2014 Spring Meeting Lille, France – May 26th - 30th

SYMPOSIUM E

E

Defect-induced effects in nanomaterials

Symposium Organizers:

Flyura Djurabekova, University of Helsinki, Finland

Eugene Kotomin, University of Latvia, Latvia

Mark C. Ridgway, Australian National University, Australia

Nikolai A. Sobolev, Universidade de Aveiro and I3N, Portugal

Published in Physica Status Solidi C

PROGRAM VIEW : 2014 Spring
MY PROGRAM : 2014 Spring

Symposium : E

Defect-induced effects in nanomaterials

26 May 2014	27 May 2014	28 May 2014	29 May 2014	30 May 2014

hide a

start at	Subject	Num.

Properties of graphene : Arkady Krasheninnikov

09:00 **Defects in two-dimensional materials and nanoparticles -- Theory and microscopy**

Authors : Sokrates T. Pantelides, Stephen J. Pennycook
Affiliations : Department of Physics and Astronomy, Vanderbilt University, Nashville, TN, USA and Oak Ridge National Laboratory, Oak Ridge, TN USA; University of Tennessee, Knoxville, TN USA

Resume : Calculations based on density functional theory using high-performance computers have made enormous strides in describing the atomic-scale properties of complex materials. In parallel, aberration-corrected scanning transmission electron microscopy has reached extraordinary levels of spatial and energy resolution, in both imaging and electron-energy-loss spectroscopy. The combination of theory and microscopy provides an unparalleled probe of the atomic-scale structure, properties, and dynamics of complex systems, especially defects, boundaries, interfaces and nanoparticles. Here we describe recent results on defects in graphene, MoS2 monolayers, and CuInS2 nanoparticles. More specifically, we will discuss plasmon enhancement at Si impurities in graphene [1], Si6 clusters and Si-passivated nanovoids in graphene [2], nanowire formation in MoS2 monolayers [3], and a unique form of crystalline order observed in CuInS2 nanoparticles [4]. Primary collaborators: Theory: Jaekwang Lee, Xiao Shen, Junhao Lin; microscopy: Wu Zhou, Juan C. Idrobo, Junhao Lin, Matt Chisholm; This work was supported by the US Department of Energy Basic Energy Sciences, Materials Science and Engineering directorate. 1. W. Zhou et al., "Atomically localized plasmon enhancement in monolayer graphene", Nature Nanotechn. 7, 161 (2012). 2. J. Lee et al., Direct visualization of reversible dynamics in a Si6 cluster embedded in a graphene pore, Nature Commun. 4, 1650 (2013); J. Lee et al. "Stabilizaion of graphene nanopores", under review. 3. J. Lin et al., "Flexible metallic nanowires with self-adaptive contacts to semiconducting transition-metal dichalcogenide monolayers", under review. 4. X. Shen et al., "Interlaced crystals: 'Perfect Bravais lattices with interlaced chemical order revealed by real-space crystallography", under review.

EO11

add to my program (close full abstract)

09:30 **Scanning Probe Microscopy Characterization of Grain Boundaries in CVD Graphene and Nanolithography**

Authors : L. P. Biró1, 4, L. Tapasztó1, 4, G. Magda1, 4, P. Nemes-Incze1, 4, G. Dobrik1, 4, P. Vancsó1, 4, Z. Osváth 1, 4, G. I. Márk1, 4, Ph. Lambin2, X. Jin3, 4, Y. S. Kim3, 4, C. Hwang3, 4
Affiliations : 1Institute of Technical Physics and Materials Science, Research Centre for Natural Sciences, 1525 Budapest, PO Box 49, Hungary, http://www.nanotechnology.hu/; 2Department of Physics of Matter and Radiations, University of Namur (FUNDP), 61 Rue de Bruxelles, B-5000 Namur, Belgium; 3Center for Nano-metrology Division of Industrial Metrology Korea Research Institute of Standards and Science, 267 Gaejeong-ro, Yuseong-Gu, Daejeon 305-340, Republic of Korea; 4Korean-Hungarian Joint Laboratory for Nanosciences (KHJLN), P.O. Box 49, 1525 Budapest, Hungary

EO12

Resume : Graphene is an excellent candidate to replace silicon in nanoelectronics, to mention only the most exciting from its many potential applications [1]. Chemical Vapor Deposition (CVD) is the industrially most viable way of producing large area graphene layers [2]. The CVD graphene is

polycrystalline [3], therefore the characterization of the grain structure and the effect of individual grain boundaries (GBs) is a must, if any serious practical application is intended. AFM [4], and STM [5, 6] in combination with numerical simulations [7] are extremely useful in understanding the structure and electronic properties of the GBs in CVD graphene. Furthermore, STM is very well suited for the nanolithography of the material with nanometer precision and full crystallographic orientation control of the edges of the nanoarchitectures. [1] Novoselov, K. Rev. Mod. Phys. 83, 837–849 (2011). [2] Bae, S. et al. Nat. Nanotechnol. 5, 574–578 (2010). [3] Biró, L. P. & Lambin, P. New J. Phys. 15, 035024 (2013). [4] Nemes-Incze, P. et al. Appl. Phys. Lett. 99, 023104–1–023104–3 (2011). [5] Tapasztó, L. et al. Appl. Phys. Lett. 100, 053114 (2012). [6] Nemes-Incze, P. et al. Carbon N. Y. 64, 178–186 (2013). [7] Vancsó, P., et al., Carbon N. Y. 64, 101–110 (2013).

add to my program (close full abstract)

09:45 **Dirac-states in a Ta-doped TiO2 nanowire: basis for a new type of high-speed field effect transistors.**

Authors : Peter Deák,1 Bálint Aradi,1 Alessio Gagliardi,1,2 Huynh Anh Huy,1 Gabriele Penazzi,1 Binghai Yan,1 Tim Wehling,1,3 and Thomas Frauenheim1
Affiliations : 1 Bremen Center for Comp. Mater. Sci., University of Bremen, P.O. Box 330440, D-28334 Bremen, Germany; 2 Department of Electronic Engineering, University of Rome "Tor Vergata", via del Politecnico 1, I-00133 Roma, Italy; 3 Institute for Theoretical Physics, University of Bremen, Otto-Hahn-Allee 1, D-28359 Bremen, Germany

Resume : Dirac-states in graphene nanoribbons or topological insulators have very high mobility, but the lack of a sizeable gap results in electronic switching devices with a much too low on-off ratio [1]. Based on theoretical calculations, we have discovered [2], that [001] nanowires of anatase-TiO2 posses Dirac-states near the wide fundamental band gap, just above the conduction band edge. A gate voltage could shift the Fermi-level into the Dirac-region, switching the system between the "classical" high-resistivity semiconducting and a relativistic high-mobility metallic range. The band gap of an anatase-TiO2 nanowire is too wide, to tune the Fermi-level from its intrinsic position at midgap above the conduction band edge. Therefore, n-type doping is necessary. Here we present computational studies on Nb- and Ta-doping of anatase [001] nanowires. We show, that the solubility is good and the dopants prefer high symmetry sites inside the wires. We also show that Ta does not destroy the Dirac-states, and a random distribution does not give rise to Anderson localization either. [1] F. Schwierz, Graphene transistors. Nat. Nanotechnol. 5, 487 (2010). [2] Deák, B Aradi, A. Gagliardi, H. A. Huy, G. Penazzi, B. Yan, T. Wehling, and T. Frauenheim, Possibility of a Field Effect Transistor Based on Dirac Particles in Semiconducting Anatase-TiO2 Nanowires. Nanoletters, 13, 1073-1079 (2013).

EO13

add to my program (close full abstract)

10:00 **Break**

Two-dimensional materials : Sokrates Pantelides

10:30 **Native and irradiation-induced defects in two-dimensional materials**

Authors : Arkady V. Krasheninnikov
Affiliations : Department of Applied Physics, Aalto University, Finland

Resume : Following the isolation of a single sheet of graphene, many other 2D systems such as h-BN, transition metal dichalcogenides (TMD), and SiO2 sheets were later manufactured. All these materials have native defects, which naturally affect their properties. Moreover, defects can deliberately be introduced by ion and electron irradiation to tailor the properties of 2D materials. In my talk, I will summarize our knowledge about defects [1,2] in graphene and other 2D systems. I will also touch upon defect production in 2D systems under impacts of energetic ions and electrons and present theoretical data obtained in collaboration with several experimental groups [3-6]. I will also dwell upon impurity and defect-mediated engineering of the electronic structure of 2D materials such as BN or TMDs. I will finally touch upon defects in bilayer 2D silica [8] and show that point and line defects in this system are strikingly similar to those in graphene with their morphology being governed by the hexagonal symmetry of the lattice. 1. F. Banhart, et al. ACS Nano, 5 (2011) 26. 2. O. Lehtinen et al. Nature Comm. 4 (2013) 2098. 3. M. Kalbac, et al. Adv. Mat. 25 (2013) 1004. 4. J. Meyer, et al. PRL 108 (2012) 196102. 5. H.-P.

