ADDENDUM - Symposium A

Monday, September 6th

Structural stability of In2O3 films deposited by spray pyrolysis

17:30 - 17:45
oral

Ghenadii Korotcenkov[1)], **Vladimir Brinzari, Mihail Ivanov, Albert Cornet, Joan Morante, Joan Morante, Albert Cirera**

1) Technical University of Moldova (TUM), Bld. Stefan cel Mare, 168, Chisinau 2004, Moldova

STRUCTURAL STABILITY OF In2O3 FILMS DEPOSITED BY SPRAY PYROLYSIS, G.Korotcenkov1, V.Brinzari1, M.Ivanov1, A.Cornet2, A.Cirera2, J.Morante2, 1Technical University of Moldova, Chisinau, Moldova, 2University of Barcelona, Barcelona, Spain
The results of analysis of In2O3 film properties stability during thermal annealing in the temperature range from 500oC to 1100oC are presented in this report. In2O3 films used for gas sensor applications were deposited by spray pyrolysis from InCl3-water solution. The change of parameters such as film morphology; grain size; texture; intensity of catodoluminescence, and Raman scattering were controlled. For structural analysis we used XRD, SEM, and AFM techniques.
It was determined that the change of In2O3 film structure during thermal treatment in oxygen containing atmosphere goes through the following 4 standard stages of structure transformation of polycrystalline materials: the stage of structural stability of the film (25-500oC); the stage of coalescence of grains forming agglomerates (500-700oC); the stage of local structural reconstruction (700-1000oC); and the stage of global (comprehensive) structural reconstruction (>1000oC). The influence of grain size (10-60 nm), film thickness (20- 400 nm), and deposition parameters (Tpyr= 390-520oC) on structural stability of In2O3 films is discussed as well. Besides we established the following regularities: thin films have better structure stability; grain coalescence is accompanied by recrystallization; grain growth during thermal annealing at T(an)> 700 oC does not obey the law t{1/2}; high temperature annealing at T(an)> 1000 oC gives possibility to form In2O3 crystallites with flat surface planes, sufficient for conducting experiments connected with STM method using.

Porous silicon prepared by high-energy ball-milling and pressing

17:50 - 18:05
oral

Jaroslaw Jakubowicz

In the past 50 years there has been great effort to develop porous structures based on silicon. Commonly use technique preparation of porous silicon base on electrochemical etching. The thickness of the porous layer is usually in the micrometer range and the porosity of such prepared layer is in the range of 20-80%. Porous silicon is a material composed from wires and open spaces. In the nanometer size range such structure can be prepared as a quantum wires and quantum dots. Recent investigations shows that ultrafine silicon particles shows luminescence comparable to those reported for porous silicon films. Hence the ball milling can be accurate to achieve highly dispersed structures with properties comparable to electrochemically etched wafer.
The formation of porous silicon by high-energy ball-milling and sintering was studied. The coarsely crushed silicon wafer was ball milled in a time up to 72h. After that, the average crystallite size is close to 15nm. Between 24 and 72h there was not significant change in crystallite size. The fine particles were then isostatically pressed at a pressure of 300 and 400 MPa. The green compacts are porous and after sintering at 1173K/60min the samples have still porous nature. In comparison etching of silicon wafer in diluted NH_4F was done, which results in regular porous layer. The advantage of powder metallurgy is a preparation of the porous structure in whole volume of the sample in spite of etching.

TRANSFORMATION OF SILICON WAFER SURFACE UNDER LOW-ENERGY HYDROGEN ION-BEAM TREATMENT

18:10 - 18:25
oral

Alexander K. Fedotov[1)], **Svetlana P. Kobeleva**[2)], **Sergyei I. Tyutyunnikov**[3)], **Serguei V. Chigir**[1)], **Olga V. Zinchuk**[1)], **Alexander V. Mazanik**[1)], **Nikolai A. Drozdov**[1)], **Yuri S. Kovalev**[3)], **V A. Yakovlev**[4)]

