard' PLD system behavior but also some droplet reduction techniques used in PLD (e.g. shadow mask technique, back-side deposition ...) The model combined the advantages of Monte-Carlo and Finite Element methods, being able to give a detailed image of particles behavior, both from microscopic and macroscopic points of view. Some significant results and theoretical interpretations together with proposal for experimental system adjustment are also presented.

Multi-component structures with varying configuration

poster H-16

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Multi-component structures (heterophases, layered, porous, composite) present a stable interest for different fields of science and engineering. In the present paper the equations are discussed describing the dependence of several effective properties (electrical, thermal, galvanomagnetic, etc.) of such systems with varying concentration and configuration of inclusions. The examples are given of calculation of complex properties like thermoelectric effectiveness and figure of merit of multi-component structures. The approach offered may be used for optimal design of complex multi-component structures with advanced effective characteristics.
The work has been supported by the Russian Foundation for Basic Research (RFBR) - Gr. No. 04-02-16178, and by the INTAS (Ref. Nr. 03-55-629).

Molecular dynamics simulations of cyanoadamantane multilayers between graphite substrates

poster H-17

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The constant pressure molecular dynamic (MD) simulations have been carried out to investigate structural and dynamical properties of the multilayer cyanoadamantane ($C_{10}H_{15}CN$) between the graphite substrates. We consider a temperature range spanning from 100 to 900 K. Results for diffusion coefficient, as well as for the pair distribution function, are reported for several numbers of layers and compared among each other. The interaction between cyanoadamantane molecule and basal planes of graphite was studied theoretically using a semi-empirical potential approach, where graphite is treated as a static surface providing the external holding potential for the molecules [1]. Complicated structures of real cyanoadamantane molecule have been simplified by three site model of cyanoadamantane (CNadm) [2].

References
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Computer Simulations study of solid C_{60} doped by hydrogen cyanide molecules

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poster
H-18

Using spherical averaged Girifalco potential model of interacting fullerenes C_{60}, we have simulated (MD method) the relaxation processes of hydrogen cyanide molecule embedded in fullerene host. The dynamics of molecules in the system has been studied by inspecting the calculated dipolar absorption spectrum and Arrhenius like plot. Moreover, the translational and rotational correlation functions of HCN in fullerene environments have been calculated and interpreted in terms of phenomenological model.

Molecular dynamics of cholesterol in thin film surrounded carbon nanotube

Przemysław Raczyński[1), Aleksander Dawid, Mariusz Sokół, Zygmunt Gburski
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poster
H-19

We have performed molecular dynamics (MD) simulations of the system composed of a single walled carbon nanotube (SWNT) surrounded by thin film of: a) cholesterol plus water and, b) cholesterol. The translational and rotational correlation functions and their Fourier transforms for both cholesterol and water molecules have been calculated for several temperatures and concentrations. The interpretation of translational and rotational dynamics of both cholesterol and water molecules in such specific environment is presented.

Molecular dynamics study of the fullerene - cholesterol mixture cluster

Przemysław Raczyński[1), Aleksander Dawid, Zygmunt Gburski
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poster
H-20

Molecular dynamics (MD) studies are presented of the cluster composed of the fullerene and cholesterol molecules mixture. We have investigated several dynamical quantities of fullerene and cholesterol as a function of temperature and their concentration in the cluster. The radial distribution function, mean square displacement and diffusion coefficient of both fullerene and cholesterol in the mixture have been calculated. We have shown that the dynamics of cholesterol molecules is strongly modified by the presence of the strong fullerene-cholesterol interaction potential.

Molecular dynamics and dielectric relaxation of nitrogen oxide near fullerene "sphere" - computer simulation

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poster
H-21

Computer simulation (MD method) studies are presented of the nanosystem composed of nitrogen oxide molecules surrounded single fullerene. The calculations were performed for several temperatures and densities (solid and fluid phases of nitrogen oxide thin layer). The radial distribution function, mean square displacement and diffusion coefficient of NO have been obtained. The influence of fullerene on the calculated dielectric loss spectra are visible as compared to the calculated spectra of bulk sample of nitrogen oxide.

The search for minimum energy structures of small atomic clusters - application of the ant colony algorithm

poster H-22

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We have applied the ant colony algorithm to the problem of finding the minimal energy configurations of the small physical system (cluster) of atoms interacting via Lennard-Jones phenomenological potential. The ants were positively motivated if their activity (displacement of atomic positions) leads to the lower total potential energy of the system. Starting from a random spatial distribution of atoms, during the optimalization process, the ants were able to find the configurations with much lower energy than at the begining. The obtained configurations were compared with the ones calculated by Monte Carlo method. The optimized configurations generated by the ant colony algorithm can be used as a good starting point of the classical or ab initio molecular dynamics (MD) simulations.

Origin of the negative thermal expansion in perovskite-type $PrGaO_3$

poster H-23

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Perovskite-type rare-earth gallates attracted much attention because of their interesting physical qualities. Most important properties of $RGaO_3$ compounds are used in substrate materials, either for high-temperature superconductors (HTSC), for doped manganese perovskite $LnMnO_3$ films with colossal magnetoresistance (CMR) and for GaN films. Recently it was proposed to use rare-earth gallates as superionic conductors. Among such rare-earth perovskite-type gallates, $PrGaO_3$ is outstanding. Our recent studies of the $PrGaO_3$ structure using high-resolution powder diffraction techniques and synchrotron radiation revealed negative thermal expansion in the temperature range 12 - 80 K. Nevertheless, no negative expansion could be seen in isostructural $LaGaO_3$, $CeGaO_3$ and $NdGaO_3$.
Considering the structure of $RGaO_3$ (R=La-Nd) and its solid solutions $R_{1-x}R_xGaO_3$ allows us to conclude that many of such compositions are promising candidates for negative expansion at low temperatures. This is because a significant contribution of the overall thermal expansion is caused by rotations of the GaO_6-octahedra. There is, however, a subtle balance between the rotations and distortions of the polyhedra. The negative thermal expansion of $PrGaO_3$ seems to be related to the violation of this balance caused by interactions between octahedral rotational modes and Pr-ion excitations.
Negative thermal expansion has also been observed in Pr-containing solid solutions ($La_{0.19}Pr_{0.81}GaO_3$, $La_{0.4}Pr_{0.6}GaO_3$) [Aleksiyko et al]. Hence, we performed semiclassical simulations of the thermal expansion of $PrGaO_3$ using the GULP code based on pairwise interactions. We did, however, not observed traces of negative expansion, which indicates possible electronic effects involved in the nature of such negative thermal expansion of Pr-containing rare-earth gallates.

This work was supported by WTZ (UKR-012-97),UMS (M/85-2003) and PCSR (N7 T08A 00520).

The diffusion model of nitrogen and carbon during carbide phases transformation into nitrocarbides

poster H-24

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The model of diffusion of nitrogen and carbon during nitriding of NC11 steel, which demonstrates phenomena occurring during chromium carbides of type Cr7C3 transformation, is shown in this paper.
The determination method of diffusion coefficient, of nitrogen in steel, basing on chemical profiles researches by means of EDS is also presented.
The method is based on results coming from carbon concentration profiles determination on the cross section of the layer in areas free from carbides precipitations and in areas of their presence. The diffusion coefficient was calculated by converse problem solution.
The diffusion equation was solved by means of finite difference method. The simulation of nitriding process of NC11 steel was performed, thanks to that the model of diffusion controlled transformation: chromium carbide-nitrocarbide, was obtained.
The numerical model verification was made on the base of researches with use of X-Ray microanalysis.
The carried out experiments allowed developing a model of transformation kinetics of chromium carbide

into nitrocarbide in dependence from nitrogen flow.
The mathematical model of nitrogen diffusion both in steel NC11 and chromium carbide of type Cr7C3 is presented in this paper. The details of 1D, preliminary numerical model were also presented. The detailed visualization and analysis were done in 2D space. The calculations realized in 2D space allowed precise description of diffusion mechanism of nitrogen around carbides and accurate determination of process kinetics in dependence from nitrogen diffusion direction. The 2D model was applied only in small areas (nearby carbide) because of high calculation complexity. The nitrogen diffusion in areas free from precipitations was calculated in 1D space.

DEPOLARIZED LIGHT SCATTERING FROM THIN FULLERENE LAYER CONFINED BETWEEN GRAPHITE PLAINS - MD STUDY

Michał Skrzypek[1), **Zygmunt Gburski** poster H-25
1) University of Silesia, Katowice, Poland

The dynamical properties of fullerene cluster, confined between graphite walls, have been investigated by molecular dynamics (MD) simulation method. The fullerenes form the monolayers parallel to the graphite walls. The monolayers are quite stable, we have not observed the migration of fullerenes between monolayers. The interaction induced light scattering spectrum (depolarized Rayleigh scattering) of confined fullerenes has been calculated and it seems to be the sensitive indicator of phase transition in the fullerene film.

FULLERENE LAYERS BETWEEN GRAPHITE WALLS - COMPUTER SIMULATION

Michał Skrzypek[1), **Zygmunt Gburski** poster H-26
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The properties of ultra-thin fullerene layers, located between graphite plains, have been studied using the molecular dynamics (MD) technique. In this ensemble we have a competition between the energetic gain from the molecule-molecule versus molecule-graphite wall interactions. It appears that the confined fullerenes form the ultra-lubricated system. The mean square displacement, velocity autocorrelation function and radial distribution function of fullerene molecules have been calculated for several temperatures and a range of distances between graphite walls.

MOLECULAR DYNAMICS STUDY OF SOLID AND LIQUID PHASE OF $(C_{60})Ar_{44}$ MIXTURE CLUSTER

Michał Skrzypek[1), **Aleksander Dawid**, **Zygmunt Gburski** poster H-27
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The particle near rough surface exhibits different dynamical properties than near featureless surface. In this work we have studied the solid and liquid phases and phase transition in Ar_{44} thin layer covered C_{60} surface. The interaction is taken to be Lennard-Jones site-to-site potential.. We have calculated the mean square displacement, Lindemann index and velocity autocorrelation function of argon atoms. The phase transition (melting) between solid and liquid phase of confined argon film has been detected.

Cholesterol molecule adsorption on carbon nanotube

Mariusz Sokół[1), **Marcin Kaczmarski**, **Przemysław Raczyński**, **Zygmunt Gburski** poster H-28
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We studied single-walled carbon nanotube (SWNT) surrounded by cholesterol molecules using ab initio molecular dynamics simulations. Our DFT calculations were performed within the LDA (with and without spin polarization) and the GGA using the code Siesta. The equilibrium position and adsorption energy are obtained for several nanotubes with different chirality and twist angle.

Dynamical properties of $C_{60}(H_2O)_{50}$ mixture cluster - molecular dynamics simulation

poster H-29

Mariusz Sokół[1)], **Aleksander Dawid**, **Zygmunt Gburski**
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Nanoscale aggregates of molecules exhibit different properties than bulk compounds [1]. Using the molecular dynamics simulation method [2] we study the system composed of fifty water molecules spread out evenly over fullerene surface. In our calculations we have applied the well-known Lennard-Jones interatomic potential. We have calculated the radial distribution function, velocity autocorrelation functions (linear and angular) and theirs corresponding spectra. Both solid and liquid state phases of $(H_2O)_{50}$ over C_{60} surface have been investigated. The considerable differences between dynamical properties of pure water cluster $(H_2O)_{50}$ and $C_{60}(H_2O)_{50}$ cluster are observed.

Atomic-scale Ab-initio computations of the B2-RuAl

poster H-30

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First Principles calculations based on Density Functional Theory (DFT) and the pseudopotential method have been used to study B2-structured RuAl. Formation and energies of points defects in RuAl intermetallic compound are computed by the ab initio pseudopotential method with the plane-wave basis set and the generalized gradient approximation (GGA). The bulk moduls is also calculated and the deformation under applied pressure. The results are in good agreement with available experimental data.

Ab-initio calculations of elastic properties Ni3Al and TiAl under pressure

poster H-31

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The structural parameters and the elastic stiffness coefficients of Ni_3Al and TiAl under pressures are computed by the ab initio pseudopotential method with the plane-wave basis set and the generalized gradient approximtion (GGA). The pressure dependence of the elastic constants is an important characteristic for both Ni_3Al and TiAl as these materaly are frequently subjected to varying pressure during their processing. The bulk moduls is also calculated. Stress-strain relations are used to obtain the elastic constants. For zero-pressure lattice constants, binding energy are calculated. The results are in good agreement with available experimental data.

Multifractal description of fracture morphology: quasi 3D analysis of fracture surface

poster H-32

Sebastian Stach[2)], **Jan Cwajna**[1)], **Stanisław Roskosz**[1)], **Jerzy Cybo**[2)]
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The paper presents verification of the multifractal analysis proposed in papers [1, 2]. It has been found that such analysis of simulated profiles formed by removing overlaps and secondary cracks from a real profile (which corresponds to a file obtained from a profilographometer), ensures a proper diversity of fractal characterization, adequately to the degree of fracture surface development of the investigated sintered carbide grades measured using a Taylor-Hobson's Talysurf 2 profilographometer.

Multifractal description of fracture morphology: full 3D analysis of fracture surface

Sebastian Stach[2], **Jerzy Cybo**[2], **Jan Cwajna**[1], **Stanisław Roskosz**[1] poster H-33

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An experimentally verified theoretical basis has been presented of the methodology of a materials' fracture morphology description using a multifractal analysis of a stereometrically examined surface (full 3D analysis). High effectiveness of a multifractal analysis has been shown for a diversified multifractal spectrum width and for a quantitative description of overlaps. The values obtained are very similar to those obtained by the quasi 3D method [1] as well as by a conventional analysis which is an analysis of profile images obtained from transverse microsections.
The presented method, however, is the least time-consuming, the cheapest and seems to be the most objective in the scope of fracture morphology analyses.

Symmetry on the plane - the CPD function

Kazimierz Stróż[1] poster H-34

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Symmetry of atomic layers as well as symmetry of mosaics, lattice designs, symmetry of electron diffraction patterns or any pattern with two-dimensional periodicity can be classified by their symmetry groups. For comparative studies of crystallographic structures the finer methods of classification / description are more appropriate (for example: "circle packings" -Niggli , "isohedral tilings" - Sinogowitz, "lattices complexes" - Niggli, "crystallographic orbits" - Wondratschek"). All these concepts are related with a set of symmetry equivalent points (G-orbit). The orbits are visualised as "crystallographic mosaics" (by connection of the closest points of the orbit), they can be characterised by Shubnikov or Laves nets and there always exists a number (circle packing density or shortly CPD) that is related to a given orbit. The CPD function introduced by the author and specially its contour map is a good frame for locating symmetry elements, asymmetric units or points with higher plane symmetry into a unit cell. Some conclusions relating the position of an atom in the unit cell and their dimension can also be drawn. The properties and constructions of CPD contour maps for all 17 plane groups will be given in this work.

NEW POSSIBILITIES OF LIGHT MICROSCOPY RESEARCHES RESULTING FROM DIGITAL RECORDING OF IMAGES

Agnieszka Szczotok[1], **Stanisław Roskosz**[1] poster H-35

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The article presents some examples of a digital camera application in acquisition and analysis of images obtained with light microscopy. The latest digital cameras for research microscopes employ an innovative shifting CCD system together with fast hardware processing to give high resolution of images and high speed imaging for easier focusing. An integration into the appropriate software makes possibilities for image acquisition, archiving and analysis. The new research microscopes are fully automated and motorized. All functions can be controlled using a PC (e.g. functions connected with focusing or stage positioning).
An unconventional technique used to create perfectly focused images presented in the article is an extended focus imaging. This is a module of microscope software which enables to acquire images of limitless depth of focus. Possession of a microscope equipped with a motorized stage is indispensable to this technique. Zinc layers on the cast iron, thermal barrier coatings on heat-resisting alloys and carbides in matrix of cobalt-base superalloy are the examples of using the extended focus imaging.
In this work using of automated stage management is also shown. It enables to create an overview image by combining single images of high resolution. It is important because the resolution of the overview image can be adjusted and new positions required for further analysis can be easily defined. This is particularly important in quantitative materialography because this technique enables significant decrease of edge effect. The results of using the stage management are presented for the following cases: duplex steel, elements made by nickel-base superalloy, weldings and during revealing macro grain in cobalt-base superalloy.
For these reasons the digital microscope with the automation assures a high performance and diversified program of examinations.

Methods of estimation of the Hurst exponent - the analysis of the usefulness in research of the surface fracture

poster
H-36

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The optical or mechanical registration processes introduce same systematical and accidental disfigurement in the fracture image. Differentiation between chaotic and determined components of the investigated images is a main problem of the presented work. Fractals and Multifractals based-theory and estimating of the Hurst exponent have been used for this differentiation. The aim of the paper was the selection of the most suitable method for the fracture surface analysis using modern tools to the mathematical verification of dataset containing irregular data values and the considerable variability of the amplitude. In the paper, the efficiency of several most popular methods used of this exponent has been checked on several chosen examples. There are three methods of the estimations of the Hurst exponent: R/S method, Roughness - Length (R - L) method and Variogram. The basic dependences have following forms [1÷4]:
1.) $R_{(w)}/S_{(w)}{}^{*}=cw^{H}$, 2.) $S_{(w)}=cw^{H}$, 3.) $V_{(w)}=\{[y(x)-y(x+w)]^2\},^{*}$
4.) $V_{(w)}=cw^{2H}$
where: $R_{(w)}$ - the difference of the height of the profile in the window, c - the constant , $S_{(w)}$ - the standard deviation, H - the Hurst exponent,w the width of the window (section), x and y are data coordinates . Exponent H is a slope of interpolated straight line in the log - log system.
(The mark * denotes of the mean value for the data on each of the windows)
The surface research of the fracture could be executed on the light microscope with two situated lenses in relation to the examined surface at an angle of 45^0. The noise in the range of high frequencies is generated on the edge dark and lucid areas of the microscopy images. Proposed procedure of the Hurst exponent calculating is verified for profiles obtained from the surface of the fracture of steel 18G2A in the rough and after Wavelet approximations. Described methods give considerably differed results. The R - L method is offering the best approximation for the investigated case

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Simulation on Production Process of Chalcopyrite Semiconductors under High Pressure

poster
H-37

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2) Kyushu University, Fukuoka, Japan

The I-III-VI2 compounds are direct energy-gap semiconductors showing very interesting electrical and optical properties, which can be applied in various fields. Solar cell technologies using Cu-III-VI2 based chalcopyrite semiconductors have made rapid progress in recent years. In particular, CuInGaSe2 (CIGS) based solar cells have been extensively reported in comparison to other chalcopyrite semiconductor based solar cells, primarily because of its large absorption coefficient (more than 105 cm-1 near the bandgap region) and its bandgap energy of between 1.0 and 1.7 eV at room temperature. Conversion efficiencies for polycrystalline CIGS based solar cells have been significantly improved over recent years and the best cell is now reported at 19.2 % [1]. On the other hand, Ag-III-VI2 based chalcopyrite semiconductors, especially AgGaS2, is promising material for nonlinear optics. AgInS2 is also respected for nonlinear optics as well as AgGaS2 material. However, AgInS2 has two crystal forms such as chalcopyrite and orthorhombic. The orthorhombic form is stable at more than 620 ? and the chalcopyrite form is stable at less than 620 ?. Therefore, a growth of chalcopyrite AgInS2 crystal is difficult .
In this work, molecular dynamics simulation was carried out in the following scheme. Atom positions, volume and velocity were revised in each time-step in the calculation using Gear?s fifth-order algorithm [2]. We cleared that diffusion constants of vacancy were also independent of high pressure and a vacancy diffuses with a switching mechanism to the nearest-neighbor in lattice site. Using this result, we could obtain AgInS2 single phase at 700 ?C under 22.5 MPa. The sample indicated a chalcopyrite structure, nearly stoichiometry and n-type by means of X-ray diffraction, electron probe microanalysis and thermo-probe analysis, respectively.

[1] K. Ramanathan, M. A. Contreras, C. L. Perkins, S, Asher, F. S. Hasoon, J. Keane,
D. Young, M. Romero, W. Metzger, R. Noufi,
[ABSTRACT TRUNCATED TO 2000 LETTERS]

Specific heat releated to details of the vibrational modes for a 2D nanocrystalline material

poster H-38

Wolfgang Hahn[1)]

1) Polish Academy of Sciences, High Pressure Research Center (UNIPRESS), Sokolowska 29/37, Warszawa 01-142, Poland

The relationship between specific heat and details of the vibrational modes of a twodimensional nanocrystalline model material (NCM) as a function of grain size and temperature has been investigated. The specific heat of the NCM was raised respective to that of a single crystal in the temperature range of about 28 K. This raise could be related to differences in the occupation of vibrational modes: The VDOS was subdivided in subspectra by means of the participation ratio (PR), which measures the fraction of the atoms contributing effectively to a given mode. The differences in the specific heat could be largely attributed to parts of such a subspectrum.

Mechanical properties of microcrystalline Ni3Al intermetallic alloy

poster H-39

Pawel JOZWIK[1)], **Zbigniew BOJAR**[1)], **WOJCIECH PRZETAKIEWICZ**[1)]

1) Military University of Technology (WAT), Kaliskiego 2, Warszawa 00-908, Poland

A significant influence of heat and thermo-mechanical treatment and additional plastic working parameters on structure and properties of two-phase (gamma prim + gamma) Ni3Al (Zr, B) intermetallics with zirconium and boron was shown in this paper.
As a result of long-lasting heat annealing at the temperature up to 1473 K, in duration up to 100-hours on effective modification of structure homogeneity (up to single gamma prim phase) and mechanical properties (tensile strength and yield point on the level of 700MPa and 300MPa adequately in as-cast, and 600MPa and 200MPa after annealing at 1273K/50h/air).
Using optimalized parameters of plastic and thermo-mechanical treatment, over 1000-times refinement of grains was obtained in investigated alloy (from irregular - shape crystals of 4 mm in linear dimension to 4 micrometers in diameter polyhedral grains). It was shown that fine- grained structure of investigated intermetallic alloy results in their plastifying. On the samples of fine - grained alloy it was confirmed that fractures occurred during tensile testing were ductile, the proof stress was low and the tensile strength was quite high (in chosen cases of Ni3Al based intermetallics after processing, the proof stress of 400MPa, the tensile strength of 1400MPa and over 50% unit elongation during tensile testing at room temperature were recorded).
Possibility to strengthening of fine-grained Ni3Al by cold rolling up to 50% reduction (100% reduction is also possible). Thin foils with thickness below of 0,4 mm without cracking were obtained. The yield point over 2200MPa, tensile strength over 2300MPa and unit elongation about 2% during a tensile testing at room temperature, in air were obtained for the material a such strengthened condition.
Singes of fracture by shear as results of tensile testing were shown and the fractures obtained were ductile.

Tuesday, September 7th

Morning session

Main Building, room 231

11:00 - 12:30

The Role of Quantum Mechanics in Virtual Aluminum Castings

11:00 - 11:30 invited oral

Chris Wolverton[1)]

1) Ford Motor Company (Ford), MD 3083/SRL, P. O. Box 2053, Dearborn, MI 48121, United States

Increasing demands to further reduce emissions and simultaneously improve fuel economy in automobiles has expanded the need for lightweight materials (such as Al, Mg, and their alloys). In order to optimize alloy design and processing conditions to quickly achieve Al-alloy castings with suitable mechanical properties, researchers at Ford Research Laboratory are developing

the Virtual Aluminum Castings methodology: a suite of predictive computational tools that span length scales from atomistic to macroscopic to describe alloy microstructure, precipitation, solidification, and ultimately, mechanical properties.

The role of first-principles atomistic computations in the Virtual Aluminum Castings methodology will be described, as will the connection between these atomistic methods and other computational approaches (phase-field microstructural models, computational thermodynamics methods, cluster expansion methods, etc.). Because of their highly accurate and predictive nature, there is a growing desire to use these types of theoretical approaches to predict properties of new, experimentally unexplored, or difficult-to-synthesize solids. Application to problems of precipitation, thermal growth, and microstructure evolution during heat treatment has proved very fruitful. Combining these quantum-mechanical results with other modeling and experimental efforts, one can suggest heat treatments which optimize thermal stability and hardness of industrial alloys.

Superconductivity and the grand periodic table of the chemical elements

11:30 - 12:00
invited oral

Wojciech Grochala[1)]

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

Existence of the various families of superconducting materials and their T_C values are rationalized within a simple model. "Magic ground electronic state" of superconducting matter is assumed to originate from the nontrivial avoided crossing between the electronic levels of the component chemical species, which enter the binary backbone of the multinary materials. Novel families of superconducting materials, particularly those based on fluoride and hydride anions, are predicted. Superconductivity is discussed in a broad framework including metallization of nonmetals and semiconductors, influence of the external pressure on the Peierls distortion, and dynamics of nuclear motion of the localized/delocalized mixed-valence species (molecular and in the extended phases).

Influence of the packing effect on stability and transformation of nanoparticles embedded in random matrices

12:00 - 12:15
oral

Helmut Hermann[1)], **Antje Elsner**[1)], **Dietrich Stoyan**[2)]

1) Leibniz-Institute for Solid State and Materials Research, P.O.Box 270116, Dresden D-01171, Germany

2) Freiberg University of Mining and Technology, Institute of Stochastics, Agricolastr. 1, Freiberg D-09596, Germany

We use the model of hard spheres to analyse the packing effect and its contribution to stability or instability of nanoparticles embedded in disordered structures. For each simulation the initial structure is generated in a cubic box including 10^4 to 10^5 spheres. The system is subjected to a densification procedure (force biased algorithm) under periodic boundary conditions. The structural analysis is based on the S-Voronoi tessellation. Each sphere and its neighborhood is characterised by its local packing fraction defined by the ratio of sphere volume and volume of the corresponding Voronoi cell.
If the initial coordinates of the sphere centres are chosen at random according to the Poisson distribution and if all sphere diameters are equal, the structure obtained after densification to the mean packing fraction of 0.64 corresponds to the well-known homogeneous dense random packing model of hard spheres (DRPHS). Enhancement of the mean packing fraction of monodisperse systems to values above 0.64 leads to the formation of nanocrystals embedded in the DRPHS matrix. The results point to the existence of a critical radius of the nanocrystals having face-centred cubic order and the local packing fraction of 0.74. If a sphere is surrounded by 12 neighbours touching the central sphere and being situated on the vertices of an icosahedron, the central sphere has a local packing fraction of 0.76. The simulation of systems containing such icosahedral clusters shows that maximum local and global packing density are competing principles.
The results of our computer simulations are discussed in connection with recent experimental results on the structure of liquid metals and alloys.

12:15 - 12:30
oral

ATOMISTIC MODELLING OF SUPERSTRUCTURE REFINEMENT IN CRYSTALLINE MATERIALS

Rafal Kozubski[1)], **Ewa Partyka**[1)], **Mirosław Kozłowski**[1)], **Veronique Pierron-Bohnes**[2)], **Wolfgang Pfeiler**[3)]

1) Jagiellonian University, Institute of Physics (IF UJ), Reymonta 4, Kraków 30-059, Poland

2) Institut de Physique et Chimie des Materiaux de Strasbourg, UMR7504, CNRS - ULP, 23, rue du Loess, BP 20, Strasbourg 67037, France

3) University of Vienna, Institute of Materials Physics, Vienna, Austria

Chemical ordering in multicomponent crystalline systems is of fundamental technological importance and knowledge of its dynamics (kinetics) is crucial in materials engineering. The process, however, always competes with the general tendency for entropy maximization and hence, at any non-zero temperature T finite concentration of antisite defects is observed and increases with increasing T. Consequently, a change of system temperature is followed by generation/annihilation of antisite defects, so-called "order-order" relaxation, whose mechanism (atomic migration) is the same as that of diffusion. The kinetics of both phenomena are different due to non steady-state conditions during relaxation. "Order-order" relaxation may be successfully modeled by computer simulations, which involves the following tasks: (i) approximation of system energetics (Hamiltonian), (ii) energetics and thermodynamics of structural defects (vacancies, interphases, surfaces), (iii) implementation of particular atomic-jump mechanism, (iv) adaptation/elaboration of computer codes.