EO21

Komsa, et al. PRL 109 (2012) 035503; PRB 88 (2013) 035301. 6. R. R. Nair, et al. Nature Comm. 4 (2013) 2010. 7. Y. Lin et al. Adv. Mat. (2014) accepted. 8. T. Björkman et al. Sci. Rep. 3 (2013) 3482.

add to my program (close full abstract)

11:00 **Excitons and stacking order in h-BN**

Authors : A. Zobelli, R. Bourellier, M. Amato, L.H.G. Tizei, C. Giorgetti, A. Gloter, M.I. Heggie, K. March, O. St□ephan, L. Reining, M. Kociak
Affiliations : Laboratoire de Physique des Solides, Univ. Paris-Sud, CNRS UMR 8502, F-91405, Orsay, France; Laboratoire des Solides Irradi□es, Ecole Polytechnique, Route de Saclay, F-91128 Palaiseau and European Theoretical Spectroscopy Facility (ETSF), France; Department of Chemistry, University of Surrey, Guildford GU2 7XH, United Kingdom

Resume : The strong excitonic emission of hexagonal boron nitride (h-BN) makes this material one of the most promising candidate for light emitting devices in the far ultraviolet (UV). However, single excitons occur only in perfect monocrystals that are extremely hard to synthesize, while regular h-BN samples present a complex emission spectrum with several additional peaks. Despite a large number of experimental and theoretical studies, the microscopic origin of these additional emissions has not yet been understood. In this work we address this problem using an experimental and theoretical approach that combines nanometric resolved cathodoluminescence, high resolution transmission electron microscopy and state of the art theoretical spectroscopy methods. We demonstrate that emission spectra are strongly inhomogeneus within individual h-BN flakes and that additional excitons occur at structural deformations, such as faceted plane folds, that lead to local changes of the h-BN stacking order.

EO22

add to my program (close full abstract)

11:15 **Enhancement of carrier mobility in high dielectric 2D MoO(3-x)**

Authors : Sivacarendran Balendhran,* Sumeet Walia, Jian Zhen Ou, Sharath Sriram, Madhu Bhaskaran, and Kourosh Kalantar-zadeh,
Affiliations : Functional Materials and Microsystems Research Group, School of Electrical and Computer Engineering, RMIT University, Melbourne, Australia

Resume : Since the discovery of graphene, exploration of alternative 2D materials with intrinsic bandgap for electronic applications has been afoot. Layered MoO3 has a relative high dielectric (k) of ~500 and can be exfoliated to minimum resolvable 2D layers. The bandgap of MoO3 can be easily manipulated to desirable values by several techniques such as hydrogen ion intercalation, UV irradiation, electron beam bombardment etc. Such techniques produce partially reduced non-stoichiometric MoO(3-x) which has increased carrier concentration and a high-k value, that highly favours the enhancement in charge carrier mobility. In this work, room temperature charge carrier mobilities exceeding ~1100 cm2/Vs were established for non-stoichiometric 2D MoO3 based field effect transistors (FETs). The experimental mobilities and the theoretical behaviour of the mobility, calculated using Borne approximation with respect to temperature are presented. As, the acoustic and optical phonon scattering effects are independent of the k value, in a low-k material coulomb scattering effect seems to be the limiting mechanism of the overall mobility. In a high-k material the coulomb scattering effect is minimized and acoustic phonon scattering emerges as the dominant mechanism that limits the overall mobility. The experimental mobilities observed in the MoO(3-x) FET are in the same order of magnitude and closely match the theoretically predicted trend of the overall mobility. In summary, this work demonstrates the enhancement of the overall carrier mobility in a high-k 2D material, achieved by introducing non-stoichiometry.

EO23

add to my program (close full abstract)

11:30 **Formation of defects and defect healing during carbon nanotube and graphene growth**

Authors : Feng Ding, Qinghong Yuan, Lu Wang
Affiliations : Institute of Textiles and Clothing, Hong Kong Polytechnic University, Hong Kong S.A.R., China

Resume : The number of polygons in the wall of a macroscopic sized carbon nanotube (CNT) can be billions or more. Simple geometrical analysis shows that the formation of any topological defects (such as pentagons, heptagons or their pairs, etc) would lead to a change of the CNT's intrinsic chiral structure and the electronic properties. Experimentally, the synthesis of perfect macroscopic CNT has been observed but the mystery of the high efficiency of defect healing is still unveiled. In this presentation, I will discuss the potential routes of forming a topological defect in CNT wall and the corresponding mechanism of defect

EO24

healing. Our ab initio calculations and kinetic analysis clearly indicate that, Fe, is the best catalyst among the most used ones and the fast growth (at the rate of 1 m/hr.) of macroscopic long defect free CNTs is theoretically possible.[1,2,3] This study open a door of synthesizing of macroscopic long defect free CNTs for electronic and device applications. Besides, the mechanism of defect formation and healing in graphene CVD synthesis will be discussed as well.[4] References: 1. F. Ding, A. R. Harutyunyan, B. I. Yakobson, PNAS, 106, p2506, (2009) 2. QH. Yuan, F Ding, Q. Yuan, Z. Xu, B. I. Yakobson and F. Ding, Phys. Rev. Lett., 108, 245505, (2012) 3. Q. H. Yuan., H. Hu, F. Ding, Phys. Rev. Lett., 107(15), 156101, (2011) 4. Lu Wang, Xiuyun Zhang, Helen L.W. Chan, Feng Yan,* and Feng Ding*, J. Am. Chem. Soc. 135, 4476−4482 (2013).

add to my program (close full abstract)

12:00 **Lunch**

Nanoheterostructures : Andre Vantomme

14:00 **Defect-Induced Growth and Electronic Properties of Quantum Dot Molecules**

Authors : A.V.Dvurechenskii
Affiliations : Rzhanov Institute of Semiconductor Physics, Siberian Branch of Russian Academy of Science, Novosibirsk State University

Resume : The aim of the present work is to review present and future trends of research on quantum dot (QD) nanostructured semiconductors concerning quantum dot molecules (QDM), from fundamental issues of synthesis to some electronic properties. The synthesis should allow: a) to improve QD homogeneity in size with keeping form and elemental content; b) to control QD density and space ordering; c) to lower the defect density. Spontaneous nucleation of nanocrystals at heteroepitaxy of lattice mismatched semiconductors is described by: a) the dispersion in size averaged with 17-20% for (as example) Ge QD in Si; b) the random nanocrystal nucleation and as a result random arrangement in growth plane. Different experimental techniques such as the nanoimprint, extreme ultraviolet interference, electron-beam lithography, ion-beam induced pit-patterning of substrates and effect of vertical alignment of nanocrystal nucleation are used for the fabrication of templates with predefined dot formation sites. The epitaxy on pin-patterned surface allows to reduce QD size dispersion and QD ordering in the plane of growth. Another way of QDM growth is the strain induced epitaxy in heterophase system. The spatial localization of electrons in QDM can be controlled by the change of spacer thickness between double QDM. The two-qubit operations are performed on the physical qubits by controlling the exchange interaction. There were determined the conditions on which the exchange coupling is large enough for a fast swap operation in quantum computation and the double-occupancy probability is still low, thus maximizing the entanglement for a small computation error which allows to use coupled Ge/Si QDM in two-qubit quantum operations.

EO31

add to my program (close full abstract)

14:30 **Thermal characteristics of tapered SiGe nanowires**

Authors : Eun Kyung Lee1, Jong Woon Lee2, Junho Lee3, Won-Jae Joo4, Sung Jin Kim1, Sungwoo Hwang4, Dongmok Whang2, Byoung Lyong Choi4
Affiliations : 1. Samsung Electronics, Samsung Advanced Institute of Technology, CAE Group, Korea 2. Sungkyunkwan University, School of Advanced Materials Science and Engineering, Korea 3. Samsung Electronics, Samsung Advanced Institute of Technology, AE Group, Korea 4. Samsung Electronics, Samsung Advanced Institute of Technology, Nano Electronics Lab, Korea

Resume : In recent years, low dimensional nanostructures have been considered to be the effective way to make thermoelectric materials with low thermal conductivity by suppressing the lattice phonon contribution.1 Particularly, SiGe alloy nanowires are one of the promising candidates because they have excellent thermal and electrical properties for efficient thermoelectric materials.2 We suggest taper-shaped SiGe nanowires with plane defects in outer shell grown by vapor-liquid-solid (VLS) and vapor-solid (VS) growth mechanism, and the effects of their defects on the suppression of phonon propagation in nanowire while sustaining the electrical conductivity. The thermal conductivity of SiGe nanowires are measured using micro-fabricated devices over temperature range of 60K to 450K. Thermal conductivity of SiGe alloy nanowire (diameter ~340nm) with different composition between core and shell of nanowires is as

EO32

low as ~1.24W/m-K at 300K. The suggested defect-engineered tapered nanostructures can give a way to keep mechanical properties for the realization of nano thermoelectric systems.

add to my program (close full abstract)

14:45 **Formation of interconnected Ge nanostructures in SiO2 matrix by in-situ annealing during co-sputtering of Ge and SiO2**

Authors : B. Altuntas*1,2, S. Ilday2,3, M. Yilmaz2,4, R. Turan1,2, S. Cosentino5, R. Raciti5, I. Crupi5, A. Mio5, G. Nicotra5, A. Terrasi5, S. Mirabella5
Affiliations : 1Department of Physics, Middle East Technical University, 06800, Ankara, TURKEY 2Center for Solar Cell Research and Applications (GÜNAM), Middle East Technical University, 06800, Ankara, TURKEY 3Department of Micro and Nanotechnology, Middle East Technical University, 06800, Ankara, TURKEY 4Department of Physics, Necmettin Erbakan University, 42090, Konya, TURKEY 5Dipartimento di Fisica e Astronomia and CNR-INFM, MATIS, Università di Catania, I-95123, Catania, ITALY