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The samples of p-type (100) Cz-Si cut from wafers covered with 1 to 2 nm thick native oxide were subjected to the treatment in low-energy DC hydrogen plasma at room temperature with ions energy in the range of 100 - 800 eV.
The experiments have shown that hydrogen ion-beam treatment leads to a significant changes in native oxide state and properties of under-surface region of the samples studied.
In particular, the mean lifetime, diffusion length [U+F020] of minority charge carriers and surface conductance decreased by a factor equal to 1.5-2 even after 5 min treatment, whereas the further increase of introduced hydrogen dose didn't result to significant variation of them. Moreover, all hydrogenated wafers displayed the appearance of photo-EMF recorded without p-n junction or Schottky barrier formation that testifies energy band bending taking place in the under-surface layer of hydrogenated samples.
AFM measurements have shown that hydrogenation always transforms the nano-smooth wafers into nanostructured patterns after first 5 min of hydrogenation. The further increase of exposure time up to 40 min resulted only to the surface evening-out and decrease of AFM-roughness again. XPS and IR measurements have exhibited that nanostructuring after 5 min hydrogenation resulted in reduction of native SiO2 whereas the following flattening of the surface after 40 min exposure was accompanied by the intensive growth of oxide thickness (up to 7-8 nm) stimulated by atomized hydrogen. The measured Raman spectra have exhibited the increase (proportionate to exposure time) of long-wave wing for the basic silicon line (520 1/) after hydrogenation that can be interpreted as formation of amorphous-like layer between oxide and monocrystalline wafer.

Tuesday, September 7th

Lithium Niobate Nano- and Microtubes

14:30 - 14:45
oral

Lili Zhao[2)], **M. Yosef**[1)], **S. Schlecht**[1)], **E. Pippel**[2)], **M. Steinhart**[2)], **U. Gösele**

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We report on the preparation of lithium niobate (LiNbO3) nano- and microtubes, and on the tailoring of their wall morphology. Tubular nano- and microstructures have attracted increasing interest since they may act as a pipeline for electromagnetic waves and matter. Their intrinsically anisotropic nature allows their integration into complex architectures. Lithium niobate (LiNbO3) is considered as one of the most interesting inorganic oxides because of its outstanding features, for instance, its unique, photorefractive, piezo-electric, electro-optical and non-linear properties, as well as its pronounced mechanical and chemical stability and wide transparency range. Therefore, it is a challenging task to combine the functionality of LiNbO3 with the advantages of a tubular geometry. It is, however, particularly important to control the generation of the internal morphology of the tube walls because not only mechanical, but also electronic and optical properties of crystalline materials depend largely on the crystallite size. Wetting ordered porous templates with precursor solutions with subsequent thermolysis yields polycrystalline LiNbO3 tubes with uniform length and diameter. Their diameters are determined by the ones of the template pores and range from few tens of nm up to one micron, whereas their length amounts up to 100 microns. LiNbO3 tubes may be building blocks for a multitude of micro- and nanoelectronic devices, for instance, ferroelectric nonvolatile memories and microelectromechanical systems (MEMS).

Studies Toward Practical Synthesis of Disubstituted 3,6-Carbazoles - Electroconductive Nanomaterials for New Type of Sensors and Optoelectronic Devices

17:30 - 17:45
oral

Joanna Cabaj[1)], **Krzysztof Idzik**[1)], **Jadwiga, Maria Sołoducho**[1)], **Antoni Chyla**[1)], **Jacek Doskocz**[1)]