"Order-order" relaxations have been modeled and simulated in binary systems showing different types of superstructures by combining Monte Carlo and Molecular Dynamics methods. Particular attention has been paid to the statistics (correlations) of atomic jumps, which appeared to control specific features of the relaxations experimentally observed in particular intermetallics and being important for designing technological processes. This concerns: different time scales active in the processes, differences between the activation energies for chemical ordering and for self-diffusion, differences between statically and dynamically modeled activation energies for atomic jumps, effective role of the high concentration of vacancies in increasing the rate of chemical ordering etc.

Current studies concern the effect of size limitation on "order-order" phenomena modelled in nanostructured intermetallics.

Lunch break

12:30 - 14:00

Afternoon session

Main Building, room 231

14:00 - 15:30

Deformation Mechanisms in Nanocrystalline Materials by Molecular-Dynamics Simulation

14:00 - 14:30
invited oral

Dieter Wolf[1)]

1) Argonne National Laboratory (ANL), 9700 South Cass Avenue, Argonne, IL 60439, United States

Large-scale molecular-dynamics simulations of nanocrystalline model microstructures were performed to elucidate the dislocation and grain-boundary mechanisms of plastic deformation in nanocrystalline materials. These simulations reveal how and why, at some critical grain size of the order of about 20 nm, the conventional dislocation-slip mechanism in fcc metals becomes ineffective in favor of a grain-boundary based deformation mechanism. In agreement with recent experimental observations, the simulations show that for the larger grain sizes, complete dislocations nucleate from the grain boundaries and grain junctions. Following their nucleation, these extended dislocations travel across the grains until they annihilate in some other grain boundary. A variety of well-known dislocation-dislocation interaction processes are identified and, for larger plastic strains (of typically $> 5\%$), extensive deformation twinning is observed. For the smallest grain sizes and in the absence of grain growth, these materials are found to deform via a mechanism involving an intricate interplay between grain-boundary sliding and grain-boundary diffusion.

Work supported by the U.S. Department of Energy, Basic Energy Sciences-Materials Sciences, under Contract W-3l-l09-Eng-38.

14:30 - 15:00
invited oral

Nucleation and polycrystalline growth in phase field theory

László Gránásy[1)], **Tamás Pusztai**[1)], **Tamás Börzsönyi**[1)]

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

A phase field theory of crystal nucleation and polycrystalline growth is presented. The model is tested for crystal nucleation in the hard-sphere system. It will be shown that evaluating the model parameters from molecular dynamics simulations, the phase field theory predicts the nucleation barrier accurately. Results of extensive simulations will be presented on transformation kinetics, particle-induced disorder ("dizzy" dendrites), and on the formation of various polycystalline structures, including spherulites. It will be shown that a broad variety of complex solidification morphologies can be recovered by changing only a few model parameters. Finally, heterogeneous crystal nucleation on foreign particles and walls, and solidification in confined volumes (channels, porous medium) will be addressed.

15:00 - 15:15
oral

Computational prediction of compositional separation, ordering and heat-capacity effects in surface-segregated binary & ternary alloy nanoclusters

MICHA POLAK[1)], **LEONID RUBINOVICH**[1)]

1) Department of Chemistry, Ben-Gurion University, Beer-Sheva 84105, Israel

The free-energy concentration expansion method (FCEM), originally derived for the theoretical prediction of surface segregation in the presence of short-range order in binary alloys [1], is an attractive tool for elucidating multicomponent nanocluster compositional structural phenomena [2] that are inaccessible by current experimental techniques. FCEM computations in conjunction with coordination-dependent energetic parameters were accomplished for Ni-Cu-Pd, Ni-Cu-Rh and Ni-Cu-Al nanocluster systems, containing up to 923 atoms with icosahedral and truncated octahedral shapes. The first two exhibit site-specific, sequentially competitive surface segregation of Cu/Pd and Cu/Ni, respectively, with resultant core separation of Ni and of Rh. Yet, remarkable differences, governed by the opposite hetero-atomic interactions, were noted in the surface segregated compositional patterns: "mixed" Cu/Pd ordering for Ni-Cu-Pd, and "demixed" order for Ni-Cu-Rh. The computations predict also in-surface rearrangement transitions reflecting the interplay of segregation and order. For Ni-Cu-Al, the much stronger Ni-Al interactions are manifested in compositional ordering that extends into the cluster core. Based on the FCEM data, thermodynamic properties such as the cluster mixing entropy and free-energy were computed for the three systems. The Ni-Cu-Rh clusters, with all-repulsive hetero-atomic interactions, were found to separate into three kinds of clusters, having different "magic number" compositions. Critical temperatures of inter-cluster compositional separation, computed for the Rh-Cu system, depend on both the cluster size and shape. Likewise, computations of the configurational contribution to the heat capacity vs. temperature reveal desegregation related characteristic features, which depend distinctly on the cluster size and shape.
[1] M. Polak and L. Rubinovich, Surf. Sci. Rep. 38, 127 (2000).
[2] L. Rubinovich and M. Polak, Phys. Rev. B 69, 155405 (2004).

15:15 - 15:30
oral

DIFFUSION MECHANISM AT THE GRAIN BOUNDARIES IN TWO-DIMENSIONAL METALS

Mikhail D. Starostenkov[1)], **Gennady M. Poletaev**[1)], **Roman Y. Rakitin**[1)]

1) Altai State Technical University (ASTU), Lenin st.46, Barnaul 656038, Russian Federation

The present paper is concerned with the research of diffusion mechanism at the grain boundaries in two-dimensional metals by the method of molecular dynamics. The diffusion of atoms was studied on the example of three metals: Ni, Al, Cu. The packing of two-dimensional crystals was corresponded to the plane [111] of FCC lattice. To describe interatomic interactions, pair Morse potentials were used. The metals under study were heated up to the temperatures, corresponded to 0.3 - 0.95 relatively to the melting temperature. Severe boundary constraints were applied on the boundaries of the calculated block.
It was found, that leading diffusion mechanism at the grain boundaries of two-dimensional metals was the result of interaction of grain boundary dislocation pairs. The creep of dislocation pairs in opposite sides was observed in the experiments. The rugged atomic row of one dislocation was lengthened at the expense of shortening of the other dislocation atomic row. In this connection, the chain of the displaced atoms was observed in the directions, connecting the nuclei of two dislocations. The inverse displacements of atoms ? the return of atoms in the initial positions, were observed. One of the important elements of similar mechanism is the appearance of the vacancy in the chains of the displaced atoms. The vacancy is the additional intensificating factor of diffusion. The trajectory of the vacancy migration from one nucleu

to the other one can have ring reserved elements, which are the cause of the appearance of ring exchange displacements of atoms at the boundary. The research showed, that the stresses, causing the migration of the boundary, temperature and density of grain boundary dislocations influence greatly on the diffusion velocity.

Wednesday, September 8th

Morning session

Main Building, room 231

09:00 - 10:30

Materials properties from ab initio approaches

09:00 - 09:30
invited oral

Raimund Podloucky[1)]

1) Institute f. Phys. Chemistry, Univ. Vienna (UNI WIEN), Liechtensteinstrasse 22A, Vienna A 1090, Austria

Based on computational results obtained in the framework of density functional theory for selected materials a variety of macroscopic quantities were investigated.
In particular, energies of formation and structural stabilities for Laves phases will be discussed in combination with their electronic, magnetic, elastic and vibrational properties in order to demonstrate the usefulness of ab initio approaches. Furthermore, by a combination of ab initio data and model potentials a model study of crack formation for materials with very different bonding properties is presented. Extending the studies on perfectly ordered compounds results will be presented for materials with point defects. Finally, the precipitation formation in a particularly interesting binary alloy will be discussed demonstrating the power of ab initio based approaches for bridging the length scales from the microscopic ab initio dimensions to dimensions for engineering.

Ab-initio thermodynamics of metal alloys: From the atomic to the mesoscopic scale

09:30 - 10:00
invited oral

Stefan Müller[1)]

1) Univesrität Erlangen-Nürnberg, Egerlanderstraße 1, Erlangen D-91058, Germany

Today, density functional theory (DFT) based calculations allow us to study a number of metal alloy properties, as e.g./ formation enthalpies, or electronic and elastic properties of intermetallic compounds. However, such so-called ab-initio calculations can only be applied as long as the alloy structure requires only small unit cells for the crystallographic description. It will be demonstrated how this limitation can be overcome without giving up the accuracy of DFT calculations by combining them with so-called Cluster Expansion (CE) methods and Monte-Carlo simulations. This concept gives access to both, huge parameter-spaces (e.g. for ground-state searches) and systems containing more than a million of atoms (e.g. for microstructure studies). It permits to treat alloy properties which possess a delicate temperature-dependence like mixing enthalpies, short-range order, coherent phase boundaries, or microstructure evolution {/em without} any empirical parameters as input, but with an accuracy that allows the {/em quantitative} prediction of experimental results. The presented examples reach from fcc- and bcc-based disordered alloys up to intermetallic compounds. Regarding microstructures the focus is on so-called coherent precipitates whose size-shape relations can be of technical relevance in alloys like Al-Li or Al-Zn. At the moment, the presented methods are extended to alloy surfaces for investigations of ordering phenomena at surfaces and surface segregation, i.e. the deviation of the alloy's composition in the near-surface region compared to the bulk. The first example represents the segregation of so-called antisite atoms in CoAl(100) and will be shortly discussed at the end of the talk.

10:00 - 10:15
oral

Modelling and ab initio calculation of electronic structure of lead and cadmium tungstate crystals doped with the rare-earth ions

Sergiy G. Nedilko[1)], **Yuriy A. Khyzhnyy**[1)], **Oksana V. Chukova**[1)]

1) Department of Physics, Taras Shevchenko Kyiv University, 6 Gloushkov avenue, Kiev 252022, Ukraine

The paper presents both theoretical and experimental study of spectral properties of the lead and cadmium tungstate crystals doped with some rare earth (RE) ions (Pr^{3+}, Sm^{3+}, Dy^{3+}, Eu^{3+}). Optical and luminescence properties of these crystals were investigated in a wide temperature region at the different excitation and registration wave length. Analysis of the Stark levels structure allows us to do conclusion about existence of two type of the emission centers formed on a basis of the RE^{3+} ions arranged in the different positions of the $PbWO_4$ and $CdWO_4$ crystal lattices.
Calculations of the electronic structure of the pure and doped crystals also were carried out.
Two methods of calculations are applied. Electronic band structures of perfect crystals are calculated by full-potential LAPW method using WIEN2k program code [1]. Electronic structures of luminescence centers of the crystal were investigated in cluster approach. The electronic structures of molecular clusters constructed by 9 - 14 formula units are ab-initio calculated by the Restricted Hartree-Fock method using GAMESS program [2]. Results of both calculations are compared and analyzed together with experimental results on luminescence and absorption spectra of the tungstate crystals. General remarks concerning the applicability of band theory and cluster methods for investigation of the electronic properties of wide-gap dielectric crystals are made.
Comparison between electronic structure of the pure and doped crystals was done.
The work is supported by STCU Project#2042.

[1] P. Blaha, K. Schwarz, G. Madsen, D. Kvasnicka and J. Luitz, WIEN2k, An Augmented Plane Wave Local Orbitals Program for Calculating Crystal Properties (Karlheinz Schwarz, Techn. Universität Wien, Austria), 2001. ISBN 3-9501031-1-2
[2] Schmidt M.W., Baldridge K.K., Boatz J.A., et al. // J.Comput.Chem. - 1993. - v. 14. - p. 1347.

10:15 - 10:30
oral

Ab-initio studies of the electronic and optical properties of half-metallic photovoltaic materials

Perla Wahnón[1)], **Pablo Palacios, Julio J. Fernandez, Cesar Tablero**

1) ETSI Telecomunicación. Universidad Politécnica de Madrid (ETSIT-UPM), Ciudad Universitaria, Madrid 28040, Spain

Using first principles calculations, band structures properties and optical transitions for novel photovoltaic materials with improved optoelectronic properties are been studied(1). This kind of materials characterized by an isolated intermediate band located in the semiconductor energy band-gap, may absorb below bandgap energy photons to promote electrons from the valence band to the conduction band using the half filled intermediate band.
We have proposed, using accurate ab-initio calculations based on Density Functional Theory, several alloys semiconductors containing a transition metal atom, presenting an isolated half metallic intermediate band (MIB) and both direct and indirect band-gaps in their structures(2). Recent exact exchange (EXX) calculations confirm the existence of the MIB(3). Spin polarized calculations carried out on these materials present in some of them large spin-polarization at the Fermi energy level.
To present the optical transitions characteristic of this type of intermediate band solar cell, we use the wave functions already determined for the transitions matrix elements and phonons dispersions curves determined also by quantum mechanic calculations.

(1)- P. Wahnón and C. Tablero, Phys. Rev. B. 65 165115 (2002).
(2)- C. Tablero and P. Wahnón, Appl Phys. Lett, 82, 151 (2003).
(3)- J.J. Fernández, C. Tablero and P. Wahnón, J. Chem. Phys. 120, 10780(2004)

10:30 - 11:00

Coffee break

Morning session - continued

Main Building, room 231

11:00 - 12:30

Vibrational and thermodynamical properties of solids

11:00 - 11:30
invited oral

Krzysztof K. Parlinski[1)]

1) Polish Academy of Sciences, Institute of Nuclear Physics (IFJ PAN), Radzikowskiego 152, Kraków 31-342, Poland

The possibility to use density-functional theory (DFT) for description of the crystal structure, lattice dynamics, vibrational frequencies, thermodynamical functions and phase transitions will be refered. The DFT is used to provide the minimum ground state energy of a supercell and gives the crystal structure at T=0K. Phonon calculations allow to extend the properties to a finite temperature. Phonons are calculated with the direct method (http://wolf.ifj.edu.pl/phonon/) from the Hellmann-Feynman forces.
The phonon dispersion curves of GaN were predicted before confirming them by X-ray inelastic scattering measurements. We found that in SnO_2 a soft mode accompanies the ferroelastic phase transition occuring under pressure. Phonon dispersion curves and phonon density of states can be calculated in tetragonal chalcopyrites ($CuInSe_2$, $AgGaS_2$, $AgGaSe_2$), orthorhombic $MgSiO_3$ and cubic Mg_2SiO_4 minerals, and ferroelectric material $LiNbO_3$. They also allow to calculate the thermodynamical functions, and predict the properties under finite temperature. We have calculated the phonon dispersion curves of the well-known shape memory alloy NiTi. austenite, martensite and R-phase of NiTi and confirmed the R-phase to martensitic phase transition from calculated free energies. Similar phase transition temperature was computed for ceramic ZrO_2. The phonon density of states of Fe dopped intermetalic NiAl lead to a local modes confirmed by the inelastic nuclear absorption.

Atomic structure and intermediate range order in network-forming disordered materials

11:30 - 12:00
invited oral

Carlo Massobrio[1)]

1) Institut de Physique et de Chimie des Materiaux de Strasbourg (IPCMS), 23, Rue du Loess, Strasbourg F-67034, France

In network forming liquid and glasses, structural order extends well beyond nearest-neighbor distances, leading to the appearance of a first sharp diffraction peak in the total neutron structure factor. Whenever available, partial structure factors convey an even more detailed set of information on the structure of these systems. In particular, the existence of concentration fluctuations at short and intermediate range distances is revealed by the behavior of the corresponding concentration-concentration structure factor. Computer modelling at the atomic scale is ideally suited to link the presence of this signature to specific features in real space, provided chemical bonding is accurately described. We reach this goal by addressing these issues within the framework of first-principles molecular dynamics.
This talk will focus on short and intermediate range order in prototypical disorder AX_2 networks: $SiSe_2$, $GeSe_2$ and $GeSe_4$. We have obtained a picture of amorphous $SiSe_2$ fully consistent with diffraction data, the number of Si atoms in corner and edge-sharing configurations following closely the experimental estimate. By focusing on all possible sequences of three Si atoms, we show that the series made of both corner and edge-sharing connections are more numerous than those formed exclusively by edge-shared atoms.
In the case of liquid $GeSe_4$, we have focused on a comparative study of the charge-charge S_{zz} and the concentration-concentration S_{cc} structure factors. We found that the first sharp diffraction peak is present in S_{cc} while it is absent in S_{zz}. This shows the inadequacy of point-like charge models in the treatment of highly ionic disordered materials, the two structure factors being simply proportional witin this approach. Our results suggest that a structural frustration due to the constraint of charge neutrality lead to the appearance of concentration fluctuations at intermediate range distances.

Structural properties of MnTe, ZnTe, and ZnO, and phase stability of $Mn_xZn_{1-x}Te$ alloy

12:00 - 12:15
oral

Nevill Gonzalez Szwacki[1)], **Piotr Boguslawski**[1)]

1) Polish Academy of Sciences, Institute of Physics, al. Lotnikow 32/46, Warszawa 02-668, Poland

Epitaxial growth of semiconductors under pseudomorphic conditions leads to stabilization of crystallographic structures that are unstable at equilibrium is observed. For example, the stable phase of MnTe is NiAs, but epitaxial layers of MnTe with the zinc blende structure have been grown on GaAs substrates

[1]. Stability of a given phase of the overlayer depends on parameters such as its lattice constant, and also - in the case of alloys - on the alloy composition.

Using Density Functional Theory within the Local Spin Density Approximation and atomic pseudopotentials we have studied phase stability, elastic properties, and electronic structure of ZnO, ZnTe, and MnTe. We have considered NiAs, wurtzite (W), and zinc blende (ZB) structures. As a result we have obtained the equilibrium lattice parameters for all considered phases and their elastic constants, together with pressure coefficients of the band gaps. In agreement with experiment we find that the stable phase of ZnO is W, lower in energy by 10 meV/atom than the ZB phase, while cubic ZnTe is more stable by 5 meV/atom than the W phase. For both crystals, the NiAs structure is highly unfavorable, being higher in energy by 250 meV/atom. On the other hand, the stable structure of the antiferromagnetic semiconductor MnTe is NiAs, which are lower in energy than the ZB and the W phases by about 100 meV/atom. Finally, we have considered $Mn_xZn_{1-x}Te$ alloy, which according to our calculations changes the equilibrium phase from NiAs to ZB for the Mn content of about 0.75. The impact of the magnetic ordering on the stabilization of crystalline phases will be discussed. The calculated bowing parameters of the energy gap of $Mn_{0.5}Zn_{0.5}Te$ in NiAs and ZB phases are small, and equal to 0.05 and 0.09 eV, respectively. A comparison with experimental morphology [1] of $Mn_xZn_{1-x}Te$ will be given.

[1] E. Przeździecka et al., to be published.

12:15 - 12:30
oral

Atomic Configuration of Nanocontact: Ionic Shell and Sub-shell Structures

Pedro García-Mochales[2)], **Pedro A. Serena**[2)], **Carlo Guerrero**[1)], **Ernesto Medina**[1)], **Anwar Hasmy**[1)]

1) Centro de Física, IVIC (IVIC), Caracas 1020A, Venezuela

2) Instituto de Ciencia de Materiales de Madrid, CSIC (ICMM, CSIC), Cantoblanco, Madrid 28049, Spain

We perform a statistical study of the preferred atomic configuration of nanocontact breakage and their minimun cross section histogram for several elements (aluminium, nickel, gold), a wide range of temperature (4-450 K) and different initial atomic configurations. Nanowires rupture is simulated using molecular dynamics (MD) and embedded atom method (EAM). We use state-of-the-art many body EAM interatomic potentials able to fit bulk and surface properties.
Starting with a parallelepiped of hundreds of atoms ordered according to a fcc structure, first we relax the initial structure. Then we stretch the nanowire separating two frozen bilayers slabs (at the top and bottom of the supercell) at a constant velocity of $2*10^{-4}$ /s. The simulation is carried out until the nanocontact breaks (the minimum cross section is zero). The full determination of atomic position during the contact allows us to know the changes of the nanocontact geometry and to evaluate the evolution of the minimum-cross section S_N in terms of the number of atoms. By accumulating conductance traces for the same initial atomic configuration, we built minimum cross-section histograms $H(S_N)$. In several cases, the histogram is constructed using a single simulation where the nanowire is put repetitively in and out of contact.
The result helps to the understanding of the (experimental) conductance histogram peaks based on preferential geometrical arrangements of nanocontact necks. As temperature increases, lower conductance peaks decrease in favour of broader and higher conductance structures, revealing the existence of favoured shell and sub-shell structures. The relative preference of atomic arrangements depends of the stretching direction and the how the nanowire is obtained.

12:30 - 14:00

Lunch break

14:00 - 15:30

Afternoon session

Main Building, room 231

14:00 - 14:30
invited oral

Vibrational properties and thermochemistry from first principles

Walter Wolf[1)], **Jürgen Sticht**[1)], **Alex Mavromaras**[1)], **Paul Saxe**[1)], **Erich Wimmer**[1)]

1) Materials Design, 44 avenue F.-A. Bartholdi, Le Mans 72000, France

For decades, ab initio calculations have been largely viewed as being restricted to 0K, or more precisely, as being condemned to operate without the concept of temperature at all. Nowadays, this major constraint has been lifted, and routine methods to evaluate vibrational properties and temperature dependent thermodynamic functions have become available, at least within the harmonic approximation. In this contribution, the basic concepts of the so-called direct approach [1,2] to vibrational properties are summarized and a number of applications in rather diverse fields are discussed. In a routinely manner, free energies, vibrational enthalpies and entropies of solid compounds can be evaluated, thus enabling the study of thermochemistry of chemical reactions as well as phase stability from ab initio theory. As will be shown, in particular for hydrogen containing compounds, neglecting zero point vibrations may cause qualitatively wrong answers in many cases. In addition, phonon instabilities of metastable phases may point towards possible phase transformations to other stable phases. Furthermore, vibrational spectra of transition states are well suited for the study of chemical kinetics as well as transport properties, opening the field for simulating diffusion processes. The methodology is, however, not restricted to the solid state: vibrations of molecules and molecules on surfaces may help to analyze spectral data, and the calculation of surface phonons are well suited to confirm stability of a suggested surfaces or may reveal possible reconstructions, just to mention some of the rather promising though challenging applications. Complementing the successful case studies, possible computational issues and difficulties are discussed thus providing a critical assessment of the methodology.

[1] K. Parlinski, Z. Q. Li, Y. Kawazoe, Phys. Rev. Lett. 78, 4063 (1997)
[2] G. Kresse, J. Furthmüller, J. Hafner, Europhys. Lett. 32, 729 (1995)

Magnetic and Electronic Properties of new Ferrimagnet $Sr_8CaRe_3Cu_4O_{24}$

14:30 - 15:00
invited oral

Masanori Kohno[1], **Xiangang Wan**[1], **Xiao Hu**[1]

1) National Institute of Material Science (NIMS), Tsukuba, Japan

Magnetic and electronic properties of the recently discovered material $Sr_8CaRe_3Cu_4O_{24}$ are investigated by means of the quantum Monte Carlo method and the LSDA+U method. Based on the LSDA+U calculation, we show that the ground state is an insulator with magnetic moment $1.01\mu_B$, which is consistent with experimental results. Further, we specify magnetic sites and derive an effective model for the magnetic properties of this material. The resultant effective model is a three-dimensional Heisenberg model with spin-alternation. Cu sites with spin 1 (Cu1) form a cubic lattice, and Cu sites with spin 1/2 (Cu2) are located between them, where neighboring spins are coupled antiferromagnetically. Finite-temperature properties of this effective model are investigated by the quantum Monte Carlo method (continuous-time loop algorithm). Our numerical results are consistent with experimental results, indicating that the effective model is suitable for this material. Through the analysis of the effective model, we make some predictions for this material.

Phase transition in the Nd-Fe-B system

15:00 - 15:15
oral

Jacek Piechota[1], **Witold R. Rudnicki**[1], **Marek Niezgódka**[1]

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The aim of the study is to examine the high-temperature phase transitions in the Nd-Fe-B system (hard magnetic material). The problem is solved by building up a simple mechanical model, which describes a system under deformation. The pressure—degree of deformation—binding energy relation is studied. In this approach the binding energy is substituted by the total energy, and the degree of deformation is related to the deformation of the unit cell (Δa, Δb, Δc). When approaching the point of equilibrium there is a non-zero probability that the system melts. Self-consistent density functional calculations of the electronic structure of the Nd-Fe-B system are carried out in order to determine the dependence of the total energy on the deformation of the unit cell.

Poster session - continued

19:00 - 21:00

Thursday, September 9th

09:00 - 10:30

Morning session

Main Building, room 231

09:00 - 09:30
invited oral

The Embrittlement of Cu by Bi: explanation based on first-principles calculations

Mike W. Finnis[1)], **Tony Paxton**[1)], **Rainer Schweinfest**[1,2)]

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2) science and computing ag, Hagellocher Weg 71, Tübingen 72070, Germany

The fact that traces of the element Bi embrittle the normally ductile metal copper has been known for over a hundred years. There have been some previous attempts to explain this and similar phenomena in terms of a weakening of Cu-Cu bonds by withdrawal of elecrons by the impurity atoms segregated at grain boundaries. Another class of explanation refers to a possible 'stiffening' of the bonds around an impurity, thereby reducing the local ductility. We have made a series of calculations using density functional theory to study electronic structure, the strength of bonding across a grain boundary (Σ19a) and the local 'stiffness' of bonds.

Our findings cast doubt on the conventional explanations. Bi is a much larger atom than Cu. However, it has negligible effect on bond-stiffness in the direction required for dislocation mobility, on the (111) plane. Neither does it withdraw electrons from Cu-Cu bonds. The explanation instead is a simple size effect, which drives segregation to boundaries that have excess volume, where the Bi atoms 'lever' the Cu atoms apart. We have repeated our calculations for the embrittling element Pb, also an oversized impurity,and find a very similar set of results.

09:30 - 10:00
invited oral

Theoretical study on electron transport properties of an organic molecule

Jun Nara[1)], **Takahisa Ohno**[1,2)]

1) National Institute of Material Science (NIMS), Tsukuba, Japan

2) and Institute of Industrial Science, University of Tokyo, 4-6-1 Komaba, Megro, Tokyo 153-8505, Japan

Recently, the transport properties of single-organic molecules have attracted much attention. One of the most prominent systems in this field is a dithiolate molecule between gold surfaces. Since the conductance of a benzene-(1,4)-dithiolate (BDT) sandwiched with two gold electrodes is experimentally measured, it has been intensively investigated in the theoretical field. However, it is still unclear how the conductance depends on the atomic configurations around the contact. Knowing how the contact geometry influences the conductance through the metal/molecule/metal sandwich structure requires both a precise determination of the molecule/metallic-electrode interface structure and an evaluation of the conductance for different geometries with a fair accuracy. We investigated the transmission properties of a BDT molecule sandwiched between two gold electrodes by means of ab initio method, and examined the effect of the contact structures on it. The transmission coefficients are evaluated with the Lippmann-Schwinger equation. It is found that the peak energies and the peak widths in the transmission curves are sensitively dependent on the contact structures. Furthermore, the contributions of molecular orbitals (MOs) of the BDT molecule to the transmission coefficient also depend on the contact structures. Especially, only some of MOs contribute to the conductance at zero bias. It is also found that the interactions beyond first-nearest neighbors could have remarkable effect on the transport properties. These results suggest that the determination of the contact structure including the electrode system is essential to estimate the transport properties of molecular devices.