Resume : Ge nanostructures embedded in a dielectric matrix can be useful in devices like photodetectors and solar cells. These devices can utilize the quantum size effect occurring in the semiconductor quantum structures fabricated in an appropriate matrix. One can tailor the band gap and optical properties via the size of the structures. However, although quantum dots provide quantum confinement of excitons, their drawback is the difficulties in electrical transport through the insulating dielectric matrix. As an alternative, we propose fabrication of interconnected Ge nanostructures embedded in a dielectric matrix, which provides better electrical connections while preserving the quantum confinement effect by carefully tailoring the Ge content and engineering the structure of dielectric matrix. Here, we report on the fabrication of interconnected sponge-like Ge nanostructures embedded in SiOx matrix using magnetron-sputtering technique. We have annealed the thin films during the deposition and the effect of substrate temperature is investigated through a complete structural and optical analyses. We have achieved formation of interconnected Ge nanostructures by carefully tailoring the stoichiometry of the system as observed through HRTEM imaging. Structural evolution of Ge/SiOx and Ge/GeOx species, and their optical responses are scrutinized through ultraviolet-visible/near-infrared (UV-Vis/NIR), Rutherford back scattering (RBS), Raman, and X-ray photoelectron (XPS) spectroscopy analysis. Ge segregation is clearly observed in the all films in-situ annealed during the deposition. The segregation is found to be strongly dependent on the substrate temperature. A sponge-like material structure is observed even at temperatures as low as 400 oC. At higher temperatures, well separated Ge islands with peculiar shapes are observed.

EO3 3

add to my program (close full abstract)

15:00 **Nanopore formation induced by ion-implantation in Ge: optical properties**

Authors : D.Cavalcoli (1), B.Fraboni (1), G. Impellizzeri (2), L. Romano (2), E.Scavetta (3), M. G. Grimaldi (2)
Affiliations : (1) Dipartimento di Fisica e Astronomia, Università di Bologna,Viale Berti Pichat 6/2, 40127 Bologna, Italy (2) CNR-IMM- MATIS and Dipartimento di Fisica e Astronomia, Università di Catania,Via S. Sofia 64, 95123 Catania, Italy (3) Dipartimento di Chimica Industriale 'Toso Montanari', Università di Bologna, Viale Risorgimento 4, 40136 Bologna, Italy

Resume : Self-ion implantation on bulk Ge induces the formation of nanopores, and their growth, structure and transport properties have been recently reported [1]. Semiconductors containing nanopores have gained a renewed interest as they are able to adsorb and interact with atoms and molecules and can thus be used in several interesting and emerging applications. In this contribution we report on the influence of ion implantation and subsequent nanopore formation on optoelectronic properties of Ge samples. The analyses are carried out by Surface Photovoltage (SPV) Spectroscopy, a powerful technique to get detailed information on material optical properties [2]. Different nanoporous (np) structures have been investigated: crystalline and amorphous np-Ge obtained by implantation of bulk Ge, as well as crystalline and amorphous np-Ge obtained by ion implantation of Ge film grown on Si substrates by molecular beam epitaxy and sputtering. Changes in the SPV spectra as a function of ion implantation fluence and annealing treatments are discussed on the basis of the structural properties of the samples. Quantum confinement effects in nanoporous Ge film have been demonstrated, while a significant SPV enhancement in np-Ge samples decorated with Au nanoparticles has been shown. These results can be of major interest for future photovoltaic applications of thin film solar cells. G Impellizzeri et al Nanotechn 23, 395604 (2012) L Kronik and Y. Shapira, Surf Sci Rep. 37,1 (1999)

EO3 4

add to my program (close full abstract)

15:15 **Scanning tunneling microscopy of GaAs/GaAsSB Nanowires**

Authors : Adrián Díaz, Pierre Capiod, M. Berthe, Tao Xu, Jean-Philippe Nys, I. Lefebvre, Ph. Caroff, Ph. Ebert, Bruno Grandidier

Affiliations : Institut d'Electronique, de Microélectronique et de Nanotechnologie (IEMN), CNRS, UMR,8520, Département ISEN, 41 bd Vauban, 59046 Lille Cedex, France ; Key Laboratory of Advanced Display and System Application, Shanghai University, 149 Yanchang Road, Shanghai 200072, People's Republic of China; Deparment of Electronic Materials Engineering, Research School of Physics and Engineering, The Australian National University, Canberra ACT 0200, Australia; Peter Grünberg Institut, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany.

Resume : Understanding surface structure and surface composition is of particular importance for semiconductor nanowire applications, since they might strongly contribute to the electrical, optical and thermal properties of the Nanowires. A prototypical material is GaAs, where polytype inclusions consisting of zinc-blende (ZB) and wurtzite (WZ) segments form during the growth of nanowires, in particular when Sb atoms are incorporated. Here, we will investigate the structural and electronic properties of GaAs and GaAsSb nanowires with scanning tunneling microscopy and spectroscopy. These techniques gives access to the nanofaceting morphology of a single semiconductor nanowire with a detailed picture of the sidewall structural and compositional properties at the atomic scale. It will also be used to measure the band gap and the position of the Fermi level at the surface. In particular, we will show that the ZB_WZ structures on the surface of GaAs nanowires naturally introduce p-i juntions solely due to the Fermi level pinning at different energies on the non-polar WZ and ZB sidewall facets.

EO3 5

add to my program (close full abstract)

15:30 **Break**

Poster session I : Aurélien Debelle and Tiziana Cesca

16:00 **Selective Decoration of Au Nanoparticles on Monolayer MoS2 Single Crystals**

Authors : Limin Jin

Affiliations : the Hong Kong Polytechnic University

Resume : A controllable wet method was introduced to fabricate selective decoration of 2-dimensional (2D) molybdenum disulfide (MoS2) layers with Au nanoparticles (NPs). Au NPs can be selectively formed on the edge sites or defective sites of MoS2 layers. The Au-MoS2 nano-composites are formed by non-covalent bond. The size distribution, morphology and density of the metal nanoparticles can be tuned by changing the defect density in MoS2 layers. Field effect transistors were directly fabricated by placing ion gel gate dielectrics on Au-decorated MoS2 layers without the need to transfer these MoS2 layers to SiO2/Si substrates for bottom gate devices. The ion gel method allows probing the intrinsic electrical properties of the as-grown and Au-decorated MoS2 layers. This study shows that Au NPs impose remarkable p-doping effects to the MoS2 transistors without degrading their electrical characteristics.

EP1 1

add to my program (close full abstract)

16:00 **Colloidal Si and SiGe alloy nanocrystals with heavily B and P doped shells**

Authors : Minoru Fujii, Hiroshi Sugimoto, Takashi Kanno, Masataka Hasegawa, and Kenji Imakita

Affiliations : Department of Electrical and Electronic Engineering, Graduate School of Engineering, Kobe University, Rokkodai, Nada, Kobe 657-8501, Japan

Resume : Colloidal Si nanocrystals have been attracting significant attention because they can be a key material for Si-based printable electronics and are expected to be more suitable for biological applications than compound semiconductor nanocrystals due to the non-toxicity as a chemical element. In general, the surface of Si nanocrystals is functionalized by organic ligands to prevent the agglomeration in solution. However, the surface molecules hinder charge carrier transport in films produced from colloidal solutions. Recently, we have developed Si nanocrystals which can be dispersed in polar solvents without organic ligands. The structural feature of the nanocrystal is the formation of a heavily B and P doped shell on the surface. The core-shell Si nanocrystals exhibit very wide range tunable luminescence (0.85-1.8eV) in solution due to the donor to acceptor transitions. In this work, we study the structure of the heavily B and P doped shells by Raman scattering and X-ray photoelectron

EP1 3

spectroscopies. We demonstrate the evidences that a thin hard crystalline shell containing different kinds of B and P related species, e.g., substitutional B, P and B-P pairs, B clusters, B-interstitial clusters, etc., are formed on the surface of a nanocrystal. We also show that the method can be applied to SiGe alloy nanocrystals. SiGe alloy nanocrystals dispersible in ethanol without organic ligands and exhibiting size and composition controllable photoluminescence can be produced by the method.

add to my program (close full abstract)

16:00 **Optical property changes and band-gap calculations of diamond and sapphire produced by ion implantation**

Authors : Jae-Won Park, Jaeun Kim, Jun-Hyung Cho
Affiliations : Korea Atomic Energy Research Institute, Yuseong-Gu, Daejeon, 305-353, Korea

Resume : The color of N-ion-implanted diamond became glossy black with metallic luster, which was further enhanced after postimplantation annealing at 600 °C for 2 h in vacuum or inert gas atmosphere. Raman spectroscopy revealed that the crystalline diamond became completely disordered after irradiation, but the crystalline nature was restored to a mixture of well-defined diamond and diamond-like carbon after annealing. When it was annealed in air at the same temperature, however, the black color disappeared, indicating a removal of the disordered or graphitized layer by oxidation. X-ray photoelectron spectroscopy and Raman analyses indicate that the black color of as-implanted diamond is associated mainly with the disordered carbon and modified band structure. Fourier transform infrared (FTIR) analysis shows that the implanted nitrogen atoms are in N–N and symmetrical 4N-vacancy bonding states, which are commonly found in the natural diamonds with yellow and brown tint. Our DFT calculation suggests that band gap of diamond is reduced by 25% after doping N with ion implantation and then heat treating, and N has an associated energy level about 1.7 eV below the conduction band when sitting on a substitutional lattice site in the neutral charge state. Various colorations of sapphire were obtained by metallic ions implantation, including blue coloration by Co ion implatation and yellowish by Fe and Cr.