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A compounds containing carbazole units, which have substituted alkyl chains and because of the amphipilic character, were found to form stable monolayers (Langmuir-Blodgett layers) [1]. Because of the rigidity, planar rings and third-order nonlinear optical properties they can also form a novel -conjugated, processible, transparent and thermally stable materials. Most frequently a carbazoles molecules are placed in side chains of polymer (copolymer) [2]. Earlier experiences with synthesis similar structures [3] are allowed to suppose that a polymer which contain in main chain carbazoles unit between two pyrroles or thiophens, combains in a one chain electroconductive and electroluminescent properties conjugated polymers and photoactive chromophore characteristics [2] and could be applied in a large number of sensors and photonic devices.
3,6-bis(1,4-dioxane[2,3-c]thiophene)-N-alkylcarbazole and 3,6-bis(thiophene)-N-alkylcarbazole have been synthesized via a Stillle-type coupling reactions [4] in which dibromoalkylcarbazole was reacted with 2-(trimethylthin)thiophene or 2-metalated (1,4-dioxane[2,3-c])thiophene to give 3,6-bis(thiophene)-N-alkylcarbazole or 3,6-bis(1,4-dioxane[2,3-c]thiophene)-N-alkylcarbazole, using Pd(PPh3)2Cl2 or Pd(PPh3)4 as catalyst.
A series of bis(thiophenes)- and bis(dioxanethiophenes) based on carbazole rings were prepared for conductive material and characterized by 1H NMR and 13C NMR.
Further work is in progress in order to understand the role of disubstituted carbazole in these reactions and also in polymer results.

1. Y. Liu., M. Liu., New Journal of Chemistry, 2002, 26, 180-183.
2. X. Zhan, Y. Liu, D. Zhu, X. Liu, G.Xu, P. Ye, Chemical Physics Letters, 2002, 362, 165-169.
3. J.Sołoducho, S.Roszak A. Chyla, K. Tajchert, New Journal of Chemistry, 2001, 25, 1175-1181.
4. A. Afzali, T. L. Breen, C. R. Kagan, Chemistry of Materials, 2002, 14,1742-1746.

INFLUENCE OF FILLER DISPERSION ON THIN FILM POLYMER COMPOSITES SENSING PROPERTIES

17:50 - 18:05
oral

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Carbon black/polymer composite are very interesting materials already used to produce vapor sensors. Sensor responses are due to vapor absorption properties of an insulating polymer whose electrical properties are modulated by a conductive "filler".
In this work we produce thin composite films characterized by different grade of dispersion of carbon black in polymer matrix (Poly(methyl-methacrylate), Poly(2 hydroxy-ethyl-methacrylate) and atactic poly(styrene)). These samples are obtained changing some process parameters (viscosity of polymer solution and type of spinning deposition) or using different conductive filler types. We have used different fillers all made of carbon, but with different particle sizes (from micrometers to nanometers), structure and chemical functionalization. In particular, we have used commercial carbon blacks, multi-walled carbon nanotubes and home made carbon nanoparticles. In order to improve the dispersion of the filler in the polymeric solution we have modified commercial carbon black by a Fenton type oxidation. In order to evaluate the filler size influence we have prepared carbon nanoparticles (5-20 nm) obtained by flame synthesis.
Size distribution of filler in polymer suspension and deposition method strongly influence homogeneity and conductivity of corresponding polymer composite films and finally their sensing properties.
We study filler dispersion in polymer matrix by dynamic light scattering, optical and electronic scanning microscopy, profile analysis and 4 point probe measurements. This has allowed to investigate about the influence of different fabrication parameters on film morphologies (homogeneity, grade of filler dispersion, size of filler aggregates) and conductivity. Testing to different VOCs the sensor devices, will show the influence of different morphology on the characteristics of the sensors responses (sensitivity, selectivity, response and recovery time).

Assemblies of iron and TPPS porphyrins investigated by TEM, AFM and UV/vis spectroscopy