This work is supported by ACT-JST, FSIS, and the Special Coordination Funds of MEXT of the Japanese Government. The calculations were carried out using the Numerical Materials Simulator in NIMS.

10:00 - 10:15
oral

First principles molecular dynamics simulations for amorphous HfO_2 and $HfSiO_2$

Minoru Ikeda[1)], **Georg Kresse**[2)], **Hidetoshi Nabatame**[1)], **Akira Toriumi**[3,4)]

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Japan
4) Department of Materials Science School of Engineering, University of Tokyo, 7-3-1, Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

Recently, HfO_2(hafnia) grown on Si substrates is widely studied as a potential candidate for replacing SiO_2 as the gate dielectrics in scaled CMOS. This thin film grows as an amorphous phase like a SiO_2 gate oxide. In order to increase the crystallization temperature and improve the device performance, several ingredients such as Si, N and Al atoms are incorporated in the high-k gate oxides. Although Zhao and Vanderbilt reported the amorphous phase of ZrO_2 using the ab-initio method, the amorphous HfO2 has not been studied theoretically. In this report, we present the amorphous HfO_2 and $HfSiO_2$ using the Projector Augmented Plane Wave method. We also analyzed the structure of the amorphous HfO_2 and the effects of the inclusion of Si atoms by changing the atomic concentration. Amorphous HfO_2 and $HfSiO_2$ are obtained by employing Zhao-Vanderbilt prescription. Our model employed 96 and 117 atoms in the cubic cell. After elevating the temperature of the system to 4000K and melting the system in 12ps, we gradually decreased the temperature in 200ps. In our amorphous structures there exist several pore channels with diameters 3-4 A like a SiO_2 case. If we increase the Si concentration, the size of the pore channels increases and lots of space appears. The oxygen atoms with the coordination number 2 increases linearly with the Si concentration. We found that the phase separation between HfO2 and SiO2 occurs at $Hf_{0.3}Si_{0.7}O_2$. By using our pure amorphous hafnia model, we analyze the problem that boron atoms doped in the poly-Si gate penetrates into the Si substrate through the amorphous hafnia. The estimated barrier height of boron diffusion using monoclinic crystal model was 2.5 eV and contradicts with the very fast diffusion. Our estimated barrier height is 1.2 eV and fairly explains the observed boron diffusion in amorphous HfO2. And thus our amorphous structure models seem to be useful in understanding the actual systems. This work was supported by NEDO.

Ab Initio Calculations of the Critical Values of Elastic Energy Density

10:15 - 10:30
oral

Kinga T. Nalepka[1)], **Pawel Nalepka**[2)], **Ryszard B. Pecherski**[1,2)]

1) Cracow University of Technology, Institute of Structural Mechanics, Warszawska 24, Kraków 31-155, Poland

2) Polish Academy of Sciences, Institute of Fundamental Technological Research (IPPT PAN), Świętokrzyska 21, Warszawa 00-049, Poland

An energy-based approach to limit states in elastic solids of arbitrary anisotropy was developed by Rychlewski [1]. It is based on the theory of elastic eigen-states and the concept of energy orthogonal stress states, which make it possible to decompose additively the elastic energy density into not more than six disjoint parts. Such an approach can appear also helpful in the field of nanomechanics filling the gap between atomistic calculations and continuum mechanics modelling of the behaviour of different kinds of crystalline nanostructures and macroscopic material properties. Under the limit state in nanostructures, we can understand the limit of linear elastic behaviour. We propose to calculate the critical energy of pertinent elastic eigen-states from quantum mechanical theory of nc-metals [2]. The analysis is confined to the cubic crystals. In such a case, three elastic eigen-states exist. The quantum mechanical model for an ideal single crystal of Cu is studied and the comparison with the results obtained for Al crystal is made. Using the Wigner-Seitz cellular approach and the Slater method the structure of the s, d, f and p energy bands was calculated. This enables obtaining of the internal energy of the crystal volume confined in the deforming Wigner-Seitz cell. Finally the critical energy for the particular elastic eigen-state was determined.
Acknowledgement: The work supported by the Ministry of Science within the framework of the research project PBZ-KBN-095/T08/2003-2006.
1. J. Rychlewski, Elastic energy decomposition and limit criteria, Uspekhi Mekh.-Advances in Mech., 7, 51-80, 1984 (in Russian) and: Unconventional approach to linear elasticity, Arch. Mech., 47, 149-171, 1995.
2. K. Nalepka, R.B. Pęcherski, Energy-based criteria of limit states. How to calculate energy limits from first principles, Rudy Metale, R48, 533-536, 2003 - in Polish.

Coffee break

10:30 - 11:00

Morning session - continued

11:00 - 12:30

Main Building, room 231

11:00 - 11:30
invited oral

Density-functional study of oxygen adsorption on Mo(112)

Adam Kiejna[1)], **Risto M. Nieminen**[2)]

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2) Helsinki University of Technology, Laboratory of Physics (FYSLAB/HUT), Otakaari 1 M, Espoo 02150, Finland

Molybdenum surfaces attract substantial current interest because of their important applications and fundamental properties.
Mo is one of the most interesting catalysts for its various oxidation states and a wide range of chemical reactivity. Oxidation of Mo strongly alters the dissociative adsorption of several molecules.
In this work atomic oxygen adsorption on the Mo(112) surface has been investigated by means of first-principles total energy calculations. The stability of different sites and configurations of O adatoms is explored. Among the variety of possible adsorption sites it was found that the bridge sites between two Mo atoms of the top row are favored for O adsorption at low and medium coverages.
At about one monolayer coverage oxygen atoms prefer to adsorb in a quasi-threefold hollow sites coordinated by two first-layer Mo atoms and one second layer atom. Thus, a site exchange transition from bridge to quasi-threefold hollow sites is predicted. The structure and stability of an oxygen-induced p(2 x 3) reconstruction of the missing-row type is examined and discussed.

11:30 - 12:00
invited oral

Using local orbitals to compute dynamical properties of materials

Pablo Ordejon[1)]

1) Instituto de Ciencia de Materiales de Barcelona, CSIC (ICMAB), Campus UAB, Bellaterra, Barcelona 08193, Spain

The efficiency of electronic structure methods based on local orbitals makes them very competitive compared with traditional techniques such as plane waves. One of these methods, SIESTA, has proved extremely useful in hundreds of studies of a wide range of properties of materials. In this talk, I will present some results of recent efforts on studying dynamical properties of materials (both atomic and the electronic). With respect to atomic dynamics, these efforts include the calculation of difusion barriers of defects in solids, and the determination of phase diagrams in materials. Concerning the electronic dynamics, important advances have been made in calculating precise absorption spectra of clusters and molecules through Time-Dependent DFT, and non-equilibrium electronic transport in the ballistic regime in nano-scale structures. I will review selected examples of these subjects, to give a wide overview of the status of some of the current developements in the SIESTA project.

12:00 - 12:15
oral

Surface phase diagram of CoAl(100)

Ole Wieckhorst[1)], **Stefan Müller**[1)], **Lutz Hammer**[1)], **Klaus Heinz**[1)], **Ralf Drautz**[2)], **Manfred Fähnle**[2)]

1) University Erlangen-Nürnberg, Lehrstuhl für Festkörperphysik, Staudtstr. 7, Erlangen 91058, Germany

2) Max-Planck Institut fuer Metallforschung (MPI-MF), Heisenbergstr. 3, Stuttgart D-70569, Germany

The combination of density functional theory (DFT) with concepts from statistical physics is applied to construct a DFT-based phase diagram for a binary alloy surface without any empirical parameters. While treating the results of DFT calculations within a thermodynamic model reveals the stable ordered phases, application of a cluster expansion in conjunction with Monte Carlo simulations allows to treat short range order in the alloy surface.
As an example, we studied the structure and stability of the B2-CoAl(100) surface consisting of alternating Co- and Al-layers. For ideal bulk stoichiometry, the surface shows a termination by the Al-sublattice. However, a tiny surplus of Co-atoms in the bulk, equivalent to the existence of antisite atoms, i.e. Co-atoms on the Al-sublattice, leads to the segregation of such antisites to the surface. Based on DFT calculations in combination with an appropriate thermodynamic model, it is possible to construct a phase diagram for the CoAl (100) surface. While still based on the assumption of a long range ordered surface, comparison of the structural parameters of the predicted stable phases are in quantitative agreement with

those retrieved from LEED structure determinations. However, with long range order assumed the model fails to describe short range order of the antisite atoms as observed for CoAl(100). The limitations of our model, which is based only on long range ordered DFT calculations, can be overcome by combination of the DFT calculations with a cluster expansion (CE) and Monte-Carlo (MC) simulations. This approach considers both layer dependent interactions and configurational entropy. Thus, we can study ordering phenomena and segregation profiles of metal alloy surfaces.

Combined Surface Science and Density Functional Theory Approach towards Water Ordered Structures Formation on Magnetite

12:15 - 12:30
oral

Maria E. Grillo[1)], **Wolfgang Ranke**[2)], **Carsten Menke**[1)]

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2) Max-Planck-Gesellschaft, Fritz-Haber-Institut, Faradayweg 4-6, Berlin D-14195, Germany

The interaction of water with iron oxide surfaces is relevant for several processes of practical interests. Three different adsorbed water species were distinguished on Fe-terminated Fe_3O_4 multilayer films using thermal desorption spectroscopy (TDS), and ultraviolet photoelectron spectroscopy (UPS) measured under adsorption-desorption equilibrium conditions [1]. By means of density functional theory (DFT) calculations, the first species (γ-water) were confirmed to correspond to dissociative water adsorption with the resulting hydroxyl (OH) groups of water on the surface iron (Fe) sites and the H-atoms adsorbed onto surface oxygen (O) sites. The DFT result for the γ-water structure is consistent with the two OH-stretch lines observed by infrared-reflection-adsorption-spectroscopy (IRAS) [2], and the UPS study [1]. The DFT calculations confirm the subsequent formation of mixed molecular- and dissociated-water structures (β-water) formed by H-bonded molecular water to the surface OH-groups on surface-Fe, and the H on the surface-O sites, respectively, as suggested by the IRAS [2] and LEED experiments [2]. The DFT results reveal that formation of the γ-water overlayer structure results from the diffusion of the mobile H-atoms from the initially molecular adsorbed water on iron sites followed by formation of a transition structrure with the H-atom adsorbed the nearest-neighboring oxygen sites, diffusing over the surface to adsorb on-top onto the next O-sites.

[1] W. Weiss and W. Ranke, Prog. Surf. Sci. 70, 1 (2002).
[2] U. Leist, W. Ranke and K. Al-Shamery, Phys. Chem. Chem. Phys. 5, 2435 (2003).

Lunch break

12:30 - 14:00

Afternoon session

Main Building, room 231

14:00 - 15:30

PLASTIC PROPERTIES OF GaN AND Al_2O_3 CRYSTAL: FEM-SIMULATION OF NANOINDENTATION CONFIRMED BY HIGH-RESOLUTION MICROSCOPY

14:00 - 14:30
invited oral

Roman Nowak[1)], **Timo Manninen**[1)], **Kari Heiskanen**[1)], **Ari Lehto**[1)], **Fusahito Yoshida**[2,6)], **Mike Leszczynski**[3)], **Jozef Lelatko**[4)], **Henryk Morawiec**, **Krzysztof J. Kurzydlowski**[5)]

1) Helsinki University of Technology, Materials Science & Rock Engineering (HUT / TKK), Vuorimiehentie 2 A, Espoo FIN 02015, Finland

2) Department oFaculty of Engineering, Hiroshima University, (HU), Kagamiyama 1-4-1, Higashi-Hiroshima 739, Japan

3) Polish Academy of Sciences, High Pressure Research Center (UNIPRESS), Sokolowska 29/37, Warszawa 01-142, Poland

4) University of Silesia, Institute of Material Science, Bankowa 12, Katowice 40-007, Poland

5) Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland

6) Faculty of Engineering, Hiroshima University, Kagamiyama 1-4-1, Higashi-Hiroshima, Japan

The elastic properties of GaN were evaluated by Schwarz et al.,[1] Yu et al.[2] and finally confirmed by Nowak's et al.[3] nanoindentation testing that agreed with the earlier first principles calculations.[4−5] Our previous results run contrary a common expectation that GaN is particularly brittle material.[3] Despite its high Young's modulus (295 GPa) and hardness (20 GPa), the nanoindentation stress-strain curves suggest elasto-plastic behaviour of the crystal. Consequently, the present research aims to resolve the surface deformation of GaN by using both microscopic observation of the surface features and structure, as well as finite element simulation of the nanoindentation deformation.
The HRTEM of the GaN structure revealed perfect atom arrangement in the crystals obtained by the self-seeding process under the pressure of $15x10^8$ Pa and supplied by High Pressure Research Centre. The AFM examination of residual impressions, led to registration of the profile of the deformed surface that was compared with the FEM-simulated surface pile up around indenter. This resulted in FEM-based correction of the yield point of GaN. The lack of indentation cracks and the pile-up served as a qualitative experimental proof of low-brittleness of GaN - predicted by numerical simulation.
The FEM-simulation of nanoindentation deformation of Al_2O_3 crystal was a proper comparison for a less-examined GaN and proved effectiveness of the analysis.[6]

1. R. Schwarz et al., Appl. Phys. Lett. 70, 1122 (1997)
2. G. Yu et al., J. Cryst. Growth 189, 701 (1998)
3. R. Nowak, M. Pessa, M. Suganuma, M. Leszczynski, I. Grzegory, S. Porowski and F. Yoshida, Appl. Phys. Lett. 75, 2070 (1999)
4. V. Fiorentini et al., Phys. Rev. B 47, 13353 (1993)
5. K. Shimada et al., Jap. J. Appl. Phys, 37, L1421 (1998).
6. R. Nowak, T. Manninen, K. Heiskanen, T. Sekino, A. Hikasa, K. Niihara and T. Takagi, Appl. Phys. Lett. 83, 5214 (2003)

Ab-initio calculation of the influence Cr-microalloying on the mechanical properties of NiAl

14:30 - 14:45
oral

Petr Lazar[1,2)], **Raimund Podloucky**[1,2)]

1) Institute f. Phys. Chemistry, Univ. Vienna (UNI WIEN), Liechtensteinstrasse 22A, Vienna A 1090, Austria

2) Center for Computational Material Science (CMS), Gumpendorferstrasse 1A, Wien A-1060, Austria

NiAl is a very promising high temperature material but it is brittle at low temperatures.
We present ab-initio calculations of the influence of chromium impurities on the mechanical behaviour of NiAl, because chromium alloying is believed to improve the ductility of NiAl. By a supercell approach we derived ideal cleavage energies and γ surfaces in main slip directions for both, pure NiAl and NiAl(Cr). Based on these data the dislocation core structure and Peierls' barrier for the slips at the most important (110) glide plane are calculated in terms of the Peierls-Nabarro dislocation model with general restoring forces. The changes in dislocation properties due to Cr additions are discussed.

COMPOSITION AND PRESSURE EFFECTS ON BANDGAPS AND BAND OFFSETS IN II-VI HETEROSTRUCTURES

14:45 - 15:00
oral

Özden Akinci, Hikmet H. Gürel, Hilmi Ünlü

We present a second nearest neighbor sp3 empirical tight binding study of alloy and pressure effects on the energy bands and band offsets in group II-VI semiconductor heterostructures. The resulting band structure for ZnSe/GaAs, ZnSSe/ZnSe, ZnCdTe/ZnTe and ZnCdSe/ZnSe, HgTe/CdTe and HgCdTe/CdTe heterostructures is analyzed using nonlinear tight binding parameters and bond lengths as a function of composition, interface lattice mismatch strain and external pressure. The model reproduces real band structure of all binaries at the , L and X points of the Brillouin zone. Using these parameters band offsets between ternary/binary II-VI compounds are calculated by screening the valence band energies with the optical dielectric constant function of composition, interface lattice mismatch strain and external pressure. It is gratifying to note that by screening of the valence band energy at point, the second nearest neighbor sp3 tight binding model describes very accurately the valence band offsets, in good agreement with experiment for many heterostructures. The model predicts that the growth orientation dependence of band offsets for lattice matched heterostructures is due to lattice thermal expansion difference across the interface and that in mismatched heterostructures is due to the change in sign of lattice mismatch strain. The electron-phonon interaction has very little effect on the valence band offsets but some effects on conduction band offsets as temperature is increased.

A DFT study of the oxidation of the
clean and hydrogenated Si-rich SiC surface

15:00 - 15:15
oral

Elwira Wachowicz[1)]

1) University of Wroclaw, Institute of Experimental Physics, Wydzial Fizyki i Astronomii (IFDUWr), plac M.Borna 9, Wroclaw 50-204, Poland

SiC-based microelectronics is a candidate for a future replacement of the current Si-based technology. One of the main advantages of SiC over other wide band-gap semiconductor materials is the existence of a native oxide (SiO

2

). We present our theoretical study of the very first stages of oxidation on the clean and H-saturated Si-rich 3C-SiC(001) surface. Total-energy density functional theory (DFT) calculation of different on- and near-surface O adsorption sites on both clean and hydrogenated surfaces were performed. All calculations were done with the {/tt siesta} code using GGA and a large basis set. We determine both the most favorable and stable adsorption sites and correlate the adsorption energy with the lattice distortion. We find that the near-surface adsorption is strongly favored and can arise both as intra-bond and interstitial oxygen incorporation. Finally, we use extensive DFT calculations to study the double-oxygen adsorption and test for correlation effects in the clean SiC surface oxidation process.

Symposium I

Metal Based Nanomaterials, Thin Films and Surface Structures

Introduction

Nanometals, that means metal particles of diameter in the range of a few nanometers or thin films in the same thickness range, are interesting not only because of their special mechanic properties but also because of other physical and chemical properties, sometimes totally different from those of coarse-grained metals. Metal based magnetic materials are of great interest for the field of information storage. Encapsulated (for example in a carbon matrix) metals are protected against oxidation, without loosing their magnetic properties. Encapsulated or supported nanometals are more resistant against sintering at elevated temperatures. Metallic thin films may find their application in electronic industry, for example as interconnect lines or magnetic or electric layers. Nanometals have been used for a long time in catalysis, before the prefix "nano" has become famous and has come to be frequently used. Nowadays, using modern techniques, it is possible to study kinetics and mechanisms of catalytic reactions in nanoscale. In order to investigate processes occurring on the surface of thin films and bulk nanometals, numerous UHV surface scientific techniques are applied. These studies, carried out on a model (single crystal) or on nanocrystalline metal surfaces enable the investigation of phenomena occurring on an atomic level.

The aim of this EMRS Symposium is to offer an opportunity for discussion and exchange of ideas for scientists working with nanometals at different levels - from bidimensional surface structures, through thin films, to nanocrystalline metals.

Organisers

- Urszula NARKIEWICZ, Institute of Chemical and Environment Engineering, Centre of Knowledge Based Nanomaterials and Technologies, Technical University of Szczecin
- Yves PAULEAU, National Polytechnic Institute of Grenoble, CNRS-LEMD
- Klaus WETZIG, Institute fur Festkorperanalytik und Strukturforschung des IFW Dresden
- Jean-Francois HOCHEPIED, Ecole Nationale Superieure des Mines de Paris
- Walerian ARABCZYK, Institute of Chemical and Environment Engineering, Centre of Knowledge Based Nanomaterials and Technologies, Technical University of Szczecin
- Nikolaous GOUSKOS, Solid State Section, Department of Physics, University of Athens

Proceedings

The proceedings of the Symposium "I" will be published in Reviews on Advanced Materials Science.

Monday, September 6th

Poster session 1

19:00 - 21:00

Microstructure evaluation in an Al-Li alloy processed by severe plastic deformation

poster I-01

Bogusława Adamczyk-Cieślak[1)], **Jarosław Mizera**[1)], **Malgorzata Lewandowska**[1)], **Krzysztof J. Kurzydlowski**[1)]

1) Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland

The high stiffness and low density of Al-Li alloy make them particularly interesting for aircraft applications. Their properties may be improved by grain refinement to nanometer scale. To this end various severe plastic deformation methods can be used. The aim of this work was to describe the microstructure of an Al-Li alloy subjected to two different severe plastic deformation methods.
The Al-1.6wt.%Li alloy was used in this study. It was severely deformed up to strain of 4. The microstructure was studied using optical and transmission electron microscopy. TEM observations have revealed the grain refinement from 300 μm to below 1 μm. It has also been found that the materials processed in these methods have different mechanical properties.

Phase transformations during mechanical alloying of nickel aluminides and subsequent heating of milling product

poster I-02

Anna Antolak[1)], **Marek Krasnowski**[1)], **Tadeusz Kulik**[1)]

1) Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat), Wołoska 141, Warszawa 02-507, Poland

It is known that the reduction of grain size to nanometer scale is an attractive way to improve the mechanical properties of alloys. This reduction may be obtained by mechanical alloying. In this work, nanocrystalline powders with stoichiometrie Ni_3Al composition were prepared by ball milling of AlNi or Al_3Ni_2 intermetallic compounds with addition of Ni powder. The powders at different stages of the milling process were investigated by X-ray diffraction and differential scanning calorimetry to study phase transformations that occurred during mechanical alloying and during subsequent heating in a calorimeter. It was found that in both cases at the first stage of the milling process, a metastable Ni(Al) solid solution was formed, and this phase remained as the only milling product. Upon heating of these powders in the calorimeter, the Ni(Al) solid solution became ordered and transformed into the Ni_3Al intermetallic compound. The results obtained show that during heating in the calorimeter, a limited growth of grains occurred and nanocrystalline structure of powders was preserved.

Microstructural changes in upper surface of austenitic steel under low energy plasma

poster I-03

Jolanta Baranowska[1)]

1) Technical University of Szczecin, Institute of Materials Engineering, Al. Piastow, Szczecin 70-310, Poland

The application of cathode sputtering to austenitic steel enable to gas nitriding of this material by removing of protective layer of chromium oxides. But beside of this activating influence the additional effect is observed. Depending on the sputtering parameters the various composition of the nitrided layer after gas nitriding can be obtained in the same condition of gas nitriding. The author presents results of her investigation on influence of low temperature plasma on upper surface of austenitic steel. Plasma was made as a result of glow discharge with voltage 900-1800 V in nitrogen, argon and hydrogen atmosphere. The ion density was 0.7-5 mA/cm^2.
The investigations include the microstructural and phase evaluation of the uppers surface after treatment. It was stated that depending on the plasma characteristic some physical changes in the surface layer can occur till the depth of ca 0.5 microns.

Structural characterization of TiC/C and TiN/C films prepared by sol-gel method

Anna Biedunkiewicz[1], **Dariusz Moszyński**[2]

poster I-04

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Nanocrystalline ceramic materials are being extensively studied today with the aim to develop hard but non-brittle materials. The nonhydrolytic sol-gel process has been employed successfully for preparing nanocrystalline TiC/C and TiN/C coatings. The following techniques were applied for the samples characterization: scanning microscopy, X-ray diffraction, microanalysis (WDS and EDS), transmission electron microscopy and electron diffraction and X - ray photoelectron spectroscopy. The bonding states and structures were investigated as functions of the carbon - titanium and nitrogen - titanium relations. The microscopic and microanalysis results suggest that the TiC and TiN are homogenously dispersed in a carbon matrix and the ratio of C:Ti>1. The TEM investigations of the TiC and TiN particles showed that they were formed with the average grain size below 100nm. The comprehensive XPS analysis of the coatings have been presented.

The XRD study of the nanostructured TiC/C and TiN/C composites.

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poster I-05

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Nanocrystalline carbides, nitrides and carbonitrides are being studied today with the aim to develop hard but non-brittle materials. Carbides and nitrides are materials that have desirable properties for a variety of applications. Their key properties are high hardness and strength along with resistance to heat, corrosion and wear.The nonhydrolytic sol-gel process has been employed successfully for the preparation of the nanocomposites TiC/C and TiN/C in form powders. In this study, the results about characterization of nanostructured TiC/C and TiN/C composites elaborated by sol-gel method. The TiC and TiN crystallite sizes and lattice parameters have been determined through X-ray diffraction method by measuring the full width at half maximum (F.W.H.M.) and the intensities of the TiC or TiN powder peaks.

The obtained the TiC/C and TiN/C powders were additionally characterized by the microanalysis (wavelength dispersive and energy dispersive spectroscopies) using an IBEX System Noran Instruments and an Oxford ISIS 300, scanning electron microscopy (JEOL JSM 6100), X-ray diffraction (PHILIPS X'PERT), transmission electron microscopy and electron diffraction (JEOL JEM 1200EX).

Microstructure of Ni(Cr)-Cr_3C_2 -Cr_7C_3 -TiC composite powder

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poster I-06

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The Ni(Cr)-Cr3C2-Cr7C3-TiC composite powder was prepared by SHS (Self-propagating High-temperature Synthesis) process using elemental powders as starting materials. As-prepared powder was ground by a high-energy mill. The morphology of as-prepared and ground powders was analyzed by SEM method; the microstructure of powders was also observed by light microscopy. The X-ray diffraction methods were applied for the structure analysis of the studied samples. The Rietveld method appeared to be very useful in the verification of the qualitative phase composition and in the determination of phase abundance in the studied material. 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. It

was found that during high-energy milling a significant decrease of crystallite size to nanoscale is observed only for Ni(Cr) phase.

Annealing temperature effect on residual stresses in 316L steel subjected to HPT process

poster I-07

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The paper describes results of the studies curried out on specimens of nano-316L steel obtained by severe plastic deformation (SPD). Specimens were prepped by High Pressure Torsion (HPT) and cold rolling. Size of grains in SPD-316L was determined by TEM observations. Residual stress and microhardness have been measured for as deformed and additionally annealed samples. The results are discussed in terms of the combined effect of grain size refinement and residual stress on the properties of nano-ausenitic stainless steel.

Formation of BCC martensite in the stable FCC materials under severe plastic deformation

poster I-08

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Stable austenitic steels are not prone to formation of a strain-induced martensite and do not experience FCC-BCC transformations during high-temperature annealing.
Some alloyed Fe-Mn steels with FCC phase (austenite structure) were examined by the balance magnetometer and transmission electron microscopic methods. It was shown that nearly 0.01% of a fine BCC phase was formed in the Hadfield ($Fe_{85.8}Mn_{13}C_{1.2}$) steel after a cold plastic deformation to epsilon = 50%. The BCC phase had crystallites 200 nm in size, which did not allow identifying it by transmission electron microscopic methods. The presence of BCC phase nucleation centers in the deformed steel constrain reduced of the temperature of the precipitation austenite by 180 ^{o}C.
Fine crystals of a BCC martensite nearly 30 nm in size, whose concentration was as high as 2.3%, were detected in an austenitic steel $Fe_{79.5}Mn_{17}Al_3C_{0.5}$ after a cold plastic deformation to epsilon = 95%. Those crystals appeared in fragmented regions of a non-crystallographic shear band. As a result, the austenite decomposed during annealing at T = 500 C and about 45% ferrite was formed.
A high nitrogen-alloyed austenitic steel $Fe_{61.3}Cr_{18}Mn_{20}N_{0.7}$ contained 0.02 mass % fine crystals of a strain-induced BCC martensite 20 nm in size after a plastic deformation to epsilon = 30% at $T_d$ef = -196C. The strain-induced martensite, which was formed under the given conditions, had an extremely low Curie temperature T_C = 400C. When the steel was strongly deformed (e= 8) by shear under a high quasi-hydrostatic compression at room temperature, a strain-induced BCC martensite having a normal Curie temperature T_C = 600C appeared and initiated a FCC-BCC transformation in the stable steel during annealing.