EP1 4

add to my program (close full abstract)

16:00 **Defect Analysis in Graphenic Materials with Coupled Double Resonance Raman Scattering**

Authors : Stephane NEUVILLE
Affiliations : TCE

Resume : Considering that sp2 clusters imbedded in amorphous carbon material correspond to graphenic particles, Raman results achieved with graphene are expected to provide improved insight of many carbon materials and in order to check abundance of atomic point defects in form of vacancies and voids in graphene, SWCNT and DLC materials. However, in spite of significant progress achieved, many Raman results remain confusing especially concerning the so-called ?D disorder? Raman peak, the ?2D? band and some side peaks of the ?G? peak of graphene. Analyzing in more details current double resonance (DR) theory used for graphene Raman peak assignment and associating them to published results achieved with Micro-Raman, some questions suggest that commonly used assumptions need to be modified. This is especially concerning the locality principle of the corresponding Raman scattering model for which energy and momentum conservation conditions are not always fulfilled. Basing on dual quantum mechanical/classical representation of electron and phonon, we propose a Coupled Double Resonance theory (CDR) with which we discuss why some intense ?2D? peak can be observed where no ? D disorder? peak exists suggesting then, contrary to what established theory claims that the ?2D? is not only corresponding to a second harmonic overtone of the so called ?D disorder? peak of graphene at ~1350 cm-1 and why no second harmonic overtone of the G peak has never been observed. These effects can be used to depict the existence of point defects in graphene and SWCNT and to sort out the paradoxical case where the so-called ?D disorder? peak is superimposed by some stress upshifted ?D diamond? peak in glassy carbon for instance, which is known to contain significant amounts of voids.

EP1 5

add to my program (close full abstract)

16:00 **Adsorption and diffusion of Thorium and Uranium adatoms on graphene nanoribbons: A first principle study**

Authors : Cheng Cheng and Han Han
Affiliations : Shanghai Institute of Applied Physics, Chinese Academy of Sciences; Key Laboratory of Nuclear Radiation and Nuclear Energy Technology, Chinese Academy of Science

EP1 6

Resume : In the ceramic coated particle nuclear fuel of Gen IV reactor, the interactions between the actinide materials and graphite structures are significant for the performance and safety. In this article, we carried out the first principle calculations on Th adatom on the surface of planar graphene. We found that the Th atom prefer to locate at the hollow site with the binding energy of 3.09eV for local spin density approximation (LSDA) and 2.14eV for Perdew-Burke-Ernzerhof approximation (PBE). With the dimensionality of graphene reducing to a quasi-one-dimension, the presence of edge effects of both Th and U adatoms adsorption and diffusion on armchair and zigzag edges have been studied. We found that the edge effects in the zigzag nanoribbons are more pronounced than in the armchair case. The actinide elements was found can be easily diffused at the edge of graphite surface, and this edge effects in the zigzag nanoribbons are more pronounced than in the armchair case.

add to my program (close full abstract)

16:00 **Negative Quantum Capacitance Induced by Midgap States in Single-layer Graphene**

Authors : Lin Wang, Yang Wang, Xiaolong Chen, Wei Zhu, Chao Zhu, Zefei Wu, Yu Han, Mingwei Zhang, Wei Li, Yuheng He, Wei Xiong, Kam Tuen Law, Dangsheng Su, Ning Wang

Affiliations : Department of Physics and the William Mong Institute of Nano Science and Technology, The Hong Kong University of Science and Technology, Hong Kong, China; Department of Physics and Astronomy, California State University, Northridge, California 91330, USA; Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang, China

Resume : We demonstrate that single-layer graphene (SLG) decorated with a high density of Ag adatoms displays the unconventional phenomenon of negative quantum capacitance. The Ag adatoms act as resonant impurities and form nearly dispersionless resonant impurity bands near the charge neutrality point (CNP). Resonant impurities quench the kinetic energy and drive the electrons to the Coulomb energy dominated regime with negative compressibility. In the absence of a magnetic field, negative quantum capacitance is observed near the CNP. In the quantum Hall regime, negative quantum capacitance behavior at several Landau level positions is displayed, which is associated with the quenching of kinetic energy by the formation of Landau levels. The negative quantum capacitance effect near the CNP is further enhanced in the presence of Landau levels due to the magnetic-field-enhanced Coulomb interactions.

EP1 7

add to my program (close full abstract)

16:00 **Ab initio calculations of the transfer and aggregation of F centers, as well as bulk and nano-surface H centers in CaF2, BaF2 and SrF2**

Authors : R. I. Eglitis(a), H. Shi(b) and R. Jia(c)

Affiliations : (a) Institute of Solid State Physics, University of Latvia, 8 Kengaraga Str., Riga LV1063, Latvia; (b) School of Science, Beijing Institute of Technology, 100081, Beijing, PR China; (c) Institute of Theoretical Chemistry, State Key Laboratory of Theoretical and Computational Chemistry, Jilin University, 130023 Changchun, PR China

Resume : Our hybrid B3PW calculations show that the F-center diffusion barrier is equal to 1.84, 1.67 and 1.83 eV in SrF2, CaF2 and BaF2 crystals [1-3]. During the F center transfer, the trapped electron is more delocalized than that in the regular F center case, and the gap between defect level and CB in the alpha spin state decreases. The F center in CaF2, BaF2 and SrF2 is strongly localized inside vacancy, it contrasts with F centers in ABO3 perovskites, for example KNbO3, where two F center electrons are considerably delocalized. The calculation of total energies of different nano-surface H center configurations in BaF2 implies that H centers have a trend to locate near the surface [4]. The energy difference between H centers with different orientations shows that the H centers oriented in the [111] direction in SrF2, CaF2 and BaF2 crystals are the most stable configuration [5]. References: 1. H. Shi, L. Chang, R. Jia and R.I. Eglitis, Comput. Mater. Sci. 79, 527 (2013). 2. H. Shi, L. Chang, R. Jia and R. I. Eglitis, J. Phys. Chem. C 116, 4832 (2012). 3. H. Shi, R. Jia and R. I. Eglitis, Solid State Ionics 187, 1 (2011). 4. H. Shi, R. Jia and R. I. Eglitis, Phys. Rev. B 81, 195101 (2010). 5. L. Yue, R. Jia, H. Shi, X. He and R. I. Eglitis, J. Phys. Chem. A 114, 8444 (2010).

EP1 9

add to my program (close full abstract)

16:00 **Healing Defective CVD-graphene through Vapor Phase Treatment**

Authors : Do Van Lam,1, 2 Sang-Min Kim,2 Youngji Cho,3 Jae-Hyun Kim,2 Hak-Joo Lee,2 Jun-Mo Yang, 3 Seung-Mo Lee 1, 2, *

Affiliations : 1 Nano Mechatronics, University of Science and Technology (UST), 217 Gajeong-ro, Yuseong-gu, Daejeon 305-333, South Korea 2 Department of

EP1 10

Nanomechanics, Korea Institute of Machinery and Materials (KIMM), 156 Gajeongbuk-ro, Yuseong-gu, Daejeon 305-343, South Korea 3 Department of Measurement & Analysis, National Nanofab Center, 291 Daehak-ro, Yuseong-gu, Daejeon 305-701, South Korea
Resume : Structural defects present on chemical vapor deposition (CVD)-graphene are usually originated from growth stage and transfer process. Those limit the electronic transport properties of the graphene and degrade performance of related devices. Here we report that those inherent atomic defects could be selectively healed by simple vapor phase treatment performed in equipment conventionally used for atomic layer deposition (ALD). The unique chemistry of Al2O3 ALD facilitated selective depositions of AlxOy compounds on the defects, which was able to be readily probed and visualized using AFM imaging. The healing agent, AlxOy, was observed to bind tightly to the defects and lead to doping of the CVD-graphene, which were reflected in noticeable improvement in the electrical sheet resistance. In contrast with the chemically doped graphene, the ALD treated graphenes revealed notable long term stability under environmental conditions. Our approach promises selective healing of defects present in most of materials and likely ensures considerable enhancement in electrical and mechanical properties. The ALD with a broad spectrum of material selection could be a versatile tool for upgrading materials' properties.

add to my program (close full abstract)

16:00 **Interlayer Diffusion, Defect Creation, and Thermo –stability of Nanostructure of TM:Cu,Pd,Ni/Graphene Interfaces. MD-simulation**

Authors : Valery Polukhin, Elmira Kurbanova, Evgeny Galashev
Affiliations : Institute of Material Studies and Metallurgy of Ural Federal University, Institute of Metallurgy of Ural Branch of the RAS, Institute of Industrial Ecology of Ural Branch of RAS
Resume : The thermal evolution of transition metal nanoclusters and thin films deposited on a single- and two-layered grapheme (G) have been studied in a molecular-dynamics model for interval 300 K ≤ T ≤3900 K to analyze the formations and thermal stabilities of structure interfaces TM/G so as the diffusion processes and defect forming. The initial arrangement of TM atoms on the graphene sheet is optimal from the standpoint of their interaction with the substrate, but it was not equilibrium for a metallic system with a regular atomic packing at a temperature of 300 K. The longitudinal film size of two- layer graphene was decreased more smoothly with increasing temperature, but the transverse size was decreased not so fast as in the case of single-layer graphene. Because of non-equilibrium of interface metallic substructure even at this temperature, the TM atoms significantly approach to each other, so that the metallic film size was decreased, and this reduction was more substantial in the transverse ("armchair") direction as compared to the longitudinal ("zigzag") direction. The self-diffusion coefficient, which characterized the displacement of the Ni atoms in the horizontal and vertical directions, also were increased at temperatures above 1800 K. The advantages of a copper substrate as compared to, e.g., a nickel substrate ware that the formation of graphene on copper was occured without carbon diffusion to the metal bulk, i.e., it took place directly on the copper foil surface.