18:10 - 18:25
oral

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Porphyrins and related macrocycles provide an extremely versatile nanometer sized synthetic component for a variety of materials applications. The exploration of porpfyrins and metalloporphyrins molecules as building blocks for tailored materials has found rapid growth during the last decade. Films, solids, microporous solids have been explored as field-responsive materials. Assembling molecular functional components into supramolecular architecture is envisioned to yield artificial devices of technological relevance, such as sensors, molecular sieves, energy cells.
In this work an aggregates of the tetrakis(4-sulfonatophenyl)porphyrin (TPPS) and Fe(III)TPPS, formed in acid aqueous solutions were deposited onto hydrophilic(mica, glass) and hydrophobic (graphite) substrates and imaged using Transmission Electron Microskopy (TEM), Scanning Atomic Force Microscopy (AFM) and absorbtion spectra was investigated by UV/vis spectroscopy. The AFM and TEM studies reveald an nanoroads like structures formed on the surface from the TPPS solution. The TEM study revealed aggregate geometries, ranging from spherical with diameters 20-100 nanometers and rodlike structures with the diameter 5-7 nanometers and 1micron length.The nanoroads tend to form a bundles of individual roads. The AFM investigation have shown the flat structures with the thickness of 5-7 nanometres and the wide up to 20-70 nm. It suggest that the flat structure, unlike the previous model developed by authors1 , consist of the bundle of parallel nanoroads, formed by attractive forces of single nanoroads or it is an interplay of nucleation sites of nanoroads. Iron-porphyrins consist of 20-50 nanometer size particles which are dispersed or form fractal like structures around the nucleation centers on the surface. Some fractals have a well defined crystals shape.

1 R. Rotomskis,R. Augulis,V.Snitka,.Valiokas,B.Liedberg J.Phys.Chem.B2004, 108,2833-2838

Wednesday, September 8th

Nanocomposite nickel ceria cermet for anode supported SOFCs

15:30 - 15:45
oral

Piotr Jasinski[1,2)], **Toshio Suzuki**[2)], **Vladimir Petrovsky**[2)], **Harlan U. Anderson**[2)]

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Solid oxide fuel cells (SOFCs) are one of the most efficient energy conversion devices. The main demand in the current SOFC development is lowering operation temperature to the range of 600 ° C - 800 ° C. It has been shown that in this temperature range anode supported SOFC is a very promising design. The application of thin film techniques to the electrolyte processing allows decreasing electrolyte resistance and as a result improves fuel cell performance. A nickel cermet, which contains nickel (usually from 40 to 60 vol.%) and yttria stabilized zirconia or ceria, is typically used as an anode. However, nickel cermet during oxidation and reduction is subjected to intense volume change which may lead to destruction of thin film electrolyte or cermet structure.
In this paper a novel method of preparation of nickel cermet anode is presented and evaluated. This method, which is called net shape process, is a combination of conventional ceramic sintering and polymer precursor technique. First ceria powder with carbon pore former is sintered constructing rigid and stable cermet skeleton and next the skeleton is backfilled with nickel polymer. The nickel cermet, which is obtained by this method, has several advantages over conventional one:
1.low sintering temperature of nickel backfilling allows preparation nanocrystalline nickel, which due to its high surface area has high catalytic activity over reduction of hydrogen,
2.it is possible to obtain high conductance cermet with as low as 20% vol. of nickel,
3.decrease of nickel content leads to decrease volume change during reduction and oxidation of anode and as a result increase SOFC shock resistance.
Electrical conductivity and microstructure of nickel ceria cermet as a function of nickel content has been investigated.

Investigation of microstructure and piezoelectric properties of Zr and Sm doped PbTiO3 nanostructured thin films derived by sol-gel techmology

17:30 - 17:45
oral

Arturas Ulcinas[1)], **Mohammed Es-Souni**[2)], **Valentinas Snitka**[1)]

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$PbTiO_3$ thin films are an important class of materials for sensor and actuator applications in microsystems technology due to their excellent ferroelectric and piezoelectric properties. Use of sol-gel technology for production of these films has a number of advantages, such as fine control over stechiometry and microstructure, cost-effectiveness, relatively low processing temperature, possibility to coat large areas, and reproducibility of parameters.
In this work the microstructure and piezoelectric properties of nanostructured $PbTiO_3$ thin films was investigated in order to determine the optimal processing conditions for specific applications. Scanning electron and atomic force microscopies were used to investigate surface structure, and Doppler laser vibrometry and piezoresponse atomic force microscopy were employed to characterize macroscopic and localized piezoelectric properties of the films. It was found that Sm doped films have smooth microstructure (RMS roughness ranging from 1.26 nm for PSZT ($Pb_{1.0175}Sm_{0.05}(Zr_{0.52}Ti_{0.48})$ film to 2.05 nm for PST/PSZT heterostructure) and stable properties, but low piezoelectric coefficient (d_{33}=10-15 pm/V). Corona poling increased the piezocoefficient of these films by a factor of 4. PZT ($PbZr_{0.52}Ti_{0.48})O_3$ film has a high piezoelectric coefficient (up to 1 nm/V), however is susceptible to fatigue and other aging effects. Piezoresponse AFM has been used to obtain piezoelectric hysteresis loops and write and read areas of alternate polarization in the films.