Surface nanostructures and tribological properties of metallic materials

poster I-09

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With metals in sliding friction, in the surface layer (0.01-0.02 mm), ultrafine grained structures are formed, which to a considerable extent determine the tribological properties of the surfaces. The structures can be considered to be nanocrystalline structures (NCS): micro-fragments with large-angle boundaries are 5 to 100 nm in size.
The objects of investigation were the metallic materials with a wide concentration of manganese, having in initial state: BCC, HCP and FCC phases. To compare the obtaining results, the use was made of

the tribological characteristics of NCS different alloys: $Fe_{90}Mn_{10}$, $Fe_{80}Mn_{20}$, $Fe_{76}Cr_{11}Mn_{13}$, $Fe_{60}Mn_{40}$, $Fe_{63.5}Cr_{18}Mn_{18}N_{0.5}$, $Fe_{68.3}Cr_{19}Mn_{10}Si_2N_{0.7}$ and $Fe_{61.2}Cr_{18}Mn_{20}N_{0.8}$, differing in phase composition, structure and value of the stacking fault energy. Tribological test were done at laboratory-scale plants in conditions of sliding friction for the steel-alloy and abrasive-alloy pairs.
The NCS alloys with HCP phase and NCS nitrogen-containing alloys with FCC phase possess low friction coefficients K and high abrasive wear resistance rates epsilon. In this alloys, the developed basal or planar slip characterized by a smaller quantity of the slip systems, condition the lowering of resistance NCS fragments rotation and, as a result, the improvement of tribological properties.
Thus, the essential lowering of friction coefficient K and intensity of adhesion wear Ih, as well as the increase in the abrasive wear resistance rate epsilon of NCS alloys with HCP phase and NCS nitrogen-containing alloys with FCC phase are mainly related to decreasing the quantity of slip systems in nanocrystals of these alloys (n=3). As a result, the dislocations slip to the boundaries of nanocrystals wore easier.

Structure and properties of ultrafine grained nickel after packet hydroextrusion

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Investigations of the influence of grain size on structure and properties of nickel were done by packet hydroextrusion method (one - stage route regime) within the range of relative deformation degree epsilon = 0 - 60 %. For formation the ultrafine grained structure in nickel with the initial grain size d = 0.008 mm the packet hydroextrusion method was also used (many-stage route regime) with the maximum logarithmic deformation e = 12.
The structure and properties of nickel samples were studied by methods of optical and transmission electron and field ion microscopy methods, as well as by using resistometry and durometry. Structure parameters were quantitatively analyzed by the standard secant method. Measurements of the specific electrical resistance rho were made in liquid nitrogen. The accuracy of rho estimation was 1 10^{-10} omega cm that corresponded to rho$_D$ value (dislocation density) of the order of 108 m-^{2} calculated by used coefficient eta= delta rho$_d$/rho$_D$ (for Ni - eta= 9.4 10^{-19}omega cm m^2. The degree of strain hardening was found by measuring hardness by Vickers method with a 0.98 N load.
Investigations have been done of the influence of grains size on the value of nickel strain hardening during the deformation by packet hydroextrusion method (one-stage route regime). It is shown that the grain-boundary component of the hardening is conditioned by the increase of dislocation density during the deformation. A relationship between the value of strain hardening and the grain size has been derived. It coincides with the Hall-Petch relationship for low values of the degrees of deformation.
The results of investigations of changes in structure and properties of Ni by packet hydroextrusion method (multistage route regime) show that the ultrafined grained structure is formed at the logarithmic deformation e = 8.
It was for the first time when the direct field ion microscopy method gave evidence of a high density of defects in ultrafine
[ABSTRACT TRUNCATED TO 2000 LETTERS]

NANOCRYSTALLINE Gamma TiAl BASED MICROALLOYED COATINGS AS GAS CORROSION BARRIERS

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Titanium aluminide with about 50 at. % of Al is a promising structural material for use in automotive and aircraft applications due to its low density and creep and a relatively high strength even at the temperature as high as 1200 K, however its resistance to gas corrosion at high temperatures still needs to be improved. A great improvement of this resistance has been achieved due to nanocrystalline microalloyed magnetron sputtered gammaTiAl coatings. In view of the results obtained by means of SEM, EDS, EBSD, X-Ray and microthermogravimetric analyses at 1173 K of bare commercial gammaTiAl alloy as well as the one with nanocrystalline magnetron sputtered microalloyed gammaTiAl coatings the following conclusions have been drawn in the work:
1. Magnetron sputtered Cr, Nb, Ta, Mo, Ag or Si -alloyed gammaTiAl coatings are well adhering and show a uniform, dense, nanocrystalline structure as opposed to the coarse-grained gammaTiAl substrate
2. The resistance of the gammaTiAl-based nanocrystalline coatings to oxidation is due to the formation of thin, tight Al2O3 layer on the surface of the primary deposit which lowers the oxidation rate of the

latter several orders of magnitude
3. Both the nanocrystallinity as well as the effect of the "third element" (Cr, Nb, Ta, Mo, Ag or Si) in the ternary gammaTiAl based coatings are conducive to the increase of the diffusivity of the Al atoms in the coatings and, subsequently, to preferential nucleation of the Al2O3 phase on the coatings' surface
4. The nanocrystallinity as well as the alloying elements (Cr, Nb, Ta, Mo, Ag or Si) in the gammaTiAl based coatings are conducive to the grain refinement of the oxide scale growing on the coatings' surface during oxidation
5. Any synergistic effect of the both alloying elements (Cr and Nb, Ta and Nb, Mo and Nb, Ag and Si) in the quaternary TiAl(Cr,Nb), (Ta,Nb), TiAl(Mo,Cr), TiAl(Ag,Si) coatings have not been observed in the work

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X-ray studies of nanocrystallisation in Fe-Nb-B amorphous alloys

poster I-12

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X-ray studies of nanocrystallisation process in the Fe-Nb-B amorphous alloy are studied. The samples were annealed in argon atmosphere in a range of temperatures till 1025 K. The first diffraction lines typical for αFe were detected after annealing at 740 K temperature. The full crystallisation was observed after annealing at 1025 K/1h and leaded to formation of αFe crystalities and borides Fe_3B and Fe_2B as well. It was also shown that the enhancement of soft magnetic properties (optimisation) effect studied for the same samples takes place at lower temperatures than the nanocrystallisation.
The essential aim of the presented paper is to study a correlation between magnetic properties of the Fe-Nb-B amorphous alloy and a degree of advancement of the nanocrystallisation process examined in detail by applying X-ray technique. The determination of the nano-grain size and magnetic permeability for the same samples should allow controlling the nanocrystallisation process, thus in other words, it should allow controlling material properties.

The influence of twin bands density on microstructure of 316LVM austenitic stainless steel subjected to transverse rolling

poster I-13

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Standard metallic orthopedic materials include stainless steel, cobalt-based alloys, commercially pure titanium and titanium-based alloys. Although Ti and its alloys are preferred nowadays, stainless steel is still the most used metal for internal fixation devices. This is due to its useful combination of mechanical properties, acceptable biocompatibility and cost effectiveness in comparison to other metallic implant materials.
Recent development in fabrication of bulk nanostructured metals opens possibility to obtain novel properties in austenitic stainless steels. The paper presents the results of investigations of the properties and microstructure of 316LVM stainless steel subjected to transverse rolling in DUO process [1].
The specimens of the steel prior to rolling have been deformed via hydrostatic extrusion [2]. Microstructures of the DUO processed steel were investigated by light and transmission electron microscopy. The initial and post-rolling microstructure parameters were estimated using special software (MICROMETER [3]). Mechanical properties were described in terms of microhardness. The microstructures observed in the rolled material showed a considerable refinement of grain size, which affects mechanical properties of the studied material. High microstructure inhomogenity has been observed.

[1] Grosman F, Pawlicki J, Korbel A, Bochniak W, Kielpiński R, Tomecki L, Patent Declaration No: P-361148, 2003
[2] Klassek D, Garbacz H, Lewandowska M, Pachla W, Kurzydlowski KJ, The influence of hydrostatic extrusion on microstructure and mechanical properties of austenitic stainless steel for biomedical applications, in press
[3] Wejrzanowski T, M.Sc. Thesis. Warsaw University of Technol
[ABSTRACT TRUNCATED TO 2000 LETTERS]

The phase conversion in stainless steel under LSW processing

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There is such laser processing method of LSW (laser shock waves in transparent condensed medium), which provides great compression and low plastic deformation and could be used for modification of material properties.
The influence of laser shock waves in transparent condensed medium on phase conversion in stainless steel X18H10T is studied by means of Mossbauer effect and electro resistance methods. The shock waves were generated by impact of nanosecond laser pulses with density of the power q 10^9 W/sm^2.
It is shown, that shock waves passage in this material causes martensite conversion and increases corrosion stability. Austenite obtained in such a way has increased corrosion stability in liquid lithium in comparison with austenite obtained after thermo treatment. The formation of austenite by the shock waves mechanism is connected with two rival action factors: great (2 GPa) compressive stresses and low (0,001) plastic deformation degree.
The selective dissipation of LSW is the main factor, which causes the cleaning of the grain border from the impurities and the homogenizing of structure.
The similar effect of homogenizing and ordering after LSW-processing was observed in IV - VI semiconductors.

Development of microstructure and mechanical properties in nickel deformed by hydrostatic extrusion

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Bulk, ultra-fine grained metals can be produced by severe plastic deformation (SPD) techniques, as equal channel angular pressing (ECAP), high pressure torsion (HPT) cumulative rolling (CR) or multiple forging (MF). SPD technique combines intense plastic straining under high imposed pressure.
Recently, the hydrostatic extrusion (HE) gains more attention as the SPD process [1]. The goal of present work is to demonstrate that by HE the formation of bulk, ultra-fine grained microstructure can be obtained in commercial purity nickel. Deformation is performed at room temperature to wire of diameter 3mm with the total true strain 3.8. The structure is characterized by light microscopy, TEM and XRD methods and the mechanical properties by tensile tests and microhardness measurements.
It was found that the HE leads to significant refinement of the material microstructure. The remarkable microstructure refinement by three orders of magnitude (initial 200 micrometer grains –> final 200 nm subgrains) was observed). Transformation in microstructure is accompanied by an improvement of the mechanical properties. Results obtained are discussed in terms of microstructure development during the consecutive HE steps.

[1] see contributions to present conference

Effect of sever plastic deformation method on microstrucure and mechanical properties of Al and Cu

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Plastic deformation strongly affects the microstructure of materials. Severe plastic deformation (SPD) leads to the formation of sub-micron and nano-grain structures, which often show a high strength at room temperature. One of the methods that can be used for inducing SPD is hydrostatic extrusion.
The aim of the present study is to examine how different SPD methods, including hydrostatic extrusion alters the microstructure and properties of various metals with different from one another in the Stacking

Fault Energy, such as copper and aluminium.
The mechanical properties of the SPD materials were examined in a static tensile test. The results show significant increase in tensile strength and the yield stress. These effects were more marked in Cu. At same time microstructures of the extruded samples exibit very similar structure, consisting of equiaxial dislocation cells, with the average dimension of about 200 nm and very distinct, thin microbands of a large misorientation with respect to the surrounding material. The microbands in copper are of nanometric width.

Dependence of microhardness on annealing time of amorphous Al-Mm-Ni-(Fe,Co) alloys

poster
I-17

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Al-Mm-Ni-(Fe,Co) alloys of six slightly different compositions were melt spun to amorphous ribbons. DSC studies of the ribbons show that the first crystallization stage, responsible for the precipitation of fcc-Al, is well separated from the others. Mixed structures containing nanosized fcc-Al crystals, embedded in amorphous matrix were obtained by isothermal annealing of the initially amorphous ribbons for different times and thus, different crystalline fractions the fcc-Al crystals were obtained. The microhardness of the alloys increases with the increase of annealing time, reaching a "plateau" after about 20 min of annealing. Replacing Fe by Co does not significantly influence the microhardness of these alloys. The slight changes of chemical composition don't seem to have a clear effect on microhardness.

EFFECT OF INITIAL MICROSTRUCTURE ON MECHANICAL PROPERTIES OF THE Al-Cu-Mg-Mn ALLOY PROCESSED BY HYDROSTATIC EXTRUSION

poster
I-18

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Ultrafine grain and nanocrystalline materials show attractive properties - very high strength and relatively good ductility. Such metals can be produced by severe plastic deformation methods. In the previous work [1], it was shown that the hydrostatic extrusion results in grain refinement to nanometer scale of aluminium alloys. This processing method can be used to produce large fully-dense bulk elements (rods of various cross-section shapes and lengths much higher than in other techniques). The aim of this work was to show how the properties of nano-sized age hardenable aluminium alloy depend on the initial microstructure (single or two-phase) of extruded samples.
The material used in this study was an Al-4Cu-1Mn-0,5Mg aluminium alloy. In the as-received state, the material had a form of 20 mm diameter rod. The specimens were solution heat treated, water quenched and some of them aged at various conditions. Next, they were subjected to the hydrostatic extrusion under high pressure. The final diameter was 3 mm which corresponds to the cumulated true strain of 3,67. In order to characterize the mechanical properties of the materials, microhardness measurements and tensile tests were performed.
The results have shown that the highest strength is achieved for the specimen deformed in the as quenched condition. Moreover, this sample exhibits the highest value of elongation during tensile deformation. These results will be discussed in terms of microstructure evolution during severe plastic deformation (grain refinement rate, precipitates transformation).

[1] M. Lewandowska, H.Garbacz, W. Pachla, A. Mazur, K.J. Kurzydłowski: „Hydrostatic Extrusion and Nanostructure Formation in an Aluminium Alloy" Solid State Phenomena, in press.

STAGES OF THE LAYER GROWTH DURING THE IMPULSE PLASMA DEPOSITION METHOD.

poster
I-19

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The aim of our research was to investigate the stages of the layer growth during the IPD method. The materials for our studies were CN_x coatings produced by number of plasma impulses in range 80 - 8000 obtained on the Si substrates. All samples were prepared in the same process conditions. There were used nitrogen gas and a nitrided graphite (an internal electrode of coaxial accelerator) as sources of nitrogen and carbon atoms, respectively. The layers were examined by the TM AFM and SEM techniques as main investigations. We also researched our films by TEM, XPS and nanohardness for characterization of deposit material.
Based on the microscopy studies we observed that layer morphology changed significantly with a number of the plasma impulses during the deposition process. There are formed flat, width islands in result of a surface migration of clusters for the thin film. An increase of the number of the plasma impulses leads to creation of a few separated little pillars. We consider that this is the beginning of crystallization. Further increase of amount of the plasma impulses cause the accumulation of heat in the coating/substrate system. Therefore, there are generated a lot of nuclei and in the consequence we note strongly growth of pillar number. The final structure of thick layers consists of two zones: an internal area built of a homogeneous material and an external area with a highly anisotropic structure.
Up to now this type of structure was not observed during the IPD processes. The mechanism of the layer growth is difficult to explain. It is probably that this is connected with the accumulation of heat, therefore it might be a result of the layer recrystallization.

Phase transformations in M2 steel powders subjected to ball milling

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Mechanical alloying (MA) is well known processing technique to synthesise materials with various structures, starting usually from the powder mixtures of pure elements. If the powders subjected to milling are alloyed powders, the process is called mechanical milling (MM). Both processing methods (MA and MM) induce phase and structural transformations in the processed materials.
The aim of this paper was to study phase and structural changes in high speed steel powders subjected to ball milling. Two types of materials were studied: commercial powders of M2 steel and the chips obtained by machining of the rod of the same composition. For comparison MA process was also performed, using the elemental powders of metals and graphite. Fritsch P5 planetary ball mill was used for milling experiments.
Particle size analysis revealed that milling of chips resulted in very fine final particle size (below 0.3 micrometer), while milling of commercial powders led to the final particle size of about 10 micrometers. The particle size as well as the morphology was also examined by scanning electron microscopy (SEM) observations.
X-ray diffraction (XRD) investigations showed the dissolution of carbides and formation of supersaturated ferrite. The mean crystallite size of ferrite was in the range of several tens of nanometers and lattice strain was up to 1%. MA resulted in very similar structure. The changes of lattice parameter of ferrite were also analysed.
Mössbauer spectroscopy measurements allowed to distinguish between ordinary" ferrite and alloyed" ferrite in the structure after ball milling, as well as to detect the residual carbides content at the level of 3%. Differential scanning calorimetry (DSC) heating experiments showed two types of thermal effects, attributed to crystallite size increase and lattice strain decrease (at lower temperatures), and, to carbides precipitation at higher temperatures range.

Synthesis of a Silver nanowire with Anodic Aluminum Oxide Template

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Regularly-spaced, hexagonally-celled nanoporous channel array of anodized alumina has been produced and used as a base substrate for constructing various nanostructures.
We show some of those nanostructures, such as formation of self-assembled silver nanowires with a Silver-paste grown through the nanochannels of the alumina.
This is a facile methode to make a nanowire with an Anodic Aluminum Oxide(AAO) templeate.

Preparation and characterization of nanocrystalline copper layers

poster I-22

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Investigations performed by the authors of this paper are focused on copper surface layers deposited by electrocrystallization method and exhibiting nanocrystalline structures. The intention of this research is an identification of optimum parameters for the manufactur-ing process leading to such type of surface coatings as well as determination of correlations between the structure and properties of the nanocrystalline copper layers and the composition of an electrolyte on one hand and the process parameters of their deposition on the second hand.
In this paper results of structures and hardness investigations of produced layers are presented. The structural analysis of produced layers was executed with the help of the dif-fractometer of X-ray type PHILIPS PW-1830. The size of crystallites of the material of de-posited layers were appointed as results of analysis of X-ray lines profile with use of the Scherrer's formulae. The results of investigations of the topography and morphology of the copper surface layers by the method of electron scanning microscopy (SEM) are presented. The structure of deposited layers as well as sizes and shapes of their grains were determined by the use of transmission electron microscopy (TEM).
The performed investigations permitted to establish the chemical composition of the electrolyte as well as parameters of the process enabling the deposition of the nanocrystalline copper layers by the electrocrystallization method. The material of produced nanocrystalline copper surface layers is characterized by the compact polycrystalline structure with dimen-sions of the grains near 20 nm. This nanocrystalline structure layers show higher hardness than classic Cu surface layers exhibiting micrometric grain dimensions which were produced also by the electrocrystallization method.

THE INFLUENCE OF HIGH-ANGLE BOUNDARIES ON THE MECHANICAL PROPERTIES OF NANO-CRYSTALLINE IRON OBTAINED BY SEVERE PLASTIC DEFORMATION

poster I-23

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Severe plastic deformation ($e > 10$) was used to obtain nanostructured iron using two methods: (a) high pressure torsion (HPT) and (b) equal channel angular pressing (ECAP). The grain size after deformation was found to be 3 orders of magnitude smaller than the initial. Significant increase in tensile strength and microhardness was also observed. Special attention was focused on description of mechanical properties in the context of their relation to the character of grain boundaries and homogeneity of microstructure in the material processed by SPD. TEM and AFM method were used for microstructure observation. The significant differences in the mechanical properties and mictrostructure of SPD iron obtained by two processing routes have been observed. These differences can be partly related to the fraction of high-angle grain boundaries.

Studies of CVD Nanometallic Layers Prepared from Cu and Ag Carboxylates

poster I-24

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Cu(II) and Ag(I) aliphatic perfluorinated carboxylates: [Cu(OOCC6F13)] and [Ag2(RCOO)2(PEt3)2] where R = CF3, C2F5, C6F13, were characterized by MS EI, temperature-variable IR and TGA/IR methods as a new silver and copper CVD precursors. Gas phase and the thermal decomposition reaction mechanism was proposed which was used for determination of CVD parameters. Hot - wall CVD experiments were performed in the low-pressure horizontal reactor using argon as the carrier gas. Obtained silver and copper films (60 -120 nm) were characterized by XPS, XRD, SEM and adhesion tests.

Acknowledgements: Authors thank the Polish State Committee for Scientific Research grant PB 4T08C 039 23 for financial support.

Phase transformations in ball milled AISI 316L stainless steel powder and in the steel after sintering

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The paper shows the influence of the ball milling process on the structure of 316L stainless steel powder and the influence of sintering process of the powder on the structure of obtained steel. X-ray diffractometry and differential thermal analyze (DTA) results showed that ball milling results in a partial transformation of austenite into martensite. The martensite fraction in the sample was estimated from the Mössbauer spectra. The changes of lattice parameter and crystallite size of austenite were calculated. The powders after milling were compacted and sintered simultaneously by impulse plasma method. The final structure of the sinters was characterized by optical microscopy equipped with computer image analyzer, SEM and X-ray diffractometry.

Pressure-assisted synthesis of nanostructured Al-Cu-Fe quasicrystals

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Aluminium-based quasicrystals have properties of great interest for many applications, e.g. hard coatings[1], but are rather difficult to produce in large quantities, as they are stable only within a narrow composition domain[2,3].
Alloy powder with nominal composition $Al_{67}Cu_{23}Fe_{10}$ was prepared by ball-milling of elemental metallic powders. The as-milled powder consists mainly of a nanocrystalline Al(Cu,Fe) solid solution.
The structural phase transitions upon heating under different pressures were investigated by in-situ X-ray diffraction at the F2.1 beamline of DESY-HASYLAB (Hamburg, Germany)[4], in order to establish a PRESSURE-TEMPERATURE phase diagram. A single-phase quasicrystalline powder was obtained after a sequence of phase transitions taking place at temperatures between 250-300C and 700-800C, with phase transition temperatures varying with pressure. The quasicrystalline phase was shown to be stable after quenching under pressure.

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Surface condensation of material during IPD

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Convenient ways of producing nanocrystalline materials are plasma surface engineering techniques, in particular the Impulse Plasma Deposition method (IPD) [1]. The characteristic feature of this method is the nucleation on ions, which leads to the thermodynamic stabilisation of high - temperature phase clusters. The dominant opinion concerning film condensation in the IPD method is that the clusters migrating on the substrate surface collide with one another and than they coalesce in the way similar to that in sintering

[2]. The last research [3] indicate that in spite of the impulse character of the mass and energy transport to the separation surface, the IPD growth also involves a diffusion process that may lead to the formation of inter-metallic phases. Moreover, the mass transfer between the amorphous matrix [4] and the particles that proceeds through the local diffusion of atoms has been reported [5].
During the studies related to the surface condensation of the film material has been observed process of diffusion of the film material in the way similar to the Ostwald ripening [6]. The aim of the study was to investigate the mobility of the clusters, cluster agglomerates and the particles, which were produced by overgrowth of the clusters by the material supported to the substrate surface in form of ions or atoms. Based on the results, we assume that diffusion process is hardly slowed or even stopped when the dimension of the particles exceeds 50 nm.

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Nanoindentation measurements of austeno-ferritic stainless steel submitted to hydrogen charging.

poster I-28

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The influence of cathodic hydrogen charging on the nanohardness of austeno-ferritic stainless steel was investigated. As it is well known that hydrogen behaves differently in the ferrite (α) and austenite (γ) phases - in the fcc γ phase, hydrogen has a higher solubility but a lower diffusivity than it has in bcc α phase - the hardness changes of both α and γ grains before and after hydrogen charging were investigated. Because of the fact that only thin film on the steel surface suffered from hydrogen embrittlement, it was necessary to use the fine nanoindentation technique. Therefore the nanoindentation measurements using the Atomic Force Microscope were performed. Three various states of samples were examined: initial state, just after hydrogen absorption and after hydrogen desorption. It was shown that there are distinct changes of nanohardness between every state and every phase. Generally, the nanohardness of the phase is higher than in case of the phase. The increase of nanohardness of both phases after hydrogen absorption and its decrease after hydrogen desorption was noticed.

Studies of the initial stage of the carburisation of nanocrystalline iron with methane

poster I-29

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The carburisation of iron is known as a method to improve the hardness of steel. The iron carbide itself can be applied for example for the production of sensors or magnets. It is also an intermediate product in the formation of carbon deposit obtained in the reaction of hydrocarbons with iron.
The aim of this study is to investigate the carburisation mechanism in the interval of carbon concentration below that corresponding to the iron carbide formation.
The nanocrystalline iron (mean size of crystallite-17 nm) iron promoted with small amount of oxides (Al_2O_3, CaO, K_2O) was used in the experiments. The grain fraction of 1,2 1,5 mm was taken. The decomposition of methane has been studied in the temperature range of 400 to 550^{0}C under atmospheric pressure. The mass change of the sample was measured using spring thermobalance and cathetometer, with the accuracy of 0,0001g. The phase composition after carburisation process was characterized using X-ray diffraction and Moessbauer spectroscopy.
At the beginning of the carburisation process the measured increase of the sample mass does not correspond to the determined iron carbide content. The formation of the thin carbon layer on the iron surface is suggested for this area, connected with diffusion of iron atoms to this layer to form on intercalated iron graphite compounds.

KINETICS OF CARBON DEPOSIT FORMATION FROM DECOMPOSITION OF METHANE ON NANOCRYSTALLNE IRON SURFACE

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poster I-30

The studies of the kinetics of the formation of carbon deposit in the result of the decomposition of methane on the nanocrystalline iron are presented. The experiments were carried out in the thermobalance-differential reactor in the temperature range of 500-600^{0}C under atmospheric pressure. The kinetics of the carbon deposit formation has been studied in the reaction area where reaction rate has been limited by the dissociative adsorption of methane. The rate of the carbon deposit formation has been found to be proportional to the methane pressure. The activation energy of this process is about 150 kJ/mol. The dissociative adsorption of methane leading to the formation of carbon deposit occurs according to the same mechanism as the formation of iron carbide in the reaction of methane with nanocrystalline iron. The rate of the carbon deposit formation is proportional to the fraction of surface uncovered with carbon. The formation of carbon deposit occurs in the result of the thermal decomposition of iron carbide. The process of the thermal decomposition of iron carbide is slower than the process of the reduction of iron carbide with hydrogen.

Biocompatibility of thin films based on hydrothermal synthesized HAp

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poster I-31

Implant materials were made from metals such as titanium for a long period of time. Despite its good mechanical properties metals and its alloys may be toxic for the human body.
New materials have been developed for orthopedic implants and artificial teeth. Among these materials, HAp which is known for its high biological activity and its unique property to integrate with bones has attracted attention.
Different techniques for HAp based biomaterials synthesis (mechanical methods,
co-precipitation, biomimetic procedure, hydrothermal procedure) are described in the literature. Hydrothermal synthesis offers many advantages over conventional and non-conventional ceramic synthetic methods. Hydrothermal synthesis is a technology for crystallizing materials (chemical compounds) directly from aqueous solution by adept control of thermodynamic variables (temperature, pressure, composition). The objective of this paper is to demonstrate the enhanced biocompatibility of HAp thin films starting from hydrothermal synthesized powders.
Hydrothermal synthesized HAp was deposited on pure titanium substrates by PLD at 400oC in water vapor and in oxygen atmosphere, pressure value in the range 3.5 *10-1-10-1 torr. Biocompatibility tests performed on coated titanium showed the ability of the HAp layer to promote cell growth on the surface.

Evolution of VPO and VO_x catalysts under conventional XPS conditions: the role of support effects

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poster I-32

The stability of VPO and different supported VO_x catalysts for partial oxidation of small hydrocarbons under the ultra-high vacuum (UHV) conditions of standard X-ray photoelectron spectroscopy (XPS) was studied using a multi-purpose surface analysis apparatus which allows time spans of only a few minutes between the sample transfer into vacuum and the first photoelectron spectrum. The VPO catalysts showed a significant dependence of the vanadium oxidation state upon the time of exposure to UHV, as determined from the shape evolution of the $V2p_{3/2}$ peak. The initial V^V/V^{IV} ratio was found to decrease by a factor of at least 2 within the first 15 - 25 min of the XPS experiment for fresh as well as used VPO catalysts. From a careful set of experiments in a "stop and go" mode (10 to 20 s) of the X-ray source it can be concluded that the observed changes are predominantly due to the vacuum environment, with a rather minor (if at all) contribution of the X-ray excitation.
In contrast to these results on VPO, the investigated VO_x catalysts on various support materials, like Al_2O_3, TiO_2 and SiO_2, change under the same conditions to a much lesser degree and on the time scale of hours instead of minutes. The role of the V-O-support bonds has been studied by variation of the support at nearly constant vanadium concentration, and the stabilizing effect of the supporting oxide material on the vanadium oxidation state is discussed.