EP1 11

add to my program (close full abstract)

16:00 **Thermal stability of hydrogen in ZnO nanaostructures ; a kinetic monte carlo study**

Authors : M. A. Lahmer, K. Guergouri
Affiliations : Departement of physcis, university of Boumerdes,Boumerdes. Algeria Laboratoire de physique chimie des semiconducteurs, université Mentouri-Constantine, Algerie
Resume : In this work, kinetic monte carlo method was applied to study the thermal stability of hydrogen in ZnO nanowires and the effect of point defects on hydrogen thermal stability. Our simulation include differents possible events such as : interstitial hydrogen (Hi) jumps, substitutional hydrogen (HO) formation and dissociation, oxygen and zinc vacancies jumps, hydrogen-VZn complexes formation and dissociation, HO-Hi complex formation and hydrogen molecule (H2) formation and dissociation. The obtained results show that the hydrogen behaviour in ZnO nanowire is different from the thin films or the bulk cas. Our results show that the most part of interstital hydrogen is diffused out or transformed to subtitutional hydrogen rather than H2 molecule formaion which is completely different from the bulk case. We have explored in detailed manner the effect of annealing temperature, hydrogen concentration, point defects concentration and nanowire dimensions. The obtained results show that hydrogen decay and thermal stability in ZnO nanowire depend on all these

EP1 12

parameters. Finally, our results appear to be in good agreement with published data and give explanations of observed hydrogen thermal stability and decay in this nanomaterials.

add to my program (close full abstract)

16:00 **Sensitive surface states of CdS quantum dots and their application as white light emitting flourophore.**

Authors : Sesha Vempati,*1 Yelda Ertas,1,2 and Tamer Uyar.*1,2
Affiliations : 1 UNAM-National Nanotechnology Research Center, Bilkent University, Ankara, 06800, Turkey 2 Institute of Materials Science & Nanotechnology, Bilkent University, Ankara, 06800, Turkey

Resume : Rising energy crisis has motivated the researchers to produce fluorophore coating materials to convert UV light into visible/white light. Although semiconducting quantum dots (QDs) are very efficient for such application, they suffer from nonradiative recombination paths within the band gap, i.e surface defects. Quenching the defect density with inorganic materials is trivial, however, converting them into radiative channels with polymeric materials (poly (vinyl pyrrolidone), PVP) is rather intriguing about which we report an important observation forming a basis for designing future generation QD based fluorophores. The emission characteristics of CdS QDs are studied under phase change from dispersion to solid. Apparent yellow dispersion has transformed into white light emitting solid due to the conformal changes in the polymer that surrounds the QDs. In turn, these changes catalyze the emission from three specific wavelengths in the blue region of the spectrum shifting the surface defects closer to the conduction band of CdS. Previously flexible and dangling polymer chains are transformed into rigid moieties which can be attributed to a modified chemical environment. The origin of the new emission lines is interpreted via dipole interactions. We have employed TEM, optical absorption, FTIR and XPS. The proposed mechanism will be potential for designing future QDs based flurophores and explains the sensitivity of the surface states of CdS QDs.

EP1 13

add to my program (close full abstract)

16:00 **Tunable magnetic states in hexagonal boron nitride sheets**

Authors : Pascal Pochet 1 ; Eduardo Machado-Charry 1 ,2 ; Paul Boulanger 1 ; Luigi Genovese 1 and Normand Mousseau 3
Affiliations : 1 Laboratoire de simulation atomistique (L_Sim), SP2M, INAC, CEA-UJF, Grenoble, F-38054, France 2 Nanosciences Fondation, 23 rue des martyrs, 38000 Grenoble, France 3 Departement de Physique and RQMP, Universite de Montreal, C.P. 6128, Succursale Centre-Ville, Montreal, Quebec H3C 3J7, Canada

Resume : Magnetism in two dimensional atomic sheets has attracted considerable interest as its existence could allow the development of electronic and spintronic devices. The existence of magnetism is not sufficient for devices, however, as states must be addressable and modifiable through the application of an external drive. We show that defects in hexagonal boron nitride present a strong interplay between the N-N distance in the edge and the magnetic moments of the defects. By stress-induced geometry modifications, we change the ground state magnetic moment of the defects [1]. This control is made possible by the triangular shape of the defects as well as the strong spin localisation in the magnetic state. [1] E. Machado-Charry et al. Appl. Phys. Lett. 101 132405 (2012) ; http://dx.doi.org/10.1063/1.4754143

EP1 14

add to my program (close full abstract)

16:00 **Photoluminescent properties of lamellar nanocomposites obtained by Cd intercalation of GaSe and GaSe:Eu single crystals**

Authors : D. Untila*, V. Canţer**, M. Caraman*, I. Evtodiev*, L. Leontie***, L. Dmitroglo*
Affiliations : * The Laboratory of Scientific Research Photonics and Physical Metrology, Moldova State University, A. Mateevici, 60, MD-2009 Kishinev, Republic of Moldova; ** Institute of the Electronic Engineering and Nanotechnologies, Academy of Sciences of Moldova; *** Faculty of Physics, Alexandru Ioan Cuza University of Iasi, Bul. Carol I, Nr. 11, 700506 Iasi, Romania

Resume : By Cd-vapor heat treatment, at temperatures from 500 to 600°C, of GaSe and GaSe:Eu single crystals, GaSe-CdSe and GaSe:Eu-CdSe composites were obtained. The composite contains both GaSe micro- and nanolamella and CdSe microcrystallites, which presence were confirmed by XRD patterns. GaSe lamella (001) surface nanostructuration morphology is well highlighted in AFM images. In this paper photoluminescent properties of GaSe-CdSe and GaSe:Eu-CdSe composites were investigated at 78-300K temperature range. In photoluminescence (PL) spectrum of GaSe lamella, at temperatures T ≤80K, the exciton emission band is prevailing. The energy position of the n=1 exciton peak

EP1 15

is 2.11 eV. In PL spectrum of GaSe:Eu lamella, additional to GaSe characteristic particularities, Eu3+ emission bands are present, with peak localized at 2.2 eV. GaSe-CdSe composite emission spectra contains both impurity emission band (maximum at 1.74 eV) and CdSe crystallites donor-acceptor emission band (maximum at 1.79 eV). Eu3+ center emission band, with maximum at 2.17 eV amplifies its intensity by ~1.5-1.7 times and obtains a larger contour than that of GaSe:Eu. CdSe crystallites presence leads to extinction of exciton band present in GaSe:Eu crystalls.

add to my program (close full abstract)

16:00 **Structural and electronic properties of Gd doped ZnO nanowires: A first principles study**

Authors : Assa Aravindh S, Udo Schwingenschloegl , Iman S Roqan

Affiliations : Division of Physical Sciences and Engineering King Abdullah University of Science and Technology Thuwal 23955-6900 Kingdom of Saudi Arabia

Resume : ZnO is a promising semiconductor material whose electrical, magnetic and optical properties can be tuned by adding transition metal and rare earth dopants. Here we report a systematic study of non-passivated Zn48O48 nanowires grown along the wurtzite [0001] direction doped with Gd. The calculations are performed using density functional theory within the projector augmented wave method, in the framework of the generalized gradient approximation. An energy cut off of 400 eV is used to describe the plane waves included in the basis set. A Monkhorst Pack k-grid of 1x1x8 is employed for the Brillouin zone integration. The doping concentrations are 1.04% and 2.08% for one and two Gd atoms respectively. The preferred substitutional Zn site for Gd is determined by identifying all non-equivalent configurations and relaxing without geometry or spin constraints within a force tolerance of 0.01 eV/Å. We find doping at the surface to be energetically favorable and observe no significant lattice distortions. The equilibrium bond lengths as well as total and partial densities of states are calculated. All the nanowires are semiconducting and the Gd atoms exhibit atom-like magnetic moments of about 7 μB/atom. Calculations are also carried out by introducing Zn and O vacancies along with the Gd dopant. We find that Gd atoms prefer to stay away from each other, and less likely to cluster, in agreement with experimental observations.