Electron, hole and exciton spectra in opened cylindrical quantum dots embedded into the media of different dimension

17:50 - 18:05
oral

Mykola V. Tkach[1)], **Volodymyr A. Holovatsky, Olexander M. Makhanets, Oxana M. Voitsekhivska, Julia O. Sety**

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The electron, hole and exciton spectra are experimentally and theoretically studied in closed QD's in details now. Recently the opened QD's embedded into the 3D medium have been started the research. In the latter the quasiparticles can penetrate through the potential barrier and the new channel of energy relaxation arises. It can be used for the creation of new rapid devices.
In the proposed paper the electron, hole and exciton spectra and lifetimes in opened QD's embedded into the different media: quantum wires (QW), quantum wells (QW) and massive media(MM) are studied for the first time. The theoretical calculation of the spectra and lifetimes is done in the framework of the rectangular potential in the media interfaces and effective mass approximation. The analytical and numerical calculations are performed for the lifetimes and energies of quasiparticles in qusistationary states solving the Schrodinger equation and using the method of scattering S-matrix. It is shown that there exist the resonance states of Breit-Wigner type and non-resonance states too. Their evolution as a function of geometric sizes and shape of the heterosystem is obtained.
It is established that due to the difference between the electron and hole effective masses and depending on the geometric sizes of the well-shells (in multishell QD's) there are two different models od excitons localized in QD:i) electron and hole in the same shell; ii) electron and hole in different shells of nanosystem. It is shown that the exciton energy levels and lifetimes in both models are quite different.
The calculated dependences of the location and width of exciton bands on geometrical and physical characteristics of nanosystem give the opportunity to compare them with the results of experimental data.

ZnO nanowires with controlled nanomorphology

18:10 - 18:25
oral

German M. Telbiz[1)], **Olga V. Polonets**[2)], **Vasyly I. Gerda**[3)], **Mykola V. Bondar**[4)], **Volodymyr G. Ilyin**[1)]

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ADDENDUM - Symposium H

Monday, September 6th

Measuring the Grain Size Distribution of Pr-doped Zirconia Nanopowders obtained by Microwave Driven Hydrothermal Synthesis

17:20 - 17:35
oral

Roman Pielaszek[1)], **Agnieszka Opalińska**[1,3)], **Cristina Leonelli**[2)], **Hubert Matysiak**[3)], **Tomasz Wejrzanowski**[3)], **Krzysztof J. Kurzydlowski**[3)], **Witold Lojkowski**[1)]

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

Microwaves (MW) are increasingly used in chemical synthesis since: 1) they permit to heat materials and fluids faster than this is possible by conventional heating, 2) high purity of the reaction is easier to achieve, since the reacting substrates can be enclosed in a vessel made of a chemically resistant material and 3) the reaction path may by modified comparing to conventional reactions.
Properties of zirconia and Pr-doped zirconia nanopowders strongly depend on shape, grain size, grain size distribution and phase composition. Also the phase composition (relative fraction of the monoclinic and tetragonal phase) depends on the synthesis conditions. The microwave driven hydrothermal synthesis permit to precisely control the reaction regime and in consequence provide to expected properties of the resulting nanocrystalline powders.
In this work we investigated the effect of process parameters on Grain Size Distribution (GSD). The GSD was determined using two methods. The first one was based on analysis of images of the nanopowders obtained by means of transmission electron microscopy (TEM). The second one was based on analysis of the shape of X-ray diffraction (XRD) peaks. The two methods yielded identical results. In addition, the XRD based method permitted to perform a phase analysis of the powders and determine separately the GSD in the monoclinic and tetragonal phase and provide some information about the shape of the grains. Therefore, this method can be recommended for the determination of the GSD, which is a crucial parameter in the technology of nanocrystalline materials.