The kinetics of the nanocrystalline iron nitrides reduction

poster I-33

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The process of nanocrystalline iron nitrides reduction was investigated with application of the thermogravimetry and XRD methods. The kinetics of the reduction of ϵ-$Fe_{3-2}N$ phase was investigated under hydrogen atmosphere and temperature range 400 to 500 ^{0}C. It was observed that in the reduction process the average crystallite size both of iron and iron nitride Fe_4N phases increases with conversion degree of Fe_4N to Fe. Those results indicate that reduction process is limited by surface reaction and undergoes according to the Adsorption Range Model [1].
The rate of the reduction was calculated from slope of the approximately linear part of TG curve and is proportional to the hydrogen partial pressure. The kinetic equation of reaction was proposed. Based on kinetic equation the dependence of reaction constant on temperature was determined. The process is not activated and the apparent activation energy amounts -17 kJ/mol.
The Adsorption Range Model allows a better description of the process by the numerical modelling. In this way a good agreement of theoretical data with experimental ones was achieved. The free energy of nitrogen segregation as a function of bulk nitrogen concentration was obtained.

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THERMOELECTRIC PROPERTIES OF QUANTUM BI WIRE DOPED WITH SN AT ELECTRON TOPOLOGICAL TRANSITIONS INDUCED BY STRETCH AND DOPING

poster I-35

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The work is devoted to investigation of thermopower and magneto-thermopower in the longitudinal field in wires of pure Bi and Bi<Sn> alloys with concentrations of T-holes at 4.2K up to $3*10^{18}$ cm^{-3}. The diameters of wires changes from 100 nm to 3mkm.
Bi and Bi<Sn> nanowires (in glass cower) were fabrication by casting method from liquid phase. All wires had one the same orientation - wire axis make up and angle of 20^0 with the bisector axis C_S in the bisector trigonal plane.
Peculiarities of thermopower and resistance behavior caused by electron topological transitions (ETT) induced by stretch and doping are found. ETT were fixed by change of the Fermi surface cross-section detected by the ShdH oscillations on both resistance and thermopower.
On the temperature dependence of the thermopower of Bi wires with d$<$ 1 mkm in the temperature range 30-40 K the positive maximum is formed, its value depending on the wire diameter d. The thermopower decrease with the temperature lowering ($<$40 K) is caused by freezing of long-wave phonons with the energy 43 K and by increasing of degeneration of electron and hole gas. It is found that in the nondeformed state

in wires d>300nm of pure and Sn-doped bismuth the phonon drag effect is absent, i.e. the thermopower is determined only by the diffusion processes.
Influence of the size of a sample (diameter and length), impurity of Sn, a magnetic field and an elastic elongation on Phonon drag effect in nanowires Bi and BiSn was investigated.
The work was supported by the Civilian Research Defense Corporation, CGP- grant # MO-E1-2603-SI-04.

Magnetic nanostructure of Fe-Ti alloy layers produced by IPD

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poster I-36

The aim of our studies was to investigate the magnetic nanostructure and the morphology of the Fe-Ti layers using the Magnetic Force Microscopy (MFM) and Scanning Electron Microscopy (SEM) techniques, respectively.
The Fe-Ti layers were produced by the impulse plasma method (IPD) in two impulse plasma coaxial accelerators, each equipped with an internal electrode made of Fe or Ti, which functioned as the source of the alloying components of the layer material. The substrates were made of Si, and the plasma-generating gas was hydrogen. The successive portions of Fe and Ti were deposited independently at separated time intervals, according to the schedule that specified the number and proportion of the impulses generated by each accelerator.
Characteristically, the layer growth mechanism in the IPD method consists of the uncompleted coalescence of the clusters formed in the plasma itself and delivered onto the cold surface of the substrate. During the impulse plasma deposition the plasma is generated in the form of discrete packs with a life-time of about 100μs. In spite of pulse character of mass and energy supplying to the substrate, based on our previous investigation we assume that during the IPD growth of the layers, short-distance diffusion takes place between the separated iron and titanium clusters.
The surface morphology is very similar to the magnetic contrast in the layers. It is interesting that the magnetic domain size in the magnetic contrast is related to the characteristic size in the surface morphology. We suppose that the light and dark contrast in magnetic structure corresponds to Fe or bcc-Fe(Ti) as ferromagnetic phases and Ti or inter-metallic phases as paramagnetic, respectively.

Investigations of the wear resistance of nanocrystalline composite coatings Ni-SiC

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poster I-37

In present work the nanocrystalline composite electrochemical coatings were prepared with nickel matrix and particles SiC. The nickel plating bath of low nickel ion concentration (0.75 M) containing brightening organic compound with surfactants and the dispersed particle (SiC) was used for electrodeposition of composite coatings. The structure the composite coatings was established using TEM. The content of particles in coatings was examined gravimetrically. The dependence of the SiC content in the composite coatings Ni-SiC from of the concentration and kind of the organic additives was investigated. The roughness of the coatings Ni-SiC was measured using tester TR 100. The microhardness of the deposited layers was measured using a Vickers method at a load of 0.01 and 0,05 kG. The sliding wear tests for
Ni-SiC coatings were made in air, without lubrication, using a technique based on the measuring system comprising a flat surface and a ball. On the basis of the wear traces and measurement of their diameter, the depth of the wear was calculated, which was the measure of wear resistance.
The results suggest that the effect used of the organic compounds was the development of the nanostructure of the nickel matrix. The wear resistance increased with the microhardness increase.

Magnetic resonance study of PTMO - block - PET copolymer filled with a mixture of Fe_3O_4 and Fe_3C nanoparticles at low concentration

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poster I-38

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Nanocrystalline iron samples were carburised with CO/CO_2 mixture at 400 - 550C. The product obtained contained 29% Fe3C, 35% Fe_3O_4 and 36% C as carbon fibres. The sample were characterised by XRD, TOC (total carbon, Multi N/C) and SEM after carburisation. This iron-carbon composite was used as a filler for PTMO - block - PET polymer, with low concentration (0.5%) of iron-carbon composite. Electron Spin Resonance investigations of the sample were carried out in the 4-300 K temperature range. At room temperature a strong symmetrical signal with g = 2.229 $^{+}$- 0.022 and linewidth of 150 mT dominates the spectrum. With the temperature decrease the intensity of the line is decreasing, but at temperature of about 90 K another line appears with g = 2.666 $^{+}$- 0.032. This low-temperature line is very anisotropic and its low-field shoulder spreads to negative magnetic fields. With decreasing temperature, the linewidth of this line decreases slightly, in contrast to the behavior of the high-temperature line. The intensity of the low-temperature line is approximately independent on temperature, while the intensity of the high-temperature line strongly depends on temperature. The difference in behavior of these two lines suggests that they originate from different magnetic centers. Based on detailed analysis we suggest that the line visible at higher temperatures arises form Fe_3O_4 (magnetite) nanoparticles, whereas the line visible below 90 K arises from Fe_3C (cementite) nanoparticles. The disappearance of the line from magnetite may be caused by the so-called blocking effect, i.e. the interaction between paramagnetic Fe_3O_4 nanoparticles and the polymer matrix.

New nanocomposite materials with unique property combination

poster I-39

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Nowadays it is easily to suppose that the future progress in many branches of industry will be determined by the principal achievements in the creation of nanosized elements. Synthesis of new materials that at the same time combine different properties of components on the nanolevel is one of the most rapidly developing trends of up-to-date materials science. In this context, systems of nanoparticles embedded in various matrices are particularly promising. These materials have specific features and properties different from those of the bulk. For instance they can have other magnetic and electrophysical characteristics in various frequency ranges including microwave band.
In this work we demonstrate that it is possible to combine some properties typical only to polymers with the electrical conductivity and magnetization of metal-containing nanoparticles. Nanocomposite materials with wide range of concentrations of metal nanoparticles in polymer matrix were synthesized by high-speed thermal decomposition of metal-containing compounds in the solution-melt of polymer in the mineral oil. For characterization of composites we used the complex of different methods such as TEM, XRD methods and Mossbauer spectroscopy.
Cavity perturbation method of measuring of complex dielectric permittivity and magnetic permeability was applied to investigate microwave electrophysical properties of nanocomposites. The effects of the type of metal nanoparticles, their concentration in polymer matrix and phase ratio inside the particles on magnetic and dielectric permittivity and losses are presented.
This work was supported by the Russian Foundation for Basic Research (02-03-32435, 04-03-32090, 04-03-32311, 04-03-32597), ISTC (project no. 1991), Russian Science Support Foundation and the Russian Academy of Sciences through the basic research program Critical Issues in the Physics and Chemistry of Nanoscale Systems and Nanomaterials.

Anisotropic superparamagnetic resonance of Co nanoparticles in nanoporous carbon

poster I-40

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Here, we report on the synthesis and magnetic resonance study of Co nanoparticles, encapsulated in nanoporous carbon (NPC). NPC powder samples were prepared from carbide Mo_2C using the chemical removal of non-carbon carbide forming atoms. Size of nanopores was estimated as 1-7 nm. Impregnation of Co into was done from $CoCl_2$ during 48 hours at T = 980 C.
At room temperature the as grown powder samples of NPC: Co show magnetoresonance responce (ν=9.3 GHz) represented by two superposed lines, a broad and a narrow ones, with effective g-factor close to g=2.0.
The sample with separated granules of NPC: Co demonstrate only one almost symmetric line of absorption (ΔHpp = 340 G at T=300 K) determined by magnetic response of superparamagnetic Co particles above their blocking temperature. The resonance field corresponds to g-factor of g=2.22, which is close to the one of Co. As temperature decrease, parameters of the line change sufficiently being an evidence for a spectrum anisotropy. Such anisotropy could be interpreted as anisotropic superparamagnetic resonance, taking into account both anisotropy energy of the nanoparticles and effective magnetization of the non-spherical form of nanoparticles in a disordered system. Using the value of blocking temperature (about 70 K) estimated from our measurements, mean size of Co nanoparticles was obtained as 5 nm.

Intergranular interaction and ferromagnetic resonance of Ni nanoparticles in nanoporous carbon

poster I-41

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We present the results of magnetoresonance investigations for Ni nanoparticles embedded into a nanoporous carbon matrix (NPC). First, the NPC was prepared from polycrystalline powder of Mo_2C and then impregnated by Ni from $NiCl_2$.
At room temperature the as grown powder NPC: Ni samples demonstrate wide (ΔHpp = 2.7 kG) almost unstructured line of magnetoresonance absorption (ν=9.3 GHz). Intensity and width of the line increase sharply on cooling up to about T=50 K due to dipole coupling induced magnetic ordering in the interactive ensemble of Ni nanoparticles. Such ordering could be stimulated more probably by influence of mesopores as well as presence Ni on the granule surface.
Separation of granules from each other change drastically the magnetoresonance absorption spectra. Intensity of the ferromagnetic resonance line as well as coercive force (measured separately) at room temperature drop more than one order of magnitude. At the same time a new narrow resonance line (ΔHpp = 350 G) appears. g-factor of the line (g=2.19) is close to the one of Ni. The new line is determined by resonance magnetic response of superparamagnetic particles above their blocking temperature. Temperature behavior of the narrow line was measured and analyzed starting from dispersion of blocking temperature due to size dispersion of Ni nanoparticles.

Magnetic nanoparticles stabilized by organic polymer matrixes

poster I-42

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The great interest in polymer matrix composites containing metallic nanoparticles or cluster is motivated by wide application field of such materials: from catalysis to nanoelectronics. The polyethylene (PE), polyamides (PA), polypropylenes (PP), polystyrenes (PS) matrix are interesting as expansion and inexpensive polymers. The polytetrafluoroethylene (PTFE) matrix is very interesting because this polymer is very inert. At first glance, it would seem that poor solubility and swelling ability of PTFE in solvents hinder the introduction of different nanoparticles in this matrix and their uniform distribution over its bulk.
In searching for the solution of this problem, we have focused our attention of ultradispersed PTFE. The encapsulation was done by thermal decomposition of metallcontaining compounds (MCC) (MRn; M=Co, Fe, Cu, Ni, at all; R=CO, HCOO, CH_3COO and other) in dispersion system of UPTFE in mineral oil; solution-melt PE (or PA, PP, PS) in mineral oil. Materials with concentration of a metallcontaining NP up 2 to 30 wt.% have been obtained. Nanocomposites were determined by TEM, XRD, EXAFS, Mössbauer spectroscopy and magnetic measurements. TEM studies showed that the nanoparticles (NP) are dispersed on the surface nanogranules of UPTFE matrix and in to volume polymer matrix (PE, PA, PP, PS). The used methods of researches were shown, which nanoparticles to have complex internal structure. The magnetic metering was shown the high magnetic anisotropy and coercivity (at 300K) for Co NP on the surface UPTFE 800Oe, in PE matrix coercivity Co NP - 590Oe; Fe - 960Oe; Fe_2O_3 NP - superparamagnetic.
This work was supported by the RFBR (02-03-32435, 04-03-32090, 04-03-32311, 04-03-32597), ISTC (project 1991), Russian Science Support Foundation and program of Russian Academy of Sciences "Critical Issues in the Physics and Chemistry of Nanoscale Systems and Nanomaterials".

Nanometals for medical applications

poster I-43

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Hydrostatic extrusion (HE) is a plastic forming process which can be used to obtain sever plastic deformation in a single operation. As in the case of equal channel angular pressing (ECAP), torsion under compression (TUC) and multi-step forging (MSF), it can be used to fabricate ultrafinegrained metal structures, which are characterized by excellent mechanical properties.
The aim of the present study was to test the possibility of using hydrostatic extrusion for the fabrication of high strength materials for medical applications. The materials examined were 316LVM steel and pure titanium. The microstructure and mechanical properties of the materials subjected to cold extrusion were analyzed. It has been found that the HE leads to significant refinement of the material microstructure. In 316LVM steel, cold extrusion induces the deformation nanotwins. The change of the microstructure is accompanied by an improvement of the mechanical properties, such as the hardness, microhardness and the yield stress in final products increase by 30 to 50%.
HE of titanium produces a nanometric structure with a grain size of about 90 nm. The ultrafinegrained metal shows excellent strength properties-the yield stress of 1100 MPa, which is more than 200% value of the initial material.

Determination of steel surfaces roughness subjected to etching and oxidation processes

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poster I-44

The reflection studies of steel samples subjected to etching and oxidation processes have been performed with an integrating sphere. Such measurements have allowed one to separate the specular- and diffuse component intensities of light reflected from the surfaces studied in order to determine the surface quality which changes substantially after mechanical- (polishing) and chemical treatments (etching, corrosion). The performed atomic force microscopy (AFM) investigation supports applicability of the integrating sphere for determination of steel surface roughness.
It has been found that the total light reflection from the steel surfaces changes very little after mechanical treatment but contribution of specular- and diffuse components of the optical reflection changes substantially.
The integrating sphere method has been applied to follow the roughness changes as a function of time of etching. It has been found that etching in an HCl solution causes initially decreasing of roughness of both polished and non-polished surfaces but, after longer etching time, roughness increases and the observed changes are of the order of 15%.
During the optical studies of oxidation in situ in the free air, it has been found that roughness of both polished- and non-polished surfaces decreases with time; such changes occur rapidly during first 200 s and then roughnesses asymptotically go back to their initial values. The fact that area of polished surface is lower than that of non-polished one causes decreasing of susceptibility of the former on the etching and oxidation processes.

Determination of optical parameters of polyazomethine thin films by reflectance measurements.

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poster I-45

The results of study of the total, diffuse and specular reflectance of thin poliazomethine films on fused sillica and Si substrates are reported. The layers was deposited by polycondensation method of initial substrates. The main optical parameters i.e energy loss function, absorption, and scatter refraction coefficient were determined. The values of rms roughness were found using AFM microscope, Talysurf profilometer and integrating sphere.

INVESTIGATION OF NUCLEATION AND COALESCENCE PROCESS OF METALLIC FILMS (Ag. Cr) ON DIFFERENT SUBSTRATES

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poster I-46

Processes of nucleation and shaping of nanostructurity of surface of substrates with different physical - chemical nature where investigated ultra thin metallic films (Ag, Cr with thickness 20 - 100 nm) were deposited on polymer (PET) and quartz glass substrates by evaporation in vacuum. XRD and AFM were employed to study structural and morphological changes of the films. Surface composition of these films was investigated by XPS.
It is found that the size of nanostructured formations can be changed by changing the evaporation rate and substrate temperature (essentially reaching the polymer glassing temperature region). Changes of optical and electrical properties were registered by parallel optical transmittance and resistivity measurements. Nucleation and coalescence process of metallic films on different substrates at the high temperature region dependent on the used metals and substrate surface nature.

Critical current density reduction for current-induced magnetization switching

poster I-47

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There has been greate interest on current-induced magnetic excitation and switching in a magnetic nanopillar after the theoretical prediction by Slonczewski and Berger. The concept of using a spin-polarized current to switch the magnetization orientation of a magnetic layer provides great possibility on realizing future "current-driven" devices, i.e. direct switching of the magnetic memory bits by local application of current, instead of the field generated by external wires. Untill now all the reported current-induced magnetization switching (CIMS) works are concentrated on the simple ferromagnet FM/Cu/FM trilayers. In this work, the first observation of the CIMS in exchange-biased spin-valves (ESPVs) is reported. The ESPVs clearly show the CIMS behavior under a sweeping dc current with a very high current density. It is demonstrated that a Ruthenium (Ru) layer inserted between ESPV nanopillar and top electrode effectively decreases the critical current density from 10^8 A/cm^2 to 10^7 A/cm^2. In one of our well-designed ESPV structures, the critical current density can be reduced down to 1x10^6 A/cm^2. The substantial reduction of the critical current density makes it possible for the CIMS to be directly applied in spintronic devices, such as magnetic random access memory (MRAM).

Electrodeposition of conducting poly(0 -toludine) coatings on steel

poster I-48

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By using potentiodynamic , galvano static and potentiostatic polarization , conducting poly (0- toluidine) coatings are obtained on low carbon low alloy steel in aqueous oxalic acid. The growth mechanism of these coatings were studied . It has been shown that the nucleation and growth of these coatings on steel in aqueous acidic medium occurs in three steps . The corrosion inhibition properties were evaluated by open circuit potential measurements .It has been shown that corrosion control is possible by using these coatings.
Key words - Conducting poly(0 - toluidine) , nucleation and growth , corrosion control .

Influence of dopants on the physical properties of metal(Al, Ag, Li) doped ZnO Films grown by RF magnetron sputtering

poster I-49

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Metal doped ZnO (MZO, M = Al, Ag, Li) films were prepared by RF magnetron sputtering on glass substrates with extraordinary designed MZO targets. For the doping sources contained in each MZO targets, we used $Al(OH)_3$, $AgNO_3$, LiCl powders by mixing the powders into pure ZnO powder with a various rate (0 10 wt.%), respectively. We investigated dependences of a kind of dopant and dopant content in target on optical and electrical properties of the as-sputtered MZO films. All MZO films have shown a preferred orientation in the [001] direction. As metal doping amounts and a kind of dopant in the target were changed, the crystallinity and the transmittance as well as optical band gap were changed. Electrical resistivity was also changed with changing metal doping amounts and a kind of dopant. To investigate these phenomena in details, valence band structure of the MZO films were also investigated. In addition, changes of optical band gap as well as resistivity for the MZO films were also explained with the data obtained by XRD, XPS and UPS analysis.

2D periodic structures and conducting nano-wires fabricated by pulsed laser irradiation of silver and gold island films

poster I-50

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Silver and gold island films (IF) of 0.5 - 10 nm effective thickness deposited on glass or sapphire surfaces were used for direct laser recording of sub-micron two-dimensional (2D) periodic structures and conducting wires of nanometer width. The IF were irradiated by two or four coherent intersecting laser beams of 355 nm wavelength, with pulse duration of 8 ns, and pulse repetition of 10 Hz. The fabricated structures were analyzed by AFM. Two or four beams create a 1D or 2D interference field on the irradiated surface, with periodically varying light intensity in one or two directions, respectively. As a result, depending on the size and surface density of the metal islands, various 1D and 2D periodic structures were created, consisting of thin lines (walls), nano-meter hillocks, or clusters of alternating sizes. We have shown that islands located at the regions of highest intensity ("hot spots") were heated to high temperatures and even evaporated due to absorption of light energy during the pulse. During evaporation, a cloud of nanoclusters is formed in the air just above the hot spots, and after the end of the pulse, the cloud redeposits onto the substrate. At the regions irradiated by lower intensity where the island temperature is not high enough for IF evaporation, liquid islands move along the surface in local temperature gradients from hot to cold. We present theoretical analysis of temperature distributions around islands of various sizes under ns pulsed irradiation and calculate kinetics of island motion in a temperature gradient.

Diffusion barrier properties of reactively sputtered W-Ti-N thin films

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poster I-51

Initiated by the demands of high temperature and high power electronics, the long-term stability of ohmic and Schottky contacts on III-V semiconductors has been extensively studied. These contact layer systems generally include a diffusion barrier that prevents the metallurgical reaction between metallization and semiconductor substrate. The stability of thin film diffusion barriers in semiconductor high-temperature metallization is essential for successful device performance.
In this work, we have investigated the deposition processes and thermal stability of reactively sputtered W-Ti-N thin films. This study was focused on the effect of nitrogen content in these films on structural, electrical and barrier properties.
The conductivity, stress, crystal structure and chemical composition as well as surface morphology have been investigated using four-point probe sheet resistance measurements, stress measurement optical system, X-ray diffraction, Rutherford backscattering spectrometry and atomic force microscopy.
Our results show, that by optimizing the parameters of sputter deposition (W - Ti (30 at.%) target, dc power 200 W, nitrogen partial pressure 0.05 Pa, total gas pressure 0.5 Pa), the 100 nm thick amorphous $W_{65}Ti_{17}N_{18}$ film shows excellent barrier property preventing the interaction between Au and GaAs under annealing at 750^o C.

STRUCTURAL AND OPTICAL PROPERTIERS OF β -FeSi$_2$ PHASE PREPARED BY ION BEAM SYNTHESIS

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poster I-52

Semiconducting iron disilicide (β -FeSi$_2$) was prepared by ion beam synthesis (IBS) in (111)Si P-type by implantation of 195 KeV Fe ions with a dose of 2x10^{17} Fe$^+$/cm^2 and implantation temperature at 440 ^{o}C followed by annealing in a N_2 atmosphere at 900 ^{o}C for 4 h. Characterization of samples was carried out using Rutherford backscattering spectrometry (RBS), X-ray diffraction (XRD) pole figure, and Raman spectroscopy. A mixture of β -phase and α -phase was observed in the as-implanted state.
A Photoluminescence (PL) measurement at 12 K indicates the luminescence peak at the energy of about 0.81 eV corresponding to a wavelength of 1.532 μ m.

Keywords: Iron silicides; Ion beam synthesis; RBS; XRD pole figure; Raman spectroscopy; PL

Surface diffusion of potassium from iron catalyst

poster I-53

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Many catalysts are promoted by the addition of small amounts of alkali compounds which are known to change the selectivity of heterogeneous reactions in a favorable way. For example potassium is used as promoter for the iron catalyst in the Fischer Tropsch or ammonia synthesis. Taling into account an important radius of potassium atoms, they do not dissolve in the crystal lattice of iron and remain on the surface. Thus, the surface diffusion of potassium at higher temperatures is crucial for catalyst activation and deactivation. This paper is focused on the diffusion of potassium on the surface of ammonia synthesis iron catalyst studied under ultrahigh vacuum, under atmospheric pressure and under the pressure of 10 MPa. Under UHV the diffusion of potassium from iron catalyst to the iron foil has been studied using AES method. The AES spectra were taken from the iron surface in the temperature range 500-600 ^{0}C. The concentration profiles of potassium were observed in time. The diffusion of potassium on the iron surface was simulated using one dimensional second Fick$^{'}$s equation. The diffusion of potassium with a gas stream (nitrogen-hydrogen mixture) has not been observed at the temperature of 520 ^{0}C under atmospheric pressure. The intergranular diffusion of potassium has been proved during the ammonia synthesis reaction under the pressure of 10 MPa at the temperature above 400 ^{0}C.

The structure and properties of oxygen hardenend titanium and its alloys

poster I-54

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Dynamic development of application of titanium and its alloys in modern automotive and aircraft industry, forces the necessity of finding new ways of improving mechanical and chemical properties of applied materials. One of the possibility is the diffusion hardening of titanium and its alloys by such elements as nitrogen, carbon and oxygen, most often in glow discharge processes.
The results of the X-ray analyses (diffraction, chemical microanalysis) and mechanical tests (microhardness) of diffusely hardened substrates of titanium and Ti6Al4V alloy are presented in this paper. The substrates underwent the process in plasma discharge in presence of oxygen and argon mixture, and after that the series of researches were conducted.
The X-ray diffraction was used to determine the phase composition of formed layers, X-ray microanalysis to determine the chemical composition changes of alloying components (aluminum and vanadium) and oxygen, in the surface layer. The microhardness distribution test was also done. The influence of chemical composition of the substrate, on the structure and mechanical properties and thickness of hardened layer, was evaluated.

TIME EVOLUTION MODELLING OF THE SURFACE COVERAGE FOR CATALYTIC SYNTHESIS OF CARBONIC ACID GAS

poster I-55

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Carbonic acid gas synthesis in carbon mono-oxide oxidation reaction is considered. The system of differential equations for modelling of the processes based on Langmuir-Hinshelwood mechanism is written down, and the results for a reduced system with neglected diffusion and constant reaction rates are presented. The temperature T of the system equals 520°C, partial pressures of incoming components are P_{CO}=2.13*10^{-3}Pa and P_O=2.66*10^{-2}Pa for carbon mono-oxide and oxygen, respectively. Peculiar to the presented model is an attempt to take into consideration near-surface interactions through near-surface concentrations of CO and O_2. Catalyst surface layer is considered to consist of free active sites and adsorbed carbon mono-oxide and oxygen, near-surface layer consists of CO, O_2 and the product (CO_2). Results were as it would be expected: optimal incoming concentration ratio of CO to O_2 is 2:1. Deviation from the optimal conditions leads to poisoning by CO or O particles (a typical feature is the adsorption of all species on the catalyst surface). The reaction product occupies space in near-surface area instead of CO. Time of formation of the steady state is not more than 2s for the optimal initial conditions. We also suggest using the dependence between the adsorbed CO and O coverage as a qualitative index for finding the optimal initial conditions. The optimal conditions are achieved when the curve transforms to a closed loop. The critical minimal value for the closed loop formation is the 24% surface coverage by the adsorbed oxygen. Our suggestion to receive the optimal results by varying initial conditions is to increase the oxygen concentration until the optimal values are reached.

Structural determination of the low-coverage phase of Al on Si(001) surface

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For many years, the investigation of group-III metals on Si surfaces has been one of the typical studies in surface science. This system exhibits an abundance of surface structures depending on the coverage and the annealing process. Al is one of the group-III metals and a particularly important material for the device applications. But atomic structure of the low-coverage Al absorbed on Si(001) surface is still under debate. Thus, initial stages of Al growth on Si(001) surface have been studied using low-energy electron diffraction (LEED) and coaxial impact collision ion scattering spectroscopy (CAICISS). Because the low energy ion which is sent to the target material from ion source does not deeply penetrate the sample, CAICISS has been known the very surface-sensitive technique.
A standard cleaning procedure allowed us to obtain sharp (2X1) LEED patterns of Si(001) surface mainly free of contamination. Al was evaporated from a heated tungsten filament onto the substrate at the well defined conditions. After that, we investigate the atomic structure of Al on Si(001) surface. To confirm our results definitely, computer simulations with a two-dimension trajectory count method were also performed and compared with experimental results.