EP1 16

add to my program (close full abstract)

16:00 **Electronic Structure and van der Waals Interactions in the Stability and Mobility of Point Defects in Semiconductors**

Authors : Wang Gao and Alexandre Tkatchenko

Affiliations : Fritz-Haber-Institut der MPG, Berlin, Germany

Resume : Point defects are abundant in all real materials, and significantly affect the electronic, optical, and magnetic properties of solids. However, our understanding of the stability and mobility of point defects in semiconductors remains incomplete, despite decades of intensive work on the subject. In the framework of density-functional theory, Perdew-Burke-Ernzerhof functional underestimates formation energies by 0.7 eV due to the electron self-interaction error, while Heyd-Scuseria-Ernzerhof (HSE) functional yields formation energies in better agreement with high-level many-body methods, but often overestimates migration barriers by up to 0.4 eV. Using HSE functional coupled with screened long-range vdW interactions (HSE+vdW) [1], we demonstrate that HSE+vdW can simultaneously and accurately describe the formation energies and migration barriers of point defects in Si. The inclusion of vdW interactions significantly changes the transition state geometries, and brings migration barrier into close agreement with experimental values for six different defects. For multiatom vacancies and point defects in heavier semiconductors, vdW interactions are found to play an increasingly larger role [2]. [1] G. X. Zhang, et al., PRL 107, 245501 (2011); A. Tkatchenko, et al., PRL 108, 236402 (2012). [2] W. Gao and A. Tkatchenko, PRL 111, 045501 (2013).

EP1 17

add to my program (close full abstract)

16:00 **Calculation of latent track parameters for SiO2/Si and Si3N4 irradiated with fast ions**

Authors : F. Komarov1, L. Vlasukova1, V. Yuvchenko1, A.Dauletbekova2, A. Akilbekov2, A. Alzhanova2

Affiliations : 1 Belarusian State University, Minsk, Belarus, 2L.N.Gumilyov Eurasian national university, Astana, Kazakhstan

Resume : Fast ion irradiation for formation of latent tracks in SiO2 is of great interest for practical applications. These tracks can be etched in appropriated etchants with the formation of nanochannels. For reproducible formation of layers with high density (up to 1011 cm-2) of nanochannels, it is very important

EP1 18

to evaluate the crucial factors of track etching. Among these factors the most important ones are: probability of formation of the latent track around each incident ion and minimum size of pore, which may occur in the place of a latent track during etchant treatment. The effects of the fast ions passage through SiO2 and some other insulators are well described using the thermal spike model. It has been believed that the etchable track results from the quenching of a zone which contains the sufficient energy for melting. We have evaluated the possibility of nanochannel formation in amorphous SiO2 and Si3N4 during the irradiation with 19F 28 MeV; 32S 47 MeV; 35Cl 43 MeV, 40Ar 38, 54 MeV for SiO2 and with 56Fe 56 MeV, 84Kr 84 MeV, 180W 180 MeV for Si3N4. For this purpose we calculated the molten region radius for ions named above using computer simulation in the frame of thermal spike model and compared it with the criterion for "etchability" of tracks from [1]. [1] A. Dallanora et al, J. Appl. Phys. 104 (2008) 024307.

add to my program (close full abstract)

16:00 **Structural damage in LiF crystals, irradiated with swift ions under normal and oblique incidence**

Authors : A. Dauletbekova1, R. Zabels2, A. Russakova1, M. Baizhumanov1, A.Akilbekov1, M. Zdorovets1

Affiliations : 1L.N. Gumilyov Eurasian national university, Astana Kazakhstan, 2Institute of solid state physics, University of Latvia, , Riga, Latvia

Resume : Formation of single defects and bulk nanostructures in LiF crystals, irradiated with swift Au and Kr ions of different energy and dose under normal and oblique incidence, were investigated by AFM, SEM, optical spectroscopy (absorption and luminescence spectra), nanoindentation and thermal annealing. In case of normal ion beam incidence the two structural zones can be distinguished: one enriched with dislocations and another exhibiting features of mosaic-type bulk nanostructure. The observed effects have a threshold nature in terms of energy loss and fluence. The samples irradiated at angles other than normal have a similar division into zones, but are oriented in the direction of the ion beam. Variation in thickness of the irradiated layer in dependence on the angle of incidence can be observed. Thermal annealing enabled to estimate the thermal stability of nanostructures and thermal diffusion of anion vacancies, which actively participate in the process of aggregation of electronic color centers.

EP1 19

add to my program (close full abstract)

16:00 **Study of the composition and structure of nano silicide phases created on the Si by ion implantation with active metals**

Authors : X.X.Boltaev (a), D.A.Tashmukhamedova(a), M.T.Narmurodov(b)

Affiliations : a) Tashkent state technical university b) Karshi state university

Resume : In this work, the low-energy (E0□10 keV) ion implantation in combination with annealing used to create nanofilms and nanocrystals on the surface of single crystal Si (111). Our studies have shown that silicide nanocrystals nanofilms and crystallize in a cubic lattice type and crystallographic orientation is identical to that for the matrix. However, the lattice constant silicides depending on the type of implanted ions varies widely: 6,54 Å for BaSi2 and 5,35 Å for CoSi2. By varying the ion energy (E0 = 0,3 - 8 keV) at an optimal dose (D = (4 - 8)·1016 cm-2) were obtained self films with thickness from 10 - 15 Å to 80 - 100 Å. At E0 ≤ 0,3 keV film structure differed little from the structure of the films obtained by solid-phase epitaxy (pores, surface irregularities) . Analysis of RHEED pictures obtained for different film thicknesses showed that when □ decrease from 100 Å to 12 - 15 Å lattice constant CoSi2 does not appreciably change . However, the results of ultraviolet photoelectron spectroscopy showed that the width of the band gap Eg increases by ~0.1 eV and significantly change the density of electronic states in the valence electrons. And in the case of formation of a nanocrystalline phase CoSi2 with size 20 - 25 nm Eg is increased by 1,2-1,5 times the relative massive film CoSi2

EP1 20

add to my program (close full abstract)

16:00 **ELECTRON-LATTICE ENERGY TRANSFER RATE FOR DIFFERENT ELECTRONIC TEMPERATURES**

Authors : S.A.Gorbunov (1), P.N.Terekhin (2), N.A.Medvedev (3), A.E.Volkov * (1,2,4)

Affiliations : (1) LPI of the Russian Academy of Sciences, Leninskij prospekt, 53,119991 Moscow, Russia, (2) NRC Kurchatov Institute, Kurchatov Sq. 1, 123182 Moscow, Russia, (3) CFEL at DESY, Notkestr. 85, 22607 Hamburg, Germany, (4) JINR, 141980 Dubna, Russia

Resume : High energy deposited into a solid during irradiation with swift heavy ions (SHI) or femtosecond laser pulses results in extreme excitation of the electron subsystem of a target, when the temperature of the electron ensemble

EP1 21

can reach several Fermi energies. Subsequent relaxation of the excited electron subsystem accompanied by energy and momentum transfer into the lattice can lead to unusual structure and phase transformations in an irradiated material. This paper presents a quantitative model of the energy transfer from the electron subsystem to the lattice. Based on the Dynamical Structure Factor (DSF) formalism, it automatically takes into account effects of different dynamic modes of coupled atomic system on the cross-sections of scattering of an electron on the lattice. In particular, this allows taking into account both the phononic and "instantaneous" limits of dynamic response of the target lattice in the electron-lattice energy transfer rate. Molecular Dynamics (MD) modeling [1] provides accurate calculations of the DSF allowing a quantitative description of the kinetics of lattice excitation. The dependence of the electron-lattice coupling factor (for Al) on the temperature of the electron ensemble is obtained. No fittings are necessary to achieve an agreement of the calculated energy transfer rates with the experimental values. [1] S.A. Gorbunov et al., Nucl.Instr.Meth.B 315 (2013) 173

add to my program (close full abstract)

16:00 **EXCITATION OF THE ELECTRON SUBSYSTEM OF SEMICONDUCTORS AFTER IMPACTS OF SWIFT HEAVY IONS**

Authors : R.A. Rymzhanov *(1), N.A. Medvedev (2), and A.E. Volkov (1,3,4)
Affiliations : (1) FLNR, JINR, Joliot-Curie 6, 141980 Dubna, Russia; (2) CFEL at DESY, Notkestr. 85, 22607 Hamburg, Germany; (3) NRC Kurchatov Institute, Kurchatov Sq. 1, 123182 Moscow, Russia; (4) LPI of the Russian Academy of Sciences, Leninskij prospekt, 53,119991 Moscow, Russia

Resume : Swift heavy ions (SHI, E>1 MeV/nucl) lose the largest part of their energy (>95%) for excitation of the electron subsystem of solid targets. Fast relaxation of this excitation can stimulate unusual structure and phase transformations in irradiated materials. The kinetics of such modification in the nanometric vicinity of the SHI trajectory depends strongly on the parameters of the excited ensemble of electrons. The developed Monte-Carlo [1] model is used to simulate event-by-event excitation of the electron subsystem of semiconductors by a penetrating SHI. The cross sections of interaction of an ion with the electron subsystem of a target are calculated via the complex dielectric function (CDF) formalism. The formalism accounts for all the collective modes appearing in the electron ensemble. The model predicts the electron inelastic mean free paths in a very good agreement with the NIST database, and SHI energy losses in agreement with SRIM and CasP codes. The temporal evolutions of the radial distributions of valence holes, delocalized electrons and their energy densities in SHI tracks in semiconductors are determined. The collective modes of electronic excitations appear in a form of the second front of spatial propagation of the excess electronic energy. It spreads outwards the track core following after the primary front of high-energy delta-electrons. [1] N.A. Medvedev , R.A. Rymzhanov, A.E. Volkov, Nucl. Instr. Meth. B 315 (2013) 85