Percolation Threshold Model and its Application in the Electrical Conductivity of Layered BaTiO3-Ni Composites

poster
H-40

Milan Ambrožič[1)], **A. Dakskobler, M. Valant, T. Kosmač**

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We have investigated the electrical conductivity percolation threshold of the materials, composed of conductive particles embedded in the nonconductive host matrix. A statistical, numerical method is used in which the particles are randomly put, one by one, into the nonconductive host and the conductive path is searched. The influence of different types of particle shapes on percolation threshold is considered. Using this method we have found that in addition to the anisotropy in the particles' dimensions, the angular distribution of the particles' long axes plays a dominant role in the calculations of the conductivity percolation threshold. Finally the nonuniform space distribution of particles' positions is taken into account and the model is used to explain the percolation threshold in the AC conductivity of layered $BaTiO_3$-Ni composites.

Tuesday, September 7th

Fractal and Symbolic Methods for Nanomaterials Science and Nanosensors

15:30 - 15:45
oral

Wlodzimierz KLONOWSKI[1,2], **Elzbieta OLEJARCZYK**[1,2], **Robert STEPIEN**[1,2]

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Calculating materials properties from structural models has long been one of the most important problems of Materials Science (cf. [1]). There is still a need for relatively simple methods of assessment of material properties, especially surface properties, based on analysis of experimental data such as microscopic images. Fractal and symbolic methods of image and signal analysis can be very useful for these purposes. Fractal dimension of a surface in 3-dimensional space, D_s , may be assessed based on fractal dimension of an image of this surface on a plane. Fractal dimension is invariant with respect to linear scale transformations and it is simply related to power spectrum exponent β - an image of a fractal Brownian surface with the power spectrum proportional to $f^{-\beta}$ shows power spectrum proportional to $f^{2-\beta}$, where $\beta/2 = (3 - D_s)$ (cf. [2]).

Nanotechnologies provide new sensors that enable easy acquisition of biosignals for monitoring of drivers, pilots, etc. and for clinical applications. But before any signal generated by a nanosensor may be used for monitoring or clinical assessment that signal has to be appropriately processed and visualized. Data-processing algorithms based on fractal and symbolic computational methods may be used for extraction, fusion, and visualization of multi-modal information from nanosensors, for representing and managing signal complexity. These methods are computationally effective and may be applied in real-time.

[1] W.Klonowski, Probabilistic Topological Theory of Systems with Discrete Interactions,I,II, Can.J.Phys. 1989, 66, 1051-1067;
[2] W.Klonowski, Signal and Image Analysis Using Chaos Theory and Fractal Geometry, Mach.Graph.Vis. 2000, 9, 403-431.

Acknowledgements:
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Wednesday, September 8th

Surface and biological catalysts for ammonia synthesis and hydrogen evolution

15:15 - 15:45
invited oral

Berit Hinnemann[1], **Jens K. Norskov**[1]

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Ammonia synthesis is one of the most important processes both in nature and industrially, as it provides nitrogen in a chemically accessible form. Industrially, ammonia synthesis is accomplished by the Haber-Bosch process, which needs high temperatures and high pressures. In nature, nitrogen fixation is accomplished by the enzyme nitrogenase, which functions under ambient conditions. A detailed understanding of the mechanism of nitrogenase is therefore desirable, as it may lead to the development of biomimetic catalysts, which may be able to fix nitrogen under mild conditions. A detailed investigation of the structure and mechanism of the enzyme nitrogenase will be presented, and the key points of the mechanism are compared to the Haber-Bosch process. Nitrogenase is also able to catalyze hydrogen evolution and this will be discussed as well. Futhermore, it will be shown how nitrogenase can serve as an inspiration for developing new fuel cell catalysts for hydrogen evolution.