ExplosiveTreatment Effect on Structure and Properties of (gamma+epsilon) Alloy on the Basis of Fe-Mn-Solid Solution

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The samples of Fe77.95Mn20Si2C0.05 alloy were quenched in water (from T=950^{0}C) and were subjected to explosive treatment, created by explosive missile device evolving the pressure pulse 45 GPa during 1 s. The extremely energy densities, high pressures, shear stresses at explosive treatment could initiate the various chemical reactions or phase transitions. Magnetometry methods allowing to fix and to run down even insignificant concentration changes of α -phase were used.
The initial samples without explosive treatment contain 0.7% α -phase after quenching according to hysteresis dependence of magnetization on magnetic field strength (H). The crystallites' size was estimated as about 300 nm according to coercitivity force. After explosive treatment (P=45 GPa) the ferromagnetic component in the sample becomes the smaller and with respect to magnetization corresponds to 0.2% α -phase content with crystallites' size about 150 nm. The temperature investigations with heating of samples up to 460^{0}C result in weak decreasing of magnetization for both samples. Further heating up to T=600^{0}C offered to determine of the Curie temperature (which runs 650^{0}C of observed phase for both samples possible. And that was typical for α -phase.
Thus under missile explosive treatment α -phase content reduces one-third as large for Fe77.95Mn20Si2C0.05 steel with decreases of crystallites sizes. Probably this was stipulated by α -> γ inverse transformation initiated by high pressure and shear stresses.

Characterisation of newly obtained Pb(Mn1/3Nb2/3)O3 ceramics by XRD, XPS and dielectric permittivity tests.

poster I-58

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The Pb(Mn1/3Nb2/3)O3 ceramics has been newly obtained from oxides by sintering in air, using a two-step process with precursor phase. In the first step, the columbite-like phase, (Mn0.5Nb)O3 was obtained. Lead oxide was added in the second step. The final sintering temperature was equal to 1150 oC. Analysis of the XRD spectra indicates that the ceramics consThe cell parameters are: a = 12.193(3) Å, b =11.966(6) Å, c = 12.144(2) Å beta = 90o10.7'. X-ray photoelectron spectroscopy was used to study the chemical composition and electronic structure of the Pb(Mn1/3Nb2/3)O3 ceramics. A nominal chemical composition was Pb1.00(Mn0.33Nb0.67)O3 while the chemical composition obtained from the XPS measurements is Pb0.99(Mn0.43Nb0.67)O2.92. The core levels of lead, manganese, niobium and oxygen were measured and deconvoluted into the synthetic peaks. Broadband dielectric measurement was carried out in frequency range from 10-2 to 106 Hz within 90 - 600 K temperature range. From analysis of dielectric spectra two relaxation processes were distinguished. First process, manifesting at lower temperature range, is related to electric conductivity with activation energy, Ea = 0.35 eV. The second process exhibits relaxation properties characteristic for a diffused, relaxor-type phase transition.

Electronic structure of $AgNbO_3$ single crystals

poster I-59

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The electronic structure of niobiates attracts attention due to interesting ferroelectric and relaxor characteristic. Moreover $AgNbO_3$ has arisen as a new visible-light-driven photocatalyst. The XPS electronic structure measurements of the $AgNbO_3$ single crystals were performed. The results were compared with those obtained for the $NaNbO_3$ ceramic. The chemical composition determined by the XPS method is $Ag_1.1Nb_0.93O_2.97$. The core level measurements revealed a smaller negative chemical shift of the Ag 3d line (-0.3 eV) in comparison with Na (-1.1 eV). The positive chemical shift of Nb 3d line +4.2 eV is in agreement with those obtained for the Nb 3d in $NaNbO_3$. The chemical shift of the O 1s line is -1.3 eV for $AgNbO_3$ and -1.8 eV for $NaNbO_3$. These results suggest a mixed covalent and ionic bonding in the compounds. The covalent character of the bonds is between Ag (or Na) and oxygen and while the ionic with Nb. The valence band exhibits the energy gap about 2 eV which is in agreement with literature data.

Permiability of Deuterium in TiN films

poster I-60

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Permiability of Deuterium in thin films was measured. TiN, DLC and Aluminum films were deposited on stainless steels by sputtering and ion plating. The effect of temperature, thickness of films, and chemical composition of films on the permiability of Deuterium was studied. Low permiation of Deuterium in TiN films was observed.

MAGNETORESISTANCE AND HALL EFFECT CHARACTERISATION OF SOME MAGNETIC MULTILAYER STRUCTURES

poster I-61

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Structures as FM/NM/FM were deposited onto oxidized Si wafers. FM denotes NiFe (Permalloy - Py), Co layers or combination using Py-Co layers. As NM we have deposited Cu or Al_2O_3 layers. In this work are presented results for Py/Cu/Py/FeMn, Py/Al_2O_3/Py/FeMn, Py/Co/Cu/Co/Py/FeMn and for Py/Co/Al_2O_3/Co/Py/FeMn multilayers. We made magnetoresistance and Hall effect measurements in order to study the magnetic properties of the samples and the quality of the interlayer. Planar Hall Effect measurements were employed to evaluate the magnetization reversal processes and the coupling between the magnetic layers. Also, we made tunnel experiments on the structures with Al_2O_3 as NM layer. Finally, we made some correlations between these measurements. Because the conduction electrons in ferromagnetic metals are spin polarized and the spin is, usually, conserved in tunneling process, Jullires model for FM/I/FM tunneling, predicts that the tunnel junction magnetoresistance is dependent on the relative orientation of the magnetization vectors in the adjacent magnetic layers separated by an insulator, I. The results of our measurements are related with the samples microstructure. The saturation fields obtained when the magnetic field is applied normal to the film plane are less than the values predicted from the shape anisotropy and give us information regarding the films roughness.

Structure and electrical properties of the film CoFeZr-aluminium oxide nanocomposites

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The goal of present paper was to investigate the influence of phase composition on DC and AC conductance of film composites containing CoFeZr nanoparticles (6 to 10 nm dimensions) in aluminium oxide matrix for atomic concentrations of metallic fraction x = 30-65 %.
Mössbauer study are evident of strong correlation between metallic fraction x in the composite and relative contribution of Fe ions in two different valence states (2- and 3-multiple-charged). It probably shows that phase composition of metallic component depends on the ratio between metallic and dielectric components. Temperature dependencies of DC resistivity described by exponential laws are characteristic for variable range hopping with Mott or Shklowski-Efros mechanisms. In the temperature range 77-300 K static I-V characteristics of the samples displayed non-ohmic character and were attributed to co-existence of Pole-Frenkel and ohmic (linear) laws. In so doing, the exponential contribution increased with the elevation of dielectric component. It was also exhibited negative magnetoresistance effect with squared-like magnetic field dependence that can be ascribed to tunneling of carriers between metallic particles.
Both real and imaginary parts of impedance in high-ohmic samples with $x < 40$ % in the frequency range from 0.1 to 10 kHz were not dependent on applied bias voltage, at least, for electric fields up to 4 V/cm. In the samples with $x > 40$ % the dramatic increase (up to 2-3 orders of magnitude) of capacitance modulus occurs at achieving some threshold value of bias voltage. The obtained increase of capacitance modulus with bias voltage is always accompanied by the decrease of real part of impedance. The value of threshold bias voltage decreases with the growth of metallic component content in the studied composites.

Electrolytic composite nickel layers with nano-sized Si_3N_4 disperse phase

Anna Wyszyńska[1], Magdalena Kowalewska[1], Maria Trzaska[1] poster I-63

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Composite layers with nickel matrix and nano-sized Si_3N_4 disperse phase have been the subject of the authors' investigations. The composite layers used in this study have been produced by two kinds of deposition techniques, i. e., by the chemical reduction and the electrochemical method. A disperse powder of the silicon nitride with grain dimensions in order of 15 nm has been used for the depositions of the composite coatings.
Results of the morphology and diffraction analyses of the silicon nitride powder and its contents in the materials of the composite coatings are reported. The chemical compositions and the surface topography of the nano-crystalline composite layers as well as the structure of the produced composite $Ni-Si_3N_4$ and $Ni-P-Si_3N_4$ coatings have been studied. The microstructures of the coatings were examined by scanning electron microscope (SEM) equipped with EDS suitable for local chemical analysis. Moreover, studies of the used ceramic phase and the composite coatings have been performed with XRD and TEM techniques. The comparative analysis of the obtained results showed that the type of the methods applied for producing of the composed coatings has an important influence on the contents and distributions of the nano-disperse phase within the surface composite layers.

Study about burning of hydrogen isotopes on metallic catalyst in detritiation pilot plant for CANDU reactors

poster I-64

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The Nuclear Power Plant Cernavoda is equipped with a CANDU reactor and is the most powerful tritium source from Europe. This reactor is moderated and cooled with heavy water which is continuous contaminated with tritium. For these reasons, NIR&DCIT Rm. Valcea developed a detritiation technology based on catalytic isotopic exchange and cryogenic distillation. In some stage of the detritiation process the oxygen is considered like impurity in the fluid, that could product the obstruction of the pipes. The oxygen could be removed by recombination with hydrogen, using a metallic catalyst. The final product of the detritiation process is deuterated hydrogen. In the process of the catalytic burning of the deuterated hydrogen is obtained the heavy water, free of tritium, witch could be reused in the CANDU reactor. Both modules, which include the purification from the oxygen and deuterated hydrogen burning, are equipped with deoxo catalyst (palladium on Al2O3) or Pt on charcoal. The interaction between hydrogen and oxygen molecules devolves through the succession of the reactions. Superficial species which are participating at the reaction, proceed from the dissociate chemisorption of the oxygen and the hydrogen molecules. It is observed by the Gibbs energy, which is negative, that reaction is thermodynamic possible. The reaction could be release by the palladium or platinum catalyst. The catalytic oxidize of hydrogen on palladium or platinum catalysts devolve with the oxygen chemisorption on catalyst and then with the reaction of the hydrogen from gas stage. Order of the reaction is one for the hydrogen and zero for the oxygen. The paper describes a study about the platinum and palladium catalyst and the mechanism of the reaction between hydrogen isotopes and oxygen using these catalysts.

"CO oxidation on thin Pt crystals : stoichiometric and mathematical models."

poster I-65

Bogdan Gnativ[1)], **Myhaylo V. Tokarchuk**[2)], **Igor Penyak**[1)]

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The problem of developing a mathematical model of oscillatory chemical reactions accompanied by formation of chemically unstable compounds retains importance in kinetics of heterogenic systems. Oxidation of CO on Pt (110) surface is a typical example of such reaction. We performed a stoichiometric analysis of the system in order to simplify the analysis of the process and view it as a sequence of separate elementary stages for which it is easy to determine its numeric characteristics.We applied the concept of formation of active intermediate substances (coating) as reagents in elementary stages of the reaction, avoided the analysis of mass transfer processes, took into account the route of reaction, and built and analysed the stoichiometric matrix. Further, we elaborated a molecular matrix for reaction components. With regard to additional limitations of the mass balance due to the molecular matrix we determined the quantity of linearly independent stages of the process. Linking of rates of elementary reactions with rates of reaction for each component according to the principle of independent elementary reactions lead us to the system of algebraic kinetic equations. In closed systems including each elementary stage of a complex oxidation reaction, it transforms into a system of differential equations. After equalization of elementary stages of the process based on the concept of stoichiometric multipliers in order to avoid the side products of reaction in the final equation and after introduction of corresponding changes into the stoichiometric matrix according to the principles of formal kinetics we obtained the final model for quantitative investigation of time characteristics of complex heterogenic processes in kinetic part. Comparison of quantitative results of model investigation with experimental data indicates that this model can be justifiably applied for processes in kinetic part of experiments.

Conductivity in quantum wires in a homogeneous magnetic field

poster I-66

Elerlanj P. Sinjavsky[1)], **R. A. Hamidullin**[1)], **Albina A. Nikolaeva**[1,3)], **Huber T.**[2)], **Leonid A. Konopko**[1)]

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In model of parabolic potentials taken into account the anisotropy of effective mass of current carriers it is calculated electroconductivity of quantum wires in the homogeneous magnetic field, directed along a surface of the size-limited system, and field perpendicular to axis of spatial quantization. Temperature and field dependences of conductivity for nondegenerated and degenerated quantum quasy one-dimensional systems are investigated. The received results for electroconductivity are compared to experimental data [1].The features of electroconductivity, arising in quantum systems with the lowered dimension are in detail discussed. In particular it is shown, that in a perpendicular magnetic field conductivity in systems with the lowered dimension in a quantum limit $\omega_c\tau$ »1 (ω_c- cyclotron frequency, $1/\tau$ it is determined by probability of carriers scattering on acoustic oscillations) can be much more, than in bulk semi-conductor systems. This circumstance can appear one of the possible reasons of sharp increase in electroconductivity in the perpendicular magnetic field, experimentally observed in quantum wires Bi [1] with thickness about <100nm.

[1]. A. Nikolaeva, D. Gitsu, T. Huber and L. Konopko. Physica B: Condensed Matter, Volumes 346-347, 30 April 2004, Pages 282-286.

The work was supported by the Civilian Research Defense Corporation, CGP- grant # MO-E1-2603-SI-04.

Electrical conductivity of TiC and (Ti,W)C ceramic samples

poster I-67

Nikos Guskos[1,2], **Janusz Typek**[2], **Anna Biedunkiewicz**[3], **Stamatis Patapis**[1], **Konstantinos A. Kanekas**[1], **Michał Maryniak**[2]

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Three samples: crystalline titanium carbide TiC (sample I), titanium-tungsten carbide (Ti,W)C (sample II), and nanocrystalline TiC dispersed in a carbon matrix (sample III) have been selected for electrical conductivity measurements. The first two samples consisted of macron-size grains, while the third was a nanocrystalline TiC/C composite and was synthesized by a nonhydrolytic sol-gel process. All samples have been characterized by the X-ray diffraction (XRD), scanning microscopy, microanalysis (WDS and EDS), transmission electron microscopy (TEM) and electron diffraction techniques. In sample II the ratio of W:Ti was equal to 0.3. The grain sizes in sample I and II were measured by the Fisher method and the mean diameter of the grains was calculated to be below 10 m. The TEM investigation of the TiC particles in the sample III has showed that they were formed with an average grain size around 20 nm. XRD measurements of sample III has revealed that the lattice constant is smaller than observed for other titanium carbides TiC_x. The dc electrical conductivity studies have been made in the 80-330 K temperature range. Samples I and II have shown a metallic behavior but with different slopes of the conductance vs. temperature dependence. Sample III displayed at higher temperatures a pronounced thermal hysteresis in dc conductivity. The ac conductivity measurements have not shown any frequency dependence in the 1 kHz -100 MHz range.

Tuesday, September 7th

Afternoon sessionMetal structures and mechanical properties. Chairmen: W. Gulbinski

14:00 - 15:20

Main Building, Small Hall (Mała aula)

Application of diamond anvils techniques for studying nanostructure formation in massive materials directly during severe plastic deformations

14:00 - 14:20 oral

Alexey N. Babushkin[1], **Ivan V. Sukhanov**[1], **Olga V. Savina**[1]

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Progress in understanding of properties of materials at high pressures in many respects is connected to diamond anvils technique. We developed and investigated a technique of megabar range pressure valuation, applicable in the opaque high pressure diamond anvil cell (DAC) with anvils of the "rounded cone-plane" (Verechagin-Yakovlev) type made of synthetic carbonado-type diamonds, consisting of dielectric grains

of synthetic diamonds in layers of conducting materials. These anvils are good conductors, permitting measurement of the electrical properties of samples placed between the anvils in the DAC by using the anvils as the electrical contacts to the sample. We for the first time have applied this technique to research of formation of new states in metals and metals alloys. As structurally sensitive parameters we use a thermo electromotive force (TEMF). At compression of a metal sample in anvils, there are severe plastic deformations. These deformations conduct to change of a microstructure of a material. Therefore, at measurement a TEMF directly it is possible to study dynamics of changes occurring in a sample during deformation. It is possible to study dependence of structure on size of deformation and on time. These techniques represent not only scientific interest, but also can be interesting for technology.
We report the results of an investigation of the TEMF of nanostructured materials (zirconium dioxide, Ti-alloys) directly during severe plastic deformations in DAC (pressure range between 15 and 50 GPa and room temperature). This work was supported in part by grant BRHE EK-005-X1 (Ural research educational center "Advanced materials").

Excellent mechanical properties of UFG metals and alloys, subjected to combination of severe plastic deformation methods.

14:20 - 14:40
oral

Nikolay Krasilnikov[1,3], **Witold Lojkowski**[2], **Ruslan Valiev**[1]

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The Ni and Al-based alloy 2024 after different methods of severe plastic deformation (SPD) are investigated. The equal channel angular pressing (ECAP) and cold rolling nickel, subjected also to high-pressure torsion (HPT), is characterized of large strain degree, homogeneous structure with grain size 120 nm and shows at room temperature the record strength with ultimate tensile stress (UTS) (1270 MPa), but limited plasticity (6%). The combination of high strength and plasticity managed to be obtained using the annealing at 200C of Ni after ECAP and rolling. This treatment of Ni leads to UTS about 900 MPa and ductility 12%.
Using HPT under pressure 6 GPa has allowed to obtain nanostructured samples of Al-based alloy 2024 with grain size 70 nm and high-angle grain boundaries in result of torsion (5 turns) at room temperature. The nanostructured alloy at room temperature demonstrated record UTS above 1100 MPa, and superplastic behavior at temperature higher then 300. The microhardness of nanostructured alloy after superplastic deformation was 1.5 GPa and was more than after standard treatment of coarse-grained state of alloy (1.2 GPa).
Opportunity of achievement in metals and alloys of combination high strength and good ductility opens perspectives of its application in industry, particularly, for mirco-systems and for details with complex geometry, obtained due to superplastic forming.

Structure and mechanical properties of ball milled TiAl-Cr intermetallics consolidated by hot pressing and pulse plasma sintering

14:40 - 15:00
oral

Jan Dutkiewicz[1], **Andrzej Michalski**[2], **Paweł Kurtyka**[3], **Wojciech Maziarz**[1]

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

3) Pedagogical Academy, Podchorążych 2, Kraków, Poland

The TiAl-Cr alloys compositions were chosen from the g-phase stability region up to maximum 5 at. % chromium. The elemental powders were initially blended to desired composition of Ti-49,Al-49,Cr-2 and Ti-48,Al-47,Cr-5 (numbers indicate at. %). The ball milling process was performed in a high energy planetary mill Fritsch Pulverisette P/4 and detailed study of structure and micro-hardness changes during milling was described in [1].
Two consolidation methods of milled powders were applied: hot pressing at 1000C at 35MPa under argon flow and pulse plasma sintering. The conditions of latter method were optimized for pressure, voltage and pressure measuring temperature and shrinkage during the process. The micro-hardness of consolidated samples was about 860 HV1 and only small differences were observed between samples obtained by both

methods. The mean density of pulse plasma sintered compact was about 98 % of theoretical while hot pressed samples had lower density close to 95% of theoretical. The TEM observation of consolidated samples revealed that pulse plasma sintered samples has a grain size in the range of tens of nanometers while the grains in the hot pressed samples are bigger and has size below 1 micron.
The compression tests performed in the temperature range between RT and 900C with deformation rate of 4x10-1s-1 demonstrated differences in ductility and strength of consolidated samples probably due to different level of densification and grains size.

[1] W. Maziarz, M. Fujda, L. Lityńska, J. Dutkiewicz, Microstructure and microhardness changes during ball milling of TiAlCr intermetallics, revived and accepted for publication in Proceeding of Advanced Materials and Technologies Conference, Łódź 2004, Poland

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Densification and characterization of nanocrystalline hypereutectic Al-Si-Fe-X alloy powder compacts produced by mechanical milling and field assisted sintering

15:00 - 15:20
oral

Kandukuri Y. Sastry[1), **Ludo Froyen**[1), **Jef Vleugels**[1), **Omer Van der Biest**[1), **Rolf Schattevoy**[2), **Juergen Hennicke**[3)

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2) Powder Light Metals GmbH (PLM), Am Wiesenbusch 2, Gladbeck D-45966, Germany

3) FCT Systeme GmbH (FCT), Gewerbepark 11, Rauenstein D-96528, Germany

Rapidly solidified pre-alloyed Al-17Si-5Fe-3.5Cu-1.1Mg-0.6Zr (wt%) alloy powder was mechanically milled in air using stearic acid as process control agent. The resulting nanocrystalline powder was degassed at 350C for 5 hrs. Both as-milled and degassed powder were consolidated using field-assisted sintering (FAST) in steel dies under vacuum at 400C. Shrinkage along the pressure axis, temperature and electric current input were automatically stored through a data acquisition system.

As-milled powder and sintered compacts were characterized using optical microscopy, scanning electron microscopy (SEM), X-ray diffraction (XRD) and microhardness measurements. The crystal size, calculated from the line broadening of the X-ray diffraction peaks using Williamson-hall plots, of the FAST sintered mechanically alloyed materials was in the range of 53-70 nm, depending on the type and amount of process control agent used during milling and the FAST parameters. As-milled powders could not be densified to full theoretical density and the particle bonding was improper. Degassed powders on the other hand exhibited a very good interparticle cohesion and could be fully densified under identical sintering conditions.

Coffee break

15:20 - 15:50

Afternoon session - continuedReactions on metal surfaces

15:50 - 17:15

Main Building, Small Hall (Mała aula)

Oxy-dehdrogenation of NH3, Reduction of N2O on Cu(110), two challenging reactions investigated by combining in situ FT-IRAS and kinetics measurements

15:50 - 16:35
invited oral

Claire-Marie PRADIER[1), **Isabelle LOUIS-ROSE**, **Christophe METHIVIER**

1) Ecole Nationale Supérieure de chimie de Paris (ENSCP), 11 rue P. et M. Curie, Paris 75005, France, Metropolitan

Two challenging reactions, the oxy-dehydrogenation of NH3 and the reduction of N2O, were investigated on model metallic surfaces, combining characterisation of model surfaces under low pressures of reactants and kinetics measurements.
New insights into the reactions mechanisms were in particular brought by the in situ determination of the surface intermediates by FT-RAIRS. XPS was also used to characterise the catalyst surface at various extents of conversion. The influence of oxygen upon the two reactions was addressed.
On Cu(110), at 600K, in the presence of an NH3+O2 equimolecular mixture, the active catalyst surface is a mixed oxy-nitride layer. On that new surface phase, the reaction proceeds via a progressive dehydrogenation of ammonia by adsorbed oxygen. The formation of NH2, NH and of a polarised dinitrogen species, adsorbed on Cu(110), was evidenced. An excess of oxygen, or a higher reaction temperature, leads to the formation of N2O, an undesired product of the reaction.
- At temperature below 750 K, N2O dissociation leads to the formation of an oxide surface layer that rapidly blocks the reaction.
- At temperature above 750 K, N2O can be reduced by a NH3 + O2 mixture.
In situ RAIRS characterisation of the copper surface again made clear the formation of NH2, NH and a N2d- adsorbed species. The IR frequency of it's stretch mode is strongly influenced by the atomic environment of this species making this molecule a probe to assess the surface occupancy by oxygen or hydroxyls.
A surface science approach, combined with kinetics tests enables us to suggest that the reactivity of N2O is strongly related to the concentration of oxygen on the surface.

16:35 - 16:55
oral

THE DOMINANT OF CH BONDINGS IN a-C:H THIN FILMS GROWN BY DC-PECVD AT VARIOUS CHAMBER PRESSURES

Yussof B. Wahab[1], **Suriani A. Bakar**[1], **Bakar B. Ismail**[1], **Mohamad K. Saidin**[1]

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Hydrogenated amorphous carbon thin films (a-C:H) have been of great scientific interest since their advent for mechanical, chemical, optical and electrical applications, owing to their flexible properties depending on specific deposition conditions. Their final resulting properties seem to be determined from their microscopic structure compromised by the local bonding configuration among carbon-carbon and carbon hydrogen atoms in the film matrix, which can be varied by choosing the appropriate external deposition parameters. In this work the bonding configurations of PECVD's deposited a-C: H films are studied using infrared analysis under varying deposition pressures of 0.1- 0.8 torr or an equivalent electrical power between 0.30 - 0.16 W. Other fixed parameters were 5 sccm CH4 flow rate, 2.5 cm electrode spacing, and room temperature deposition for the periods of 5 hrs. It was observed that, form infrared Spectroscopy the relevant CH bonding in the stretching frequency range, 2700 - 3200 cm-1 appeared to be dominant if compared to those of CC bonding. Essentially, the stretching of the measured spectrums seemed to be in wavy-like curves associated with spmCHn configurations with m,n = 1-3, and this trend was gradually disappearing with an increase of pressure up to 0.8 torr. The curve measured at 0.2 torr indicated marked changes with detectable infrared absorption rates in a-C: H at 2959 cm-1, 2934 cm-1 and 2872 cm-1, which were corresponded to the presence of sp3CH3 (both symmetric and asymmetric) and sp3CH2 (asymmetric). A further investigation using XRD analysis confirmed the amorphousity of the as-prepared a-C:H thin films.

Wednesday, September 8th

09:30 - 10:20

Morning sessionMetallic thin films. Growth kinetics. Polymer films on metals

Main Building, Small Hall (Mała aula)

09:30 - 09:50
oral

Kinetics of Phase Formation in Mechanically Alloying Ni-Al and Fe-Al Powder Systems

Ludmila Paritskaya[1], **V. V. Bogdanov**[2]

1) Karazin Kharkov National University, Department of Crystal Physics, 4 Svoboda Sq., Kharkov 61077,

Ukraine
2) Karazin Kharkov National University, Department of Crystal Physics, Ukraine

Mechanically alloying (MA) Ni-Al multi-layered samples with alternating Ni and Al layers of tens nm thickness and Fe-Al powder systems composed of the spherical Fe particles of tens nm diameter inserted into matrix of fine-grained Fe-Al mixture were used for study the kinetics of intermetallic growth at temperatures 300-600^{o}C. X-ray phase analysis, optical microscopy and SEM were applied for measurement of the volume fraction of new phases and average thickness of intermetallic layers. The kinetics of intermetallic growth was also studied in massive Ni-Al and Fe-Al diffusion couples. The diffusion characteristics for both the MA and massive objects were calculated from the growth kinetics. The phase formation in MA systems begins at much lower temperatures (300^{o}C) compared to massive couples (550^{o}C). Low pressures up to 0.5 kbar accelerated the phase formation in MA powder objects, increasing the phase volume fraction due to increase of phase nucleus density. The mechanism of low-temperature phase formation, based on interdiffusion of both sort atoms along interfaces, phase nucleation at interfaces and their subsequent displacement, is proposed and discussed. Accelerating effect of low pressure is caused by elimination of cavities and other discontinuities at interfaces and as a result the more active phase nucleation at more perfect interfaces.

Corrosion control by conducting polyaniline

09:50 - 10:10
oral

Dilip R. Peshwe, Shailkumar U. Pathak, Pravin P. Deshpande[1)]
1) Visvesvaraya National Institute of TechnologyE (VNIT), N.Ambazari road, Nagpur 440 011, India

By using potentiodynamic , galvano static and potentiostatic polarization , conducting polyaniline coatings are obtained on low carbon low alloy steel in aqueous oxalic acid. These coatings were characterized by spectro photometry and raman analysis . It has been shown that the extent of steel protection in aqueous acidic medium is governed by amount of conducting phase of polyaniline . The coating is able to withstand defects because of Leucoemeraldine to emeraldine transformation .
Key words - Conducting polyaniline, corrosion control.