EP1 22

add to my program (close full abstract)

16:00 **Correlation between electrical properties and structure of single GaAs nanowires grown by MBE onto silicon substrate**

Authors : Bussone G. (1,2), Schaefer-Eberwein H. (3), Dimakis E. (4), Biermanns A. (2), Carbone G. (1), Geelhaar L. (5), Haring Bolivar P. (3), Schuelli T. U. (1) and Pietsch U. (2)
Affiliations : (1) European Synchrotron Radiation Facility, Grenoble, France; (2) Festkoerperphysik, Universitaet Siegen, Germany; (3) Hochfrequenztechnik & Quantenelektronik, Universitaet Siegen, Germany; (4) Helmholtz-Zentrum Dresden-Rossendorf, Dresden, German; (5) Paul Drude Institute, Berlin, Germany

Resume : Electronics, photonics and optoelectronics require more and more the use of semiconductor nanowires (NWs). Our objective is to show how the properties of GaAs nanowires, e.g. the electrical conductivity and mobility, are influenced by structural parameters such as crystal phase purity or lattice strain. Several NWs in their free standing position on the substrate have been electrically measured, by contact through micromanipulators in a Focused Ion Beam system. The analysis of the current-voltage curves via thermionic emission theory, allowed to quantify the difference in the resistances of the measured NWs. The mobility was extracted as well through a Space Charge Limited Current approach. Different trends were observed for different objects. Subsequently, the origin of this difference, in particular the phase composition and the presence of defects, has been studied using X-ray diffraction with a nano-focused synchrotron beam at beamline ID01 at the ESRF. All the NWs consist of zinc-blende (ZB) segments separated by rotational twin-planes. The size of perfectly stacked ZB units differs among the measured NWs, and has

EP1 23

been estimated through the analysis of 3D reciprocal space maps. Based on those data, we suggest that the differences of the measured I-V characteristics can be correlated to the units boundaries within the NWs, acting as scattering centres for the current flow.

add to my program (close full abstract)

16:00 **Fluorescent nanodiamonds by low energy irradiation**

Authors : Andrea Mazzocut, Paolo Coppo, Alan Reynolds, Lorna Anguilano, Ashley Howkins
Affiliations : Andrea Mazzocut, The Wolfson Centre, Brunel University; Paolo Coppo, The Wolfson Centre, Brunel University; Alan Reynolds, Experimental Techniques Centre, Brunel University; Lorna Anguilano, Experimental Techniques Centre, Brunel University; Ashley Howkins, Experimental Techniques Centre, Brunel University;

Resume : The use of nanodiamonds as luminescent biological probes is particularly intriguing, in view of their lack of reactivity and toxicity in vitro and in vivo.(1) Nitrogen-Vacancy colour centres in diamond are commonly produced by irradiation of nitrogen rich diamond (type Ib) with high energy protons, electron or ion beams, followed by annealing at 600-800?C.(2?4) Hereafter we investigated the use of a low energy (200KeV) TEM electron beam to generate the displacement of carbon atoms in commercially available nanodiamonds. The morphology, structure and optical properties of the samples were studied using a Scanning Transmission Electron Microscope coupled with a Gatan cathodoluminescence detector. XRD powder diffraction and a thorough investigation by steady state optical spectroscopy reveal new insights in this promising material. In addition we explore the possibility to induce fluorescence in nanodiamonds (FNDs) by gamma irradiation with a 60Co source, in all similar to those used in hospital environment for the treatment of cancer, in order to provide a more practical protocol to produce optically active nanodiamonds. References: 1. Wu, T.-J. et al. Nat. Nanotechnol. 8, 682?689 (2013). 2. Mochalin, V. N. et al. Y. Nat. Nanotechnol. 7, 11?23 (2012). 3. Boudou, J.-P. et al. Diam. Relat. Mater. 37, 80?86 (2013). 4. Chang, Y.-R. et al. Nat. Nanotechnol. 3, 284?288 (2008).

EP1 24

add to my program (close full abstract)

16:00 **FEATURES OF RADIATION DEFECTS FORMATION IN QUANTUM DOTS EMBEDDED IN SOLID MATRIX**

Authors : B.L.Oksengendler1), S.E.Maksimov1), O.B.Ismailova1), F.G.Djurabekova2)
Affiliations : 1)Institute of ion-plasma and laser technology, Uzbek Academy of Sciences, Tashkent, Uzbekistan; 2)Helsinki Institute of Physics and Department of Physics, University of Helsinki, Helsinki, Finland

Resume : The modification of basic radiation physics effects (elastic defect generation and amorphization) in quantum dots embedded in solid matrix, is theoretically considered. The diffusion model of formation of defects with U-negative properties is introduced, and the effect of the "quantum dot-matrix" border on the displacement energy is studied. The basic reasons why the critical dose for amorphization of quantum dots is different from the same for the bulk crystal it discussed based of percolation ideas. We show that there are regions in the quantum dot core where the probability of defect formation and hence amorphization is negligible, which explains the radiation stability of nanostructure. This phenomenon is related to radiation enhanced diffusion of interstitials proceeding through the Oksengendler-Bourgoin mechanism (1972). Some features of radiation physics of nanoobjects taking into account; the combination of elastic and athermal electron-enhanced defect processes are discussed.

EP1 25

add to my program (close full abstract)

16:00 **Computer modeling ofradiative processesin nanoparticles**

Authors : V.V. Uglov1, G.E. Remnev2, N.T. Kvasov1, I.V. Safronov1
Affiliations : 1Belarusian State University,Minsk, Belarus; 2Tomsk PolytechnicUniversity, Tomsk,Russia

Resume : In this paper, on the basis of the electronicSe and nuclearSn cross sections braking proposed space-time description of the dynamics of motion of the accelerated ions in the medium.Received the analytical expressions for the ion velocityv(t) and displacementl(t) at an arbitrary time in the material volume. Comparison of the results of the theory, experiment and computer simulation shows their satisfactory agreement. Proposed the structure of the threshold energy of the defectEd. Also dynamical processes occurring in the nano-dimensional metal object during penetration of high-energy ions are studied in detail. It is shown that the elastic and thermoelastic response of the lattice to radiation exposure forms power factors that significantly affect on the evolution of defect-impurity system resulting in a decrease of a number of structure

EP1 26

defects. A quantitative estimation of spatial distribution of defects resulting in their exit on the surface was made. Such self-organization of nanoparticles under ionizing radiation is the basis for the creation of nanostructured radiation-resistant materials capable to withstand a long-term intense radiation loads.

add to my program (close full abstract)

16:00 **Stress effects on the formation of He-plates into Si**

Authors : M. Vallet1, J. F. Barbot1, A. Declémy1, S. Reboh2, M. F. Beaufort1
Affiliations : 1Institut Pprime, UPR 3346 CNRS - Université de Poitiers - ENSMA, Department of Material Sciences, BP30179, 86962 Futuroscope Chasseneuil, France 2CEA -LETI, Minatec Campus, 17 rue des Martyrs, 38054 Grenoble, France

Resume : Helium implantation in Si is known to form 'He-plates'. These defects are similar to H-platelets regarding to their general shape, but 10 to 20 times greater. Consequently, they are potential competitors to 'H-platelets' as precursors for the Smart-Cut® process. However, few studies have been focused on the characterization of these two dimensional defects. In this work, we present a study on the effect of the Si crystalline orientation on the implantation-induced strain/stress and on the formation of He-plates by combining high-resolution X-ray scattering and transmission electron microscopy. The highest strains are obtained onto (001)-oriented implanted substrates regardless of the fluence and of the channeling effects. Upon specific thermal annealing, the formation of He-plates was found to occur only in the {001} habit planes regardless of the orientation of the substrate. Moreover the distribution of He-plates in the {001} variants was found to be strongly dependent on the angle of the habit plane with the surface and on the intensity of the implantation-induced strain/stress. The nucleation and growth of He-plates are thus discussed with regard to the implantation-induced stress.