Characterisation of conducting polyaniline coatings

10:10 - 10:30
oral

Shailkumar U. Pathak, Dilip R. Peshwe, Pravin P. Deshpande[1)]
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By using electrodeposition , conducting polyaniline coatings were obtained on steel. These coatings are characterised by cyclic voltammetry and potential time curves. The electrodeposition mechanism was studied.

Coffee break

10:30 - 11:00

Morning session - continuedMetallic thin films. Interconnects. Chairmen - H.-J. Muessig

11:00 - 12:20

Main Building, Small Hall (Mała aula)

Annealing-Induced Solid-State Amorphization and Nanocrystallization in Metallic Thin Films

11:00 - 11:20
oral

Jinn P. Chu[1)]**, T. Mahalingam**[1,2)]**, Chang-Ting Lo**[1)]
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We present a direct experimental evidence that the controllable solid-state amorphization and nanocrystallization during annealing of a metastable film could serve as a precursor for exciting new nano materials. Unlike other metallic glassy materials that exhibit devitrification during annealing, our sputter deposited film with good glass-forming ability is transformed into various nano-scale and amorphous structures due to annealing process. Upon low-temperature annealing, a metastable crystalline phase that is formed due to the non-equilibrium sputtering re-dissolves. The new interesting discovery is that the metastable phase in the form of nanocrystalline is further transformed into another metastable phase in the amorphous state, instead of a crystalline state in the supercooled liquid region, with a subsequent crystallization at higher temperatures. The measured film properties (hardness and electrical resistivity) are in good agreement with those derived from the microstructure/crystal structure evolution. Such a structural development provides the opportunity to adjust the structure/property relationships necessary to tailor specific optical, electrical, and mechanical properties. The exceptional amorphization behavior can be rationalized as a consequence of the low free energy of amorphous phases, with combined effects of thermal and interfacial energies between the nanocrystalline and amorphous phases.

11:20 - 11:40
oral

fabrication and investigation of Ni-SiC nanocomposites under triangular waveform

Fei Hu[1)], **K.C. Chan**

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The codeposition of non-metal particles and metal phases brings a significant improvement on the mechanical and physical properties of electro-coatings. The quality of the coatings depends mainly on the grain size of the matrix metal, and the volume percentage and distribution of the codeposited particles. The present project is to fabricate nanocomposites under the triangular waveform with relaxation time and to investigate their deposition behaviour. Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) were utilized to investigate surface morphology of nickel-SiC composites, and the volume percentages of silicon carbide particles were also determined.
Nanosized silicon carbide particles (β SiC) of diameter about 100nm were used in the experiments. It was found that the application of triangular waveform and SiC particles changed the shape of the nickel grain from a pyramid-like structure to a nodular-like structure, and reduced the average grain size of nickel matrix to about 30nm, comparing with those under direct current conditions.
The Guglielmi's adsorption mechanism was extended to predict the volume percentage of silicon carbide particles in the codeposition process using direct current and triangular waveform with relaxation time. It was shown that the percentage of silicon carbide particles embedded in the coating could be increased by using a triangular waveform current. The trend of the predicted volume percentage was found in good agreement with the experimental results.

11:40 - 12:00
oral

Refractory metallic borides used for gate electrode applications in CMOS integrated circuits

Wanda Zagozdzon-Wosik[1)], **Deepa Radhakrishnan**[1)], **Chinmay Darne**[1)], **Irene Rusakova**[3)], **Paul van der Heide**[2)], **Zu-Hua Zhang**[3)], **Joe Bennett**[4)], **Len Trombetta**[1)], **Prashant Majhi**[4)]

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We studied the behavior of metallic diborides TiB2, ZrB2 and HfB2 deposited by e-beam evaporation on thin 20-100A thermal oxides. The diborides films (200-500A) were tested for potential applications as metal gates in CMOS integrated circuits (IC). The most important gate parameter, besides low resistivity, is metal work function, which should be within 0.2 eV of the valence or conduction band edges of Si for PMOS and NMOS transistors, respectively. We evaluated work function values of the borides and found compatibility with PMOS transistors based on MOS capacitors and corresponding Kelvin probe measurements.
Compatibility of these metal gates with the IC processing was tested using rapid thermal processing in temperatures up to 1100C. Electrical characterization of the capacitors included C-V tests and I-V measurements. They were complemented by sheet resistance measurements. For material characterization, we used RBS, XRD, SIMS, cross-section TEM, and XPS to determine stoichiometry, composition, and crystallographic structure of the processed films as well as possible B outdiffusion. Kelvin probe combined with depth profiling was used to measure work function uniformity within the films before and after annealing.

Electrical measurements of the test structures confirm very high thermal stability of stoichiometric diborides that allows for preserving the sharp interface of metallic gates with the underlying dielectric layer without its degradation during high temperatures RTP. This is confirmed by TEM, XPS, RBS, as well as SIMS results. However, annealing causes lateral shifts of C-V characteristics indicating positive shifts of flat band voltages. These changes coincide with Kelvin probe measurements pointing at modifications of borides work functions (ex. 4.71 eV to 4.93 eV for TiB2). They are related to film recrystallization, which is detected by XRD as well as by TEM and electron diffraction. Decreasing resistivity also results from the grain growth.
[
[ABSTRACT TRUNCATED TO 2000 LETTERS]

Formation of contacts and ultra shallow junctions using diborides of Ti, Zr and Hf

12:00 - 12:20
oral

Ragesh Ranjit[1)], **Wanda Zagozdzon-Wosik**[1)], **Irene Rusakova**[2)], **Paul van der Heide**[3)], **Zu-Hua Zhang**[2)], **Joe Bennett**[4)]

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Metallic diborides TiB_2, ZrB_2 and HfB_2 were used for the formation of contacts integrated with ultra shallow junctions required in deep submicron devices in integrated circuits. The films were deposited by electron-beam evaporation on an oxide free surface of both p- and n-type Si. Rapid thermal processing (RTP) in N_2 ambient was performed using temperatures up to 1100C and time up to 30s. Test structures on p-type Si were fabricated to determine contact resistance before and after the annealing processes. The borides form ohmic contacts on p-type Si after deposition and improve their ohmic behavior after annealing; specific contact resistivity decreases with temperature (from 9.3E-05Ωcm^2 at 800C to 4.3E-6Ωcm^2 at 1100C for TiB_2). On n-type Si, the formation of Schottky diodes was determined for as deposited structures and those annealed at low temperatures. Barrier heights and ideality coefficients n were determined. With increasing thermal budget p-n junctions were identified that had low leakage currents. To evaluate possible doping of the silicon beneath the borides contacts and specific contact resistivity we used measurements of transmission line model resistor.
A set of complementary material testing including XPS, XRD, SIMS, cross-section TEM, and RBS was done to determine stoichiometry, composition, and crystallographic structure of the processed films. Electrical characterization of the films was done using sheet resistance measurements, which show decreasing resistance with increasing thermal budget and Kelvin probe, which indicated changes in the work function values during annealing. These films showed recrystallization as identified by XRD and by TEM with electron diffraction. Materials studies show very high stability of the diborides if their composition is stoichiometric. However, SIMS results combined with XRD provide evidence that nonstoichiometry deteriorates this stability and results in larger than desired B outdiffusion.
[ABSTRACT TRUNCATED TO 2000 LETTERS]

Lunch break

Main Building, Small Hall (Mała aula)

12:20 - 14:00

Afternoon sessionComposite films Chairmen - Y. Pauleau

Main Building, Small Hall (Mała aula)

14:00 - 15:20

First-principles simulations of the reactivity of barrier layers of Ti, Ta and W and their nitrides towards precursors for CVD copper deposition

14:00 - 14:20
oral

Pablo Ordejon[2)], **Eduardo Machado**[2)], **Marcin Kaczmarski**[2)], **Benoît Braida**[2,3)], **Eduardo Hernandez**[2)], **Hansong Cheng**[1)], **Diwakar Garg**[1)], **John A. Norman**[1)]

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We present first-principles Density Functional Theory calculations of the reactivity of Ti, Ta and W surfaces and their nitrides with Cu-hexafluoracetylacetonato-trimethylvinylsilane [Cu(hfac)(tmvs)], a chemical precursor used for CVD growth of copper films. We show that the surfaces of the pure refractory metals are highly reac-tive, and that the copper precursor decomposes spontaneously upon contact with the surface. The products of the decomposition attach strongly to the surface, forming fluorine, carbon and oxygen containing layer on the surface that may lower the effi-ciency of the copper deposition and the adherence of the copper layer. For the case of the metal nitrides, those surfaces prepared with an orientation such that no refractory metal atom is exposed to the surface do not show such reactivity, with the copper precursor staying intact upon interaction with the surface. Our simulations suggest strategies for improved deposition efficiency and adhesion properties of copper films deposited by CVD on refractory metal barrier layers.

14:20 - 14:40
oral

Structure and Tribological Properties of Copper/Carbon Composite Films

Witold Gulbiński[1), Sławomir Kukiełka[1), Yves Pauleau[2), Francois Thiéry[2)
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2) CNRS-Grenoble, LdC (CNRS-G/LdC), Grenoble, France

Copper/carbon composite films have been deposited on steel and silicon substrates by an hybrid technique combining sputter-deposition of copper and microwave plasma-assisted chemical vapor deposition of carbon from argon-methane mixtures of various concentrations.
The composition of films was determined by Rutherford backscattering spectroscopy (RBS) and energy recoil detection analyses (ERDA). The crystallographic structure of films was identified by X-ray diffraction (XRD) techniques. The dry friction properties of films were investigated by ball-on-disk tribological tests conducted at room temperature in room air.
Copper/carbon films containing 25 to 75 at.% of carbon were produced as the methane concentration in the gas phase was varied from 20 to 100 %. These composite films consisted of copper crystallites and hydrogenated amorphous carbon (a-C:H) phase. The size of copper crystallites was in the range 2-20 nm. An abrupt increase in carbon content in the films was observed as the methane concentration in the gas phase increased from 60 to 70%.
The tribological properties and mechanical behavior of these Cu/a-C:H composite films are analyzed and discussed as functions of their microstructure, morphology and composition.

14:40 - 15:00
oral

Influence of structural and thermal properties of new CVD precursors of copper and silver on the quality and morphology of nanometallic layers.

Edward Szłyk[1), Piotr Piszczek[1), Iwona Szymańska[1), Robert Szczesny[1)
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New Cu(I), Ag(I)and Au(I) complexes with silyllated and perfluorinated carboxylates [$RCOOMPR_3$], and tertiary phosphines PR_3; R= Me, Et and diphosphines were characterized by ^{13}C, ^{19}F, ^{31}P NMR, IR, MS spectroscopy and thermal properties studied. Thermal decomposition of complexes proceeds in a multistage processes, which yields metallic final product detected by XRD. Results of MS studies and thermal analysis exhibited were used to propose the decomposition mechnism. TGA/IR analysis of gases evolved during decomposition revealed metallated particles in gases, which decide about the transport mechnism in CVD processes. Thermal decomposition of copper complexes, in nitrogen and air yields metallic silver and a mixture of Cu_2O and $Cu_2P_2O_7$. Chemical Vapour Deposition in hot wall reactor precursors based on studied carboxylates yields nanometric metallic layers. Therefore studied complexes can be treated as a new class of silver, copper and gold precursors. The morphology and composition of the nanolayers were characterised with XRF, XRD, XPS, SEM, STEM and relations between thicknes of the metallic layer and type of precursor were discussed.

Acknowledgement
Financial support from Polish State Committee for Scientific Research grant # 3T08 039 23 is gratefully acknowledged.

Independent tuning of particle diameter and interparticle spacing in Ni nanoparticle systems

15:00 - 15:20
oral

Satoshi Tomita[1], **Kensuke Akamatsu**[2], **Hiroyuki Shinkai**[2], **Shingo Ikeda**[2], **Hidemi Nawafune**[2], **Takanari Kashiwagi**[3,4], **Masayuki Hagiwara**[3,4]

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Macroscopic properties of ferromagnetic-metal nanoparticle systems are strongly affected by two microstructural parameters; the diameter of constituent particles (d) and their spacing (r). Therefore, these parameters must be fine-tuned in order to design and realize a system for a specific purpose or application, e.g., ultra-high density magnetic recording media. Nevertheless, independent and precise modification of the d and r at the level of several nanometers still remains a challenge. In this contribution, the independent tuning of the d and r in ferromagnetic Ni nanoparticle systems has been reported.
Ni nanoparticles were chemically embedded in polymer films called polyimide by applying a surface modification technique. The structure of the films was characterized by transmission electron microscopy (TEM). The TEM observation showed that the thermal decomposition of the polyimide matrices brings about a decrease in the spacing r among Ni nanoparticles with an almost constant diameter d. Ferromagnetic resonance (FMR) in the films was investigated. The FMR studies clearly indicate that we have succeeded in controlling the magnetic dipolar interaction among Ni nanoparticles via independent tuning of d and r. The present study allows us to open a new way to realize tailor-made nanostructured magnetic materials.

Coffee break

Main Building, Small Hall (Mała aula)

15:20 - 15:50

Afternoon session - continuedAdsorption on metal surfaces

Main Building, Small Hall (Mała aula)

15:50 - 16:55

Properties of Complex Molecules at Metal Surfaces

15:50 - 16:35
invited oral

Federico Rosei[1]

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The adsorption of complex molecules on surfaces has recently been the subject of intensive investigation, both because of the molecules intrinsic properties, and for prospective applications (e.g. molecular electronics, nanosensors) [1,2]. In general, molecular ordering on surfaces is controlled by a delicate balance between intermolecular forces and molecule substrate interactions. Under suitable conditions, these interactions can be tuned by appropriate choice of substrate material and symmetry. Several studies have indicated that, upon molecular adsorption, surfaces do not behave as static templates, but may rearrange dramatically to accommodate different molecular species [3,4]. By means of high resolution, fast scanning scanning tunneling microscopy (STM) we recently gained unprecedented new insight into a number of fundamental processes such as molecular diffusion [5], bonding of adsorbates on surfaces and molecular self assembly [5,6]. In addition to the normal imaging mode, the STM tip can also be employed to manipulate single atoms and molecules in a bottom up fashion, collectively or one at a time. In this way, molecule induced surface restructuring processes can be revealed directly and nanostructures can be engineered with atomic precision to study surface quantum phenomena of fundamental interest. Here I will present a short review of recent work, in which several features of the complex interaction between large organic molecules and metal surfaces were revealed. The focus is on experiments performed using STM and other complementary surface sensitive techniques.

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3. F. Rosei et al., Science 296, 328 (2002).
4. R. Otero, F. Rosei et al., Nanoletters 4, 75 (2004).

5. M. Schunack, T. R. Linderoth, F. Rosei et al., Phys. Rev. Lett. 88, 156102 (2002).
6. R. Otero, Y. Naitoh, F. Rosei et al., Angew. Chem. Int. Ed. 43, 2092 (2004).

16:35 - 16:55
oral

Influence of hydrogen adsorption on magnetic properties of Fe films and multilayers

Krzysztof Fronc[2], Wojciech Szuszkiewicz[2], Frederic Ott[1], Bernard Hennion[1], Marta Aleszkiewicz[2], Marina Chernyshova[2], Leszek Kowalczyk[2], Roman Minikayev[2], Wojciech Paszkowicz[2]

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There is a great interest in the properties of thin magnetic layers and quantum structures containing classical ferromagnets deposited on semiconductor substrates. In particular, structural and magnetic properties of bcc Fe films on GaAs and Si substrates have been extensively investigated in the past. However, up to now, little is known about the influence of hydrogen on the magnetic properties of systems involving such films.
The goal of the present studies was to look for the modification of the magnetic properties of Fe layers deposited in the hydrogen atmosphere and for the relation between the change in the magnetic properties and in the changes in the layer structure. Both 1000 A thick Fe layers (with and without hydrogen) and Fe/Fe:H multilayers were deposited in UHV sputtering system and characterized by X-ray diffraction at the Institute of Physics of the Polish Academy of Sciences in Warsaw. Magnetic properties of the samples were investigated by means of the magneto-optical Kerr effect (in Warsaw) and the neutron scattering at Laboratoire Leon Brillouin in Saclay (France). The spin-polarized neutron reflectometry and small-angle elastic neutron scattering were applied in order to check the presence of hydrogen in the investigated layers and to estimate the upper limit of its concentration. Results of our studies were discussed and compared with a few experimental data which can be found in the literature.

19:00 - 21:00

Poster session 2

Thursday, September 9th

09:00 - 10:25

Morning sessionMagnetic properties

Main Building, Small Hall (Mała aula)

09:00 - 09:45
invited oral

Transport through magnetic grains in the Coulomb blockade regime

Jozef Barnas[1]

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Basic features of electronic transport in granular systems consisting of magnetic metallic grains distributed in a non-magnetic and non-conducting matrix will be reviewed and discussed. The discussion will be particularly focused on the mechanism of electron transport through the inter-grain barriers. When the grains are of a nanometer size, the effects due to discrete charging of the grains with single electrons become important and lead to observable effects at low temperatures. When additionally an external magnetic field is applied to the system, magnetic moments of the grains align along the field and this leads to a decrease in the resistance. Basic features of such a magnetoresistance effect will be discussed, including enhancement of the effect in the Coulomb blockade regime due to co-tunnelling processes.
An interesting limiting situation occurs when electric current flows through a single grain or through a one-dimensional array of a few grains, coupled to two ferromagnetic electrodes. Such a case may be considered as a ferromagnetic single-electron transistor, in which the discrete charging effects lead to Coulomb blockade phenomenon and Coulomb oscillations when an additional gate voltage is applied. Moreover, charging effects lead to magnetoresesistace oscillations with increasing bias voltage. An important role in electronic transport plays a nonequilibrium magnetic moment induced on the grain by flowing current (so-called spin accumulation). Spin-flip processes on the grains reduce the spin accumulation and therefore are important as well. Detailed theoretical description of such systems will be presented and the predictions will be compared with experimental results presented in recent literature.

Ferromagnetic resonance from nanoparticle agglomerates in nonmagnetic matrices

09:45 - 10:05
oral

Nikolaos Gouskos[1)], **Janusz Typek**[2)], **Urszula Narkiewicz**[3,4)], **Michał Maryniak**[2)], **K Aidinis**[1)]

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4) Technical University of Szczecin, Institute of Chemical and Environment Engineering, Pulaskiego 10, Szczecin 70-322, Poland

Samples of α-Fe and Fe3C nanoparticle agglomerates dispersed at different concentrations in various nonmagnetic matrices have been prepared. The agglomerates have been characterized by XRD and SEM spectroscopy. Magnetic resonance measurements of the samples have been carried out at different temperatures in the 4-300 K range. An intense and broad magnetic resonance absorption line has been recorded at different magnetice resonance fields for various matrices. With decreasing temperatures the resonance field has shifted and the intensity and the linewidth of that resonance line have displayed an unusual behavior. The resonance line could be fitted by a superposition of two Lorentzian-shape lines: one centered at lower magnetic field and the other placed at higher resonance magnetic field showing strongly decreased integrated intensity with decreasing temperatures. It is suggested that the magnetic resonance condition depends essentially on the internal magnetic field. This phenomenon is stronger for the Fe nanoparticle agglomerates than for Fe3C, for which the Neel temperature is higher. The magnetic exchange interaction between spins essentially influences the above processes.

Giant Magnetoresistance Dependence of Film Thickness, Annealing Temperature, Multilayer and Gas Rate in Layered Co/Cu/Co Nanotructures

10:05 - 10:25
oral

Samsudi B. Sakrani[1)], **Y.C Lau**[1)], **Yussof B. Wahab**[1)], **Rashdi Shah.B Ahmad**[1)]

1) Universiti Teknologi Malaysia, Institute of Ibnu Sina, Johor 81310, Malaysia

Experimental parameters effecting the giant magnetoresistance (GMR) of Co/Cu/Co nanostructures are investigated. The samples were fabricated using a sputtering method with varying Co layer thicknesses in vacuum, and were annealed at temperatures 200-450C for 150 minutes. GMR measurements were carried out in magnetic fields of 2500 Gauss. Apparently, a rapid 10% rise in GMR with Co layer thickness was observed between 2 - 6 nm, followed by a gradual drop along the thickness up to 20 nm. Annealing temperature has similar effect when its ascending mode attains a 24% GMR peak point at 400C beyond which the GMR starts to fall steadily to 20% at 450C. It is predicted that, the Co and Cu species become soluble to each other as they reach 400C and a solubility process is initiated between them with Co atoms gradually precipitated from the Cu matrix, thus forming the Co clusters. Due to ferromagnetic interaction occurring at temperature exceeding 400C an anti-parallel structure is established in the sample .

The GMR increases linearly with the number of bilayer, n except for (Co/Cu) x 8 due tendency of the curve to decrease between n = 5 - 8. However, it starts to rise again along the n > 8. This up-down variation is somewhat similar to periodicity, possibly due to the $[Co/Cu]_n$ acting as a parallel shunt resistance to the sandwich structure. For a 400C annealed sample plotted on similar axes the GMR shows an upward shift and much better improvement, preferably as high as 33%. The effect of argon gas rate injected into the deposition chamber was also studied. Initially, a small rise and fall in GMR was observed, resulting in a 11% peak between the Ar gas rates 8-15 sccm, with the curve sloping down gradually until the upper limit of 30 sccm. Such a variation may be attributed to the improvement of Co and Cu crystals formed during the 10 sccm Ar rate. The results are indicative of GMR dependency on selected experimental parameters.

Coffee break

10:30 - 11:00

Morning session - continued

11:00 - 12:30

Geometrical and electrical properties of ultrathin epitaxial metal nanostructures on flat and vicinal silicon surfaces.

11:00 - 11:30
invited oral

Herbert E. Pfnuer[1)], **T Block**[1)], **S Vagt**[1)], **V Zielasek**[1)], **I Vilfan**[2)]

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The understanding of the conductive properties of extremely small metallic structures is of high importance for the potential use in nanoelectronic devices and their interconnects. In this contribution we first show results of ultrathin epitaxially grown Pb films on Si(111). The magnetoconductive properties of ultrathin Pb films deposited on Si(111) are measured and compared with density-functional electronic band-structure calculations on two-dimensional, free-standing,(111) oriented Pb slabs. We show that the oscillations in sign of the Hall constant observed as a function of film thickness can be explained directly from the thickness dependent variations of the electronic bandstructure at the Fermi energy. Si(557) surfaces form regular arrays of triple steps between the terraces that are extended without defects over several hundred nm. Adsorption of several monolayers of Pb with subsequent annealing to temperatures above the melting point of bulk Pb leads to the selforganized decoration of the terraces by Pb nanowires with a typical width of 3 nm. Macroscopic conductivity measurements have revealed a remarkably anisotropic (up to a factor of 100) conductance parallel and perpendicular to the step direction, below 80 K, where a sharp phase transition towards strong anisotropy occurs. Finally, we present an alternative method to produce and study ultrathin epitaxial metallic and crystalline nanowires with dimensions down to 10 nm on an insulating support. We combine electron beam lithography in ultra-high vacuum with epitaxy of silver on silicon (001) and (111) surfaces using a SEM-STM system (JEOL) for confocal and simultaneous operation of both microscopes at variable sample temperatures in the range 80-900 K. First measurements of electrical conductance of single crystalline Ag and Pb nanowires using the TiSi contact pads and the STM tip as probes will be presented.

A study of surface and segregation energies of single crystalline Cu by means of XPS

11:30 - 11:50
oral

Nail R. Chamsoutdinov[1)], **Amarante J. Bottger**[1)], **Wim G. Sloof**[1)]

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Experimental values for segregation energies or surface energies are difficult to obtain. Surface (segregation) energies of metals can be related to peak shifts caused by the presence of a surface in an X-ray photoelectron spectroscopy (XPS) experiment. For industrially important 3-d metals this proved to be difficult because of the complicated background and large intrinsic peak widths. In this experimental study of single crystalline copper a new approach to XPS-profile fitting is applied, which allows discerning the contributions of surface and bulk to the spectra. Special emphasis was made on intrinsic XPS-background description. It was demonstrated that the intrinsic background is strongly affected by the surface, its type and quality. Proper account for these factors in fitting routines allowed us to separate the surface contribution to the total XPS-intensity and to report the first successful extraction of surface core-level shifts for copper (100) and (111) surfaces. The experimental results were compared to the surface energy estimations obtained by the semi-empirical Miedema macroscopic atom model. The experimental results were found in a good agreement with the trends predicted by this model.

Characterization of cleaved surfaces of metallic bronzes.

11:50 - 12:10
oral

Herve Guyot[1)], **Hafid Balaska**[1,4)], **Enesto Placidi**[3)], **Nunzio Motta**[2)]

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4) Universite de Skikda, BP 26, Skikda, Algeria

Several monophosphate tungsten bronzes are metallic ternary oxides with layered crystallographic structures and exhibit specific physical properties resulting from to the anisotropy of their structures. The $P_4W_8O_{32}$ bronze shows two phase transitions to charge density wave states, which are related to the quasi two-dimensionality of this metallic oxide. The low-dimensionality of this bronze has been evidenced by transport properties and by measurements of the Fermi surface and the band structure [1,2]. These measurements were performed on (001) surfaces cleaved in UHV. We have characterized these clean surfaces electron diffraction and STM imaging. The LEED patterns of (001) surfaces show at room temperature several Bragg spots reflecting a long range periodicity, that is in good agreement with the three dimensional crystallographic structure. The local investigation of (001) surfaces evidences different periodicities, which are interpreted as the presence of (001) and stepped (021) facets. The first orientation corresponds to the planes parallel to the layers, while the second orientation corresponds to the high density planes of the WO6 layers. These facets appear to be relaxed 1x1 surfaces.

[1] A. Mascaraque, L. Roca, J. Avila, S. Drouard, H. Guyot, and M. C. Asensio, PRB 66, 115104 (2002).
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Elastic Peak Electron Spectroscopy: metal surface analysis.

12:10 - 12:30
oral

Bernard Gruzza[1)]

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Elastic Peak ElectronSpectroscopy (EPES) is a recent technique sensitive to the surface of the substrates. It based on elastic reflected primary electrons with energy E_0 fixed or variable.
The important parameter is the percentage of elastically reflected electron. The aperture and the position of the analyser are playing an important role.
Quantitative interpretation can be done with the help of a Monte-Carlo simulation programme called MSEP.
The information depth is changing with the primary energy, with the M-M EPES (multi modes) method one can analyse the surface overlayers of the sample. The knowledge of the value of the inelastic mean free path of electrons is crucial for interpretation.
We will present results on different metallic substrates showing the influence of the atomic number Z of the atoms of the samples.
Between other examples of applications the interface studies are of the first importance, we will shows EPES appplied on the first stages of Au/Al_2O_3 formation.

Lunch break

12:30 - 14:00

Afternoon session

14:00 - 15:30

Main Building, Small Hall (Mała aula)

Ultra-low energy SIMS depth profile analysis of MOVPE grown InAlGaAs/AlGaAs/GaAs nanostructures

14:00 - 14:20
oral

Piotr Konarski[1)], **Michał Ćwil**[1,2)], **Marcin Zaremba**[2)], **Damian Radziewicz**[3)], **Beata Ściana**[3)], **Janusz Kozłowski**[3)]

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3) Wroclaw University of Technology, The Faculty of Microsystem Electronics and Photonic, Wrocław 50-372, Poland

Characterisation of layered nanostructures requires the use of sensitive and precise techniques in depth profile analysis. Recently sputtering with ultra-low energy (below 1 keV) ion beams is used in order to reduce ion beam mixing effects [1, 2]. Here we show the results of 880 eV argon ion beam sputtering applied in secondary ion mass spectrometry (SIMS) of metal organic vapour phase epitaxy (MOVPE) grown structures.
The analysed layered systems were different quantum wells (InAlGaAs and GaAs) and barriers (AlGaAs

and InAlGaAs). Typical obtained structure consisted of GaAs substrate, 150 ÷ 500 nm GaAs buffer, multi quantum well (MQW) region and 50 ÷ 70 nm GaAs cap layer. The MQW is a 3-layer period superlattice made of 9 nm thick $In_xAl_yGa_{1-x-y}As$ layer and 30 nm thick GaAs or $Al_zGa_{1-z}As$ layer. The structures were obtained by AP MOVPE technology using AIX200 R&D Aixtron reactor. The growth temperature (T_g) was in the range of 650 ÷ 690C, the H_2 flow rate through TMIn bubbler ($V_{H2/TMIn}$) was varied from 35 to 75 sccm/min. The other growth parameters were the same as for the InGaAs/GaAs MQW structures described in [3, 4].
SIMS analyses were performed on SAJW-05 analyser equipped with 06-350E Physical Electronics ion gun and QMA-410 Balzers 16 mm quadrupole spectrometer. The results show high depth profile resolution of MQW structures with measured 12 nm FWHM of $In_xAl_yGa_{1-x-y}As$ layers. Ion erosion of reference samples with thick (500 nm) ternary alloy layers allowed for careful calibration of sputtering rates in the layers of the analysed MQW structures and also for quantitative description of stoicheiometry coefficients in these layers.

[1] M.G. Dowsett, et al.; Appl.Surf.Sci. 203-204 (2003) 273.
[2] P. Konarski, A. Mierzejewska; Appl.Surf.Sci. 203-204 (2003) 354.
[3] M. Tłaczała, et al. Heterostructure Epitaxy and Devices-HEAD97, Kluwer Academic Publishers, (1998) 119.
[4] D. Radziewicz, et al.; Mol.Phys.Report, 21 (1998) 113.

14:20 - 14:40
oral

Nucleation and growth of gold nanoparticle

xiaoda xu[1], **Mike Cortie**[1], **Mike Stevens**
1) University of Technology (UTS), Broadway, Sydney 2007, Australia

The technology of nanoscale gold films deposited onto glass by vacuum sputtering is well known in solar glazing. However, aqueous deposition of gold for this purpose appears to be rarely, if ever, commercially exploited. Nevertheless, the uniform film texture and pleasant neutral color of coatings of gold nanoparticles suggest their use in this application. The results of this research showed the optical transmission or reflection spectra obtained from such coatings, was directly related to the interplay between the rates of nucleation and growth of the particles, the manner in which they aggregated and the nature of the prior treatment of the glass surface. Samples with a similar surface coverage of gold nanoparticles may exhibit quite different transmission spectra, depending on the morphology of the coating. Different pretreatment schemes for the glass also ostensibly influenced the results because the glass surface composition and surface tension changed accordingly.
The glass was pretreated with 1:1 sulfuric acid (H2SO4), 98% H2SO4 and buffered hydrofluoric acid (HF). For the glass pretreated with buffered HF, there was higher sodium content and lower contact angle compared with glass surface treated with H2SO4. the following gold deposition also indicated different transmitting spectrum of gold nano films on these pretreated glass. The textile of gold nano coatings on glass pretreated with HF was more uniform than that pretreated with sulfuric acid. Further study also found the glass pretreated with sulfuric acid tended to form the gold nano coating with dual peaks at around 540 nm and 700 nm, while the surface pretreated with buffered HF tended to form the gold nano coatings with a single broad peak at around the 700nm. These trends were modeled using classic heterogeneous nucleation and growth theory.

14:40 - 15:00
oral

Characterization of Nanocrystalline Al2O3 Aerogels Containing Fe and Co

Maria F. Casula[1], **Anna Corrias**, **Andrea Falqui**, **Giorgio Paschina**
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The sol-gel technique has been succesfully adopted for the preparation of composites in that it allows a homogeneous distribution of the dispersed phase thanks to the mixing of the precursors at a molecular level. Moreover, composites with tailored morphology and texture can be obtained by using the appropriate gel drying procedure.
In this work, we used the sol-gel method followed by high temperature supercritical drying to prepare Al_2O_3 aerogels containing Fe and Co. Pure Al_2O_3 aerogels were also prepared as a reference. The crystal structure of the aerogel samples was characterized by X-Ray powder diffraction (XRD), selected area electron diffraction and X-Rays absorption spectroscopy (XAFS). The texture was studied by N_2 physisorption and TEM. Thermogravimetric analysis (TGA and DTA) and calcination treatments were performed in order to study the evolution of the porous texture, the particle size and the crystal phase as a function of the heat treatment.
The aerogel sample after the supercritical drying are mesoporous and have surface areas around 500 $m^2 \bullet g^-1$. Bright field TEM observations show the presence of needle-like particles. Dark field TEM observations indicate that the needles are not single crystals, but are made out of spherical nanocrystals arranged into chains.

After calcination, the aerogels retain a mesoporous texture and exhibit a significant surface area even after heat treatment at 900C. Upon calcination, the formation of a cubic nanocrystalline phase which has a structure similar to γ -Al_2O_3 with substitutional Fe and interstitial Co is observed. Structural details are obtained by XAFS and Mossbauer spectroscopy.
On the other hand, thermal treatments in reducing atmosphere give rise to phase separation resulting in FeCo alloy-Al_2O_3 [U+F020] nanocomposite formation.

CHARACTERIZATION OF NANOSTRUCTURED METAL PARTICLES BY POSITRON ANNIHILATION SPECTROSCOPY

15:00 - 15:20
oral

Adkhamjon A. Paiziev[2)], **Asad M. Karimov**[1)]

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As is well known, small metal particles (SMP) are the main morphological element of different nanomaterials. The present work is devoted to research of electronic and defective structure of metal nanomaterials by methods of an electron - positron annihilation (EPA).
1. Applied metallical catalysts with the size of active metal (Pt, Pd, Ir, Ni) about 1-10nm, deposited on inner surface of high-porous oxids (Al_2O_3) with specific surface 500m^2/g.
2. Powders of a tungsten and molybdenum with a characteristic grain size 1-100 nm, obtained both ordinary hydrometallurgical way (d 100nm), and method of plasma sputtering(d 10nm).
Electronic spectrum and energy levels of SMP are computed . The existence of quantum size effects in spectra of an electron - positron annihilation on SMP is showed. The conditions of quantum size effects appearing in spectra of EPA are determined. As a result the following outcomes are obtained:
1. The direct correlation of EPA parameters with degree of dispersion of active metal Ir in catalyst is detected. It is showed, that on an initial stage the active metal on a surface of the carrier has structure of a charged metlical cluster.
2. In ultra dispersed metal powders W and Mo (1-10 nm) the volumetric and surface positron and electronic bound states are investigated. The electronic wave functions of a positron and adding electron in similar SMP structures are determined from experimental spectra of electron-positron annihilation . The existence of size quantum effects in electron-positron annihilation spectra of ultra dispersed metal powders is showed. The conditions of appearance of quantum size effects and the wave functions and energy levels of quantum levels in low dimensional structures are determined.

[ABSTRACT TRUNCATED TO 2000 LETTERS]

Funding Workshop

Funding and Investment Opportunities in Poland and Central Europe - a European and International Perspective

Organisers

- Dr Mark Morrison, (Nanoforum coordinator),
- Prof. Witold Lojkowski, (E-MRS Fall organizer),
- Malgosia Chmielecka, (secretary)

Acknowledgements

"**Funding and Investment Opportunities in Poland and Central Europe - a European and International Perspective**" -

XIVth Workshop of the Network of Centres of Excellence "**Nanostructured Materials**"

is supported by:

- The European Commission:
  - Contract: No. ICA1-CT-2002-60028
  - Contract: No. G1MA-CT-2002-04055
- High Pressure Research Center "UNIPRESS", Polish Academy of Sciences: SPUB-MSN, SPUB-PRENABIO and other.

Sunday, September 5th

14:00 - 17:00

Sunday session

Main Building, Small Hall (Mała aula)

14:00 - 14:30
invited oral

Nanoforum - European nanotechnology gateway

Del E. Stark[1)]

1) Institute of Nanotechnology (IoN), 6 The Alpha Centre, Stirling FK9 4NF, United Kingdom

The aim of the nanotechnology thematic network "Nanoforum" is to promote and raise the standard of nanotechnology activities throughout Europe, to strengthen links across disciplines and countries, and to promote Europe as a home for world-class research. Nanoforum is fully funded by the European Commission and undertakes a wide variety of activities including conferences; workshops; seminars on funding and investment opportunities; seminars on career options in nanotechnologies; summer schools to provide further training; reports on nanotechnology topics of interest - accessible to the general public; and, central to all these activities - the maintenance of a Nanoforum website (www.nanoforum.org) to disseminate information.

14:30 - 15:00
invited oral

Bringing Nanotechnology to Market

Michael P. Mason[1)]

1) The Institute of Nanotechnology (IoN), 6 The Alpha Centre, Stirling FK9 4NF, United Kingdom

It is recognized that spin-outs and start-ups in micro and nanotechnology will be important in the future economy of the EU. These early companies tend to be fragile and often lack relative support and the opportunity to network available to 'large' companies, so important in the early stages of development and that can mean the differences between success and failure.
Start-ups and spin-outs are the prime source of commercial applications of nanotechnology but often work in isolation from each other and from the business community. They may also become remote from sources of technology to fill knowledge gaps, and find quality advice difficult to find or too expensive to access. As a consequence, they often have to reinvent the wheel, and struggle to solve what may be simple problems to experienced entrepreneurs, which results in slow growth, the likelihood of making long-term mistakes, and even ultimate failure.
The end-product of such companies is often enabling technology that can be introduced into existing products, for example, paints. The marketing can be difficult and requires start-ups to look at their customer's customers, and beyond.
Even if a route to market can be found the issue of where to start a negotiation can be hard. Time to-market can be a critical issue.
How can you identify mentors and professional advisors that understand the technology and its unique issues and opportunities.
This paper will attempt to raise all the questions and suggest how they may be addressed.

15:00 - 15:30
invited oral

Nanotechnology in the EU Framework Programme

Angela Hullmann[1)]

1) European Commission, Brussels, Belgium

Nanotechnology is a growing field, where the resources needed are significant in terms of human creativity, scientific infrastructures and available funds, but where private investment is still limited. To benefit from the opportunities offered by nanotechnology, both scientific and technical challenges must be met: to increase our basic understanding of the nano-world; to create new materials, devices and processes; to integrate nano components in micro and macro applications; to establish new tools and techniques for industrial manufacture. There are also many challenges at a structural level: to maximise the efficiency of publicly funded pre-competitive research; to educate the next generation of students, researchers and technicians; to enhance societal awareness and perception; to develop metrology and standardisation for increased precision and accuracy; to secure an overall safe and responsible development of nanotechnology. These issues are addressed by the European Commission with a specific Communication on nanotechnology.

The 6th Framework Programme will contribute to the creation of the European Research Area. It will have both a strategic and structuring character. Research projects with a strategic, high added value for Europe will be supported. A set of initiatives will be launched for structuring European research and reinforcing its foundations. Efforts will be put to renewing the enthusiasm in Europe for science and technology, and to achieving enhanced critical mass through an enlarged international co-operation. Researchers (in academia, industry, centres, . . .) will be called to play a more prominent role in solving today's challenges in society for improving the quality of life of European citizens and boosting Europe's competitiveness within a sustainable growth.

A wide range of actions is supported within the 6th Framework Programme. First of all integrated projects and network of excellence, but also other type of
[ABSTRACT TRUNCATED TO 2000 LETTERS]

Gate2Growth, from Innovation to Business. The G2G financial services and relaed pan-European networks.

15:30 - 16:00
invited oral

Niko Van Goubergen[1)]

1) Brabo Ventures, St. Jacobsmarkt, Antwerp 2000, Belgium

A hands-on service for entrepreneurs
The Gate2Growth Business Matching team is a dedicated group of experts with excellent long term investor relations and an outstanding track record in business plan development. The team is working on a daily basis with companies and evaluates about 100 business plans per month. The Business Matching team invests quality time and represents a real 'gate to finance' for innovative start-ups looking for venture capital. The team effort in the preparation of start-ups entertains regular, pro-active contact with investors across Europe, in various industry sectors and with different focus in type and amount of investment. Their in-depth knowledge of the investment process ensures an increasedquality of investor presentations. Through the interactive network of Gate2Growth, the Business Matching team has direct links with the main European players in innovation, entrepreneurship and technology transfer.

For innovative entrepreneurs, the Business Matching team provides hands-on tools and services for business plan development and pro-active support in finding the right investor to raise money for their innovative venture. Entrepreneurs can use both online tools on the Gate2Growth website and offline support directly provided by theBusiness Matching team.

A win-win situation for entrepreneurs and investors

Win-win for entrepreneurs

Through the direct contact with the Business Matching team qualified entrepreneurs experience a pragmatic approach that puts their business plan on top of the pile of investors in Europe. This includes:
- Help in preparing information for pitching to investors
- Identification of relevant investors across Europe
- Access to a personal network of investment managers in top Venture Capital companies
- Saving management time.

Win-win for investors
Only when quality business plans have been prepared, the companies are presented to investors. Business Plan p
[ABSTRACT TRUNCATED TO 2000 LETTERS]

Financial opportunities for industry-acadamia cooperation in FP6 and structural funds - activities of Regional Contact Point for FP6

16:00 - 16:30
invited oral

Katarzyna Lazarz[1)]

1) Technical University of Szczecin, International Programmes Office (TUS - IPO), al. Piastow 17, Szczecin 71-022, Poland

In the last few years the expenditures for Research & Development covered from the national budget of the Republic of Poland have gradually decreased. In 2003 the financial means allocated to this purpose constituted 0,34 % of GDP whereas an average of GDP 1,3 % is spent for the same thing in other EU Member States.
In the face of the budget stringency, it is optimistically implied that non-budgetary and private recourses are to become the momentum for the development of research and evolutionary work supporting the progress of knowledge-based economy.
Stimulating cooperation between research and industry as well as implementation of achieved research

results, become a vital need if we want to bring about a desired and real economic effect.
According to the Economic Strategy of the Polish Government, a real chance for Poland are the participation in projects executed within the 6th Framework Programme and an effective use of structural funds. Therefore, the main aim of the ensuing presentation is to introduce Polish researchers and entrepreneurs, who seriously consider strong arise in the research world, to practical aspects and opportunities offered by Framework Programmes and its priorities, budget, instruments, application procedures. Functioning of the Network of Contact Points for the 6th Framework Programme will be demonstrated taking the RCP at the Technical University of Szczecin as an exemplum.
Moreover, financing possibilities for research activities coming from structural funds will be demonstrated during the lecture with regard to research projects producing commercially implemented results, specialized laboratories which have to be provided with top-class equipment, didactic objects destined for modernization, companies in need of technological trainings and many others.

Material Research opportunities within the COST Actions

invited oral

Piotr Swiatek[1)]

1) European Science Foundation, COST Office (COST), 149 avenue Louise, Brussels 1050, Belgium

Founded in 1971, COST is an intergovernmental framework for European Co-operation in the field of Scientific and Technical Research, allowing the co-ordination of nationally funded research on a European level. COST Actions cover basic and pre-competitive research as well as activities of public utility.
The goal of COST is to ensure that Europe holds a strong position in the field of scientific and technical research for peaceful purposes, by increasing European co-operation and interaction in this field.

At the moment COST runs over 40 material research related actions and is still open for new ides. COST supports bottom-up approach and therefore there are no calls and no defined priorities in COST Actions.

COST also established the Strategic Group on Nanoscience and Nanotechnology (NanoTech). The NanoTech builds on existing experience, activities and structures within COST, e.g. the COST Nanoscience and Nanotechnology Advisory Group (NanoSTAG) and outside COST. The NanoTech will provide a strategy of COST interests in this multidisciplinary field of nanoscience and nanotechnology within the European Research Area (ERA).

COST has clearly shown its strength in non-competitive research, in pre-normative co-operation and in solving environmental and cross-border problems and problems of public utility. It has been successfully used to maximise European synergy and added value in research co-operation and it is a useful tool to further European integration, in particular concerning Central and Eastern European countries.

Monday, September 6th

Monday sessionWitold Lojkowski

13:30 - 15:30

Main Building, Small Hall (Mała aula)

The EPO helps in obtaining patent protection in nanotechnology

14:00 - 14:30
invited oral

Leonard Kusztelan[1)]

1) European Patent Office (EPO), Munich D-80298, Germany

Some points to be adressed:
What is the EPO?
What is a patent?
How to obtain a patent ?
What do we deal with in our department (Semiconductor physics, nanotechnology, microstructures, photolithography, etc)
What specific help is given to inventors?

The topic is very large. The papers submitted will cover all aspects, but the oral presentation will be restricted to the neeeds and zhe wishes of the audience. An intensive question/answer/discussion session will take place.

I am an Examiner at the EPO-Munich and in charge of the directorate Semiconductor/Physics.

EUROPRACTICE PROGRAM: ACCESS TO MICROELECTRONICS TECHNOLOGIES FOR INDUSTRIAL COMPETITIVENESS IN EUROPE AND START UP SUPPORT

14:30 - 15:00
invited oral

Geraldine Andrieux[1)]

1) Yole Développement (YOLE), 45 rue Sainte Geneviève, Lyon 69006, France

"ACCESS TO MICROELECTRONICS TECHNOLOGIES FOR INDUSTRIAL COMPETITIVENESS IN EUROPE - START UP SUPPORT"

Jean-Christophe ELOY
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EUROPRACTICE is a European Union initiative aimed at stimulating wider exploitation of state-of-the-art microtechnologies by European industry.
Its ultimate goal is enhanced European industrial in the global market place.

EUROPRACTICE services offer users cost effective and flexible means of accessing Microsystems technology, Training, Integrated Circuits, IC & Microsystems Software.

EUROPRACTICE is aimed primarily at SMEs and large companies, but universities and research institutes are also encouraged to take advantage of the services it makes available.

EUROPRACTICE services in Microsystems field help them take their ideas from the concepts to manufacturable, tested and packaged products through access to expertise, design, prototyping and manufacturing facilities.

EUROPRACTICE is also supporting microsystems start-ups by running a competition to provide assistance for 10 projects to be presented to venture investors. All companies working on Microsystems are eligible, including components manufacturers, those offering specific process steps (front-end, back-end, packaging), dedicated microsystems equipment - or innovative MST based product manufacturers and service suppliers (CAD tools, design houses, packaging, integration, test, etc.). Companies selected are eligible for a number of days of free assistance with:

- Writing a business plan, or review of an existing plan
- Validation of the business model
- Analysis of the IPR position
- Market segmentation for the selected technologies

In order to prepare the projects presentation to VC's.

For further information, www.europractice.com.

The next industrial revolution - or just a new bubble ? The Financing of Nanotech start-ups.

invited oral

Kim Ludvigsen[1)]

1) Technology Finance, Kuttelgasse 15, Zurich CH-8001, Switzerland

Kim Ludvigsen has extensive experience in the areas of Corporate Finance and Venture Capital and has worked with young nano- and micro-technology companies for a number of years.

He will speak about how high-tech start-ups obtain financing, how they should present themselves, where they can go, what investors are looking for what mistakes should be avoided.

Joint Workshop G and I

Joint workshop of Symposia G and I of EMRS Fall Meeting, the Network "Nanostructred materials" and Center of Excellence Prenabio

Organisers

- Witold Lojkowski, High Pressure Research Center of the Polish Academy of Science, Warsaw
- Urszula NARKIEWICZ, Institute of Chemical and Environment Engineering, Centre of Knowledge Based Nanomaterials and Technologies, Technical University of Szczecin
- Radu Robert Piticescu, Institute for Non-ferrous and Rare Metals, Bucharest, Romania

Acknowledgements

Workshop is supported by:

- The European Commission:
  - Contract: No. ICA1-CT-2002-60028
  - Contract: No. G1MA-CT-2002-04055
- High Pressure Research Center "UNIPRESS", Polish Academy of Sciences: SPUB-MSN, SPUB-PRENABIO and other.

Monday, September 6th

Afternoon sessionHerbert E. Pfnuer - Keynote lectures. Common session of Symposia G and I

15:50 - 17:20

Main Building, Small Hall (Mała aula)

Nanoscale Surface Physics with Local Probes: Electronic Bandstructure of a Two-Dimensional Self-Assembled Adatom Superlattice.

15:50 - 16:35
invited oral

Wolf- D. Schneider[1)]

1) Ecole Polytechnique Federale de Lausanne (EPFL), Lausanne 1015, Switzerland

The quest of a reliable method for fabricating ordered atomic-scale structures is a prequisite for future atomic-scale technology. The interest in such nanostructured materials, consisting of building blocks of a small number of atoms, arises from their promising new optic, catalytic, magnetic and electronic poperties, which are fundamentally different from their macroscopic bulk counterparts: small is different. We succeeded in fabricating a sparse, self-assembled two-dimensional array of individual Ce adatoms (the "ultimate" building block) on a metal surface [1] by exploiting long-range interactions between adatoms mediated by surface state electrons. This has been achieved by evaporating in ultrahigh vacuum Ce atoms on a Ag(111) surface at a temperature below 10 K. Scanning Tunneling Microscopy (STM) images acquired at 3.9 K display a hexagonal superlattice, where the nearest-neighbor distance of 3.2 nm is near half the Fermi wavelength of the Ag(111) surface state electrons and corresponds roughly to the distance spanned by 11 Ag atoms in the substrate. The local density of states (LDOS) of this two-dimensional superlattice has been determined by Scanning Tunneling Spectroscopy (STS) and by tight-binding (TB) theoretical modeling. The scattering of Ag(111) surface state electrons by the Ce adatom superlattice leads to gap openings and to LDOS singularities at high-symmetry points of the surface mini-Brillouin zone which agree quantitatively with the characteristic features observed in differential conductance (dI/dV) spectra. The energy gain associated with the gap formation is maximal for superlattices with adatom distances in the range 2.3 - 3.5 nm, in excellent agreement with experiments. Finally, Ce is a magnetic atom, and such a superlattice of magnetic adatoms might be useful for the development of future atomic-scale magnetic devices.

[1]F. Silly, M. Pivetta, M. Ternes, F. Patthey, J.P. Pelz, and W.-D. Schneider, Phys.Rev.Lett. 92,016101(2004).

CATALYTIC REACTIONS ON NANOSIZED SURFACES: BRIDGING OF THE MATERIALS AND PRESSURE GAP

16:35 - 17:20
invited oral

Yuri Suchorski[1)]

1) Otto-von-Guericke-Universitaet Magdeburg, Chemisches Institut, Universitaetsplatz 2, Magdeburg D-39106, Germany

Nanosized metal particles representing the catalytically active phase of supported catalysts are hardly accessible for surface science methods. It is, therefore, beneficial to create well defined model systems which can be studied by surface sensitive techniques. The structurally heterogeneous surface of a field emitter tip can be considered as such a model system since it represents well the complex structure of a metal particle of supported catalyst. The tip surface, however, can be prepared and characterized with atomic resolution by Field Ion Microscopy (FIM). Using this and other field emission techniques (e.g. FEM, Li-FDM) one can observe in situ catalytic reactions on defined nanosized facets with a resolution close to 2 nm. Digitizing of the video-images allows processing of the reaction dynamics within the different virtual probe-holes arbitrarily located on the surface. The role of the atomic steps, size effects, diffusive coupling and microscopic fluctuations can be studied using ${O_2}^+$ and Li^+ ions as well as electrons as probing species. Monitoring the Li^+ ions which are emitted from the probed surface area enables studying of the alkali-promoted reactions by utilising the ions of the promoter itself. In addition, the microscopic surface mobility of the promoter during the reaction can be examined in situ using the surface density fluctuation approach.

The probe-hole technique realised in the FIM mode allows also the mass-to-charge resolved potential analyses of the ions emitted from the few surface atomic sites. This renders possible the derivation of the binding energy of adsorbed molecules (e.g. CO and O_2 in CO oxidation reaction) in the particular surface atomic environment. The applied electrostatic fields which are much higher in the FIM (10 to 20 V/nm) than in the FEM or Li-FDM modes cause the local pressure enhancement near to the specimen surface permitting in this way the partial bridging of the pressure gap.

Tuesday, September 7th

Morning sessionCommon session of G and I

Main Building, Small Hall (Mała aula)

11:00 - 12:30

Nanophase Production Using Solar Energy

11:00 - 11:30
invited oral

Claude J. MONTY[1)]

1) Procédés,Matériaux et Energie Solaire (PROMES), Avenue Professeur Trombe, FONT ROMEU 66120, France, Metropolitan

Nanophases of various compositions have been produced by two different methods, using solar furnaces with high concentration energy flux, in Odeillo - Font Romeu (France): a - vaporisation - condensation (PVD process) in solar reactors; b - melting and fast cooling followed by ballmilling.
Among the series of materials which have been prepared by this way, the presentation will be focused on the preparation of Zr1-xYxO2, Ce1-xGdxO2, [U+F064]-(Bi1-xYx)2O3, which are superionic conductors; Zn1-xInxO, Zn1-xSbxO, Zn1-xAlxO, expected to be optically transparent and exhibiting high densities of electronic carriers, Zn1-xCoxO, which is ferromagnetic as a nanopowder prepared in ad hoc conditions, Zn1-xBixO-(Bi1-yZny)2O3, for its electrical properties. The obtained nanopowders have been characterized by X-Ray Diffraction and Electron Microscopy. They can be used to prepare massive nanomaterials, thin or thick nanostructured films or as obtained, depending on their properties and on the aimed applications: solid electrolyte for SOFC or sensors, transparent electrodes for optoelectronics or photovoltaic cells, luminescent screens, magnetic devices or varistors.
An overview will be presented on the preparation by similar methods of metallic nanoparticles of Zn or Al, as well as the preparation of fullerens, carbon nanotubes and SiOx nanopowders.
Parts of this work results from the collaboration with several people; among them: F. Sibieude, R. R. Piticescu, Roxana Piticescu, C. Georgescu, A. Motoc, Tounsia Ait-Ahcene, Nora Boulares, K. Guergouri, N. Tabet, Amel Cheikh, H. Boussetta, C. Petot, Georgette Petot-Ervas, G. Baldinozzi, C. Roucau, Nathalie Brun, A. Thorel, B. Martinez, P. Sandiumenge, Ll. Balcells, J. Fontcuberta

Plasmon assisted growth of disk shaped silver nanoparticles and individual optical properties.

11:30 - 12:00
invited oral

Mathieu Maillard[1)], **Pinray Huang**[1)], **Louis Brus**[1)]

1) Columbia University, Department of Chemistry, 3000 Broadway, New York 10027, United States

Disk-shaped silver nanoparticles with tunable aspect ratio have been synthesized by photoreduction of silver ions by citrate. This growth mechanism is driven by the light-induced polarization. Hence, shape and aspect ratio of these particles are controlled by the irradiation wavelength due to the shape dependence of the plasmon resonance.
Single particle spectroscopy has also been used to study the individual scattering properties of such nanoparticles in air and in water.

Hydrothermal synthesis of nanomaterials: bringing materials closer to life

12:00 - 12:30
invited oral

Robert R. Piticescu[1)], **Roxana M. Piticescu**[1)]

1) Institute for Non-ferrous and Rare Metals, 102 Biruintei Blvd., Pantelimon 73957, Romania

Hydrothermal synthesis is a soft chemical method with versatility in producing a large class of nanostructured materials in the form of powders and thin films. The main advantages come from the low crystallization temperature done in one-step process, avoiding thermal treatments usually required in other processes. In situ functionalisation became thus possible. The microstructure of bulk and thin films obtained using this approach may open new applications to materials for biosensors, implants or substrates for growing biological cells.

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