EP1 27

add to my program (close full abstract)

16:00 **Origin of p-typeness in N-doped Zn-deficient ZnO nanoparticles**

Authors : A. Renaud*, B. Chavillon*, X. Rocquefelte*, E. Faulques*, P. Deniard*, M. Boujtita§, Y. Pellegrin§, E. Blart§, F. Odobel§, F. Cheviré!, F. Tessier!, L. Cario*, S. Jobic*
Affiliations : * Institut des Matériaux Jean Rouxel (IMN), Université de Nantes, CNRS, 2 rue de la Houssinière, BP3229, 44322 Nantes cedex 03, France § CEISAM, Université de Nantes, CNRS, 2 rue de la Houssinière, 44322 Nantes cedex 03, France ! UMR CNRS 6226 "Sciences Chimiques de Rennes", équipe Verres et Céramiques, Université de Rennes 1, 35042 Rennes cedex, France

Resume : Nowadays zinc oxide is regarded as a very promising material deemed to compete in the near future with GaN for optoelectronic applications. Unfortunately, the durability of p-type ZnO is yet a blockage, that singularly slows down the launching of ZnO based devices. In that context, we embarked recently on the synthesis as powdered samples of a p-type zinc oxide material with the wurtzite structure by ammonolysis at low temperature (e.g. 250 °C) of zinc peroxide (1). The nature of the charge carriers was identified without ambiguity by photo-electrochemistry, complex impedance spectroscopy and transient spectroscopy. P-typeness in ZnO would result from an extraordinary huge amount of Zn vacancies (up to 20%) coupled with the insertion of nitrogen within nanoscale spherical particles. Remarkably, the p-type conductivity remains stable for periods longer than two years and half in ambient conditions. Here the chemical route to produce p-type ZnO, as well the optical and electrical properties of the synthesized material, will be described. In addition, the origin of the strong Zn deficit, which plays a major role in the establishment of p-typeness, will be also tackled. This discovery could open the door to the achievement of n-ZnO/p-ZnO:N colorless homo-junctions. (1) B. Chavillon et al., J. Am. Chem. Soc., 2012, 134, 464

EP1 28

add to my program (close full abstract)

16:00 **Confocal micro-Raman study of defects induced by laser irradiation of single-layer graphene**

Authors : A.S. Nikolenko(1), V.V. Strelchuk(1), Yu.Yu. Stubrov(1), V.O. Gubanov(2), M.M. Biliy(2), L.A. Bulavin(2) and O.E. Belyaev(1)
Affiliations : (1) V. Lashkaryov Institute of Semiconductor Physics National Academy of Sciences of Ukraine, 45 Nauky pr., 03028 Kyiv, Ukraine (2) Kyiv National Taras Shevchenko University, Department of Physics, 64 Volodymyrs'ka str., 01601Kyiv, Ukraine

Resume : In the present work we used confocal micro-Raman spectroscopy as sensitive tool to study the nature of defects in single-layer graphene induced by laser irradiation at varied laser power densities and dozes. The minimal power threshold of the exciting radiation of the structural defects generation is found. Appearance and drastic intensity increase of zone-edge D-like modes caused by introduction of structural defects in the graphene layer were observed in the

EP1 29

Raman spectra at higher powers of excitation. Time-dependent evolution of Raman spectra is studied. From the analysis of intensities of defective D and D' bands relative to G-band, the structural defects generated under laser irradiation of graphene with power density higher than threshold are shown to be mainly vacancy-type defects [1]. The surface density of structural defects is estimated from the intensity ratio of D and G bands. Stokes and anti-Stokes components of the Raman spectra are analyzed to estimate the lattice temperature of graphene on the power density of exciting radiation. 1. Axel Eckmann et al., Probing the nature of defects in graphene by Raman spectroscopy. Nano Lett. 12, 3925-3930 (2012).

add to my program (close full abstract)

16:00 **Contribution of iron silicide nanoparticles to the magnetic behavior of annealed Fe implanted 6H-SiC**

Authors : M.L Diallo (a), A. Fnidiki (a), A. Debelle (b), L. Thomé (b), M. Viret (c), M. Drouet (d), D. Eyidi (d), A. Declémy (d)*
Affiliations : (a) Groupe de Physique des Matériaux (GPM) UMR 6634 CNRS, UFR Sciences et Techniques, Avenue de l'Université 76801 Saint Etienne du Rouvray, France (b) Centre de Spectrométrie Nucléaire et Spectrométrie de Masse (CSNSM) UMR 8609 CNRS, Université Paris-Sud, Bât 104 91405 Orsay Campus, France (c) Service de Physique de l'Etat Condensé (DSN/IRAMIS/SPEC), URA 2464 CNRS, Bât. 772, Orme des Merisiers, CEA Saclay 91191 Gif sur Yvette, France d Institut PPRIME, UPR 3346 CNRS, Université de Poitiers, ENSMA, SP2MI, téléport 2, 11 Bvd M. et P. Curie 86962 Futuroscope Chasseneuil France * corresponding author : Tel : +33 (0)5 49 49 67 07 e-mail address : alain.declemy@univ-poitiers.fr

Resume : Ion implantation of 3d transition metals in wide band gap semiconductors is a promising route to get Diluted Magnetic Semiconductors (DMS) with high critical temperature TC. Fe-implanted SiC (a wide band gap semiconductor with low spin-orbit coupling with excellent transport properties) is now recognized as a good DMS candidate. Moreover, ion implantation is a standard route of doping in microelectronics industry and the ability for 57Fe implantation allows using Conversion Electron Mössbauer Spectroscopy (CEMS). Thus Fe-implanted SiC is an interesting system in the DMS field although ion implantation induces strong microstructural defects needing post-implantation treatments for recovery. These post-implantation treatments often induce the formation of parasitic magnetic secondary phases. Thus, despite the now recognized magnetic properties of Fe-implanted SiC, a major controversy exists regarding their origin (Fe3Si-like nanoparticles, bound magnetic polarons related to randomly distributed Fe at the Si sites in the lattice, …). In parallel, many other techniques were used to incorporate Fe in Si and SiC (hot-pressed, mechanical alloying, MBE, …) leading to a wide variety of Fe-Si nanostructures of interest for spintronics devices (nanoparticles, nanodots, thin films, …). In this work, we show how Fe-implanted SiC studied with RBS/C, SQUID and CEMS can be better understood from the results of these recent studies.

EP1 30

add to my program (close full abstract)

16:00 **Evaluation of the influence of temperature on the photoluminescence of Mg-doped GaAs nanowires and films**

Authors : B. P. Falcão(1), J. P. Leitão(1), M. R. Correia(1), M. P. Leitão(2), M. V. B. Moreira(3), A. G. de Oliveira(3), F. M. Matinaga(3), J. C. González(3)
Affiliations : (1) Departamento de Física and I3N, Universidade de Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal (2) Departamento de Física and CICECO, Universidade de Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal (3) Departamento de Física, Universidade Federal de Minas Gerais, 30123-970 Belo Horizonte, Minas Gerais, Brazil

Resume : GaAs nanowires are promising building blocks for third-generation solar cells as they bring potential benefits over traditional wafer or thin-film based technologies, related mainly to cost, stronger light absorption, and charge separation mechanisms. To realize the full potential of such devices, the electronic doping of the nanowires and their optical and electrical transport properties must be controlled and thoroughly understood. Because GaAs nanowires can simultaneously crystallize in the wurtzite and zincblende structures, which influence strongly its electronic level structure, the investigation of these polytypic nanowires with different doping profiles is very important in view of future devices. Therefore, in this work, we present a report on the photoluminescence of Mg-doped GaAs nanowires and thin-films with different levels of doping. In the case of the thin-films, it is only observed a single radiative transition related to Mg acceptors that redshifts with increase concentration, due to the bandgap energy narrowing effect. The photoluminescence from individual nanowires and from a bunch of several

EP1 31

hundreds of nanowires is analyzed over a wide temperature range, and is compared to that of the thin-films. It is found that in the nanowires the radiative transitions are critically influenced by the staggered type II band alignment, due to the existence of polytypic regions along the nanowires, and seems to be independent of the Mg concentration.

add to my program (close full abstract)

16:00 **Controllable synthesis and catalytic performance of rich defected PdAu nanodentrites catalysts for selective hydrogenation**

Authors : Chao Ma, Dianqing Li, Junting Feng*
Affiliations : State Key Laboratory of Chemical Resource Engineering, Beijing University of Chemical Technology

Resume : Organizing nanocrystals into 1D, 2D, or 3D superstructures with defined morphologies opens up the possibilities of fabricating new materials. Nanodendrites are a special kind 3D supersructure assembled by many small nanoparticles, which usually demonstrate some intrinsic features, such as rough surface, high internal porosity, complex morphologies and especially, high densities of crystalline defects. Recently, Pd, Pt and Pt-on-Pd nanodendrites as novel catalysts have been controllable synthesized. However, detailed studies about the relationship between catalytic performance and the structure, especially how complex morphology and abundant defects work in catalysis are still needed. In this work, we report the research on the fabrication of superstructured PdAu nanodendrites as a novel heterogeneous catalyst for selective hydrogenation of acetylene. The obtained PdAu nanodentrites were found to be alloyed, typically dentritic shaped and rich defected. A disoriented self-assembling mechanism is proposed according to the observation of growth process. PdAu nanodentrites were then sol-immobilized onto Mg-Al mixed metal oxide (MMO) support. As expected, the dentritic PdAu/MgAl-MMO catalyst exhibits an enhanced performance including activity, selectivity and lifetime due to its special structure, particularly abundant defects and cooperative interaction between building units.

EP1 32

add to my program (close full abstract)

16:00 **Effect of boron ion doping on dislocation-related luminescence in silicon**

Authors : D. Tetelbaum, A. Mikhaylov, A. Belov, D. Korolev, A. Shushunov, A. Bobrov, D. Pavlov
Affiliations : Lobachevsky State University of Nizhni Novgorod, Nizhni Novgorod, Russia

Resume : A promising trend in the development of modern optoelectronics is the search for the ways of creating the effective emitters in the wavelength range of 1,5-1,6 um. Fabrication of such emitters on the basis of silicon fits the requirement of compatibility with traditional microelectronic technologies. One of the approaches to fabricate silicon-based light emitters is based on the use of dislocation-related D1 line luminescence in silicon. The improvement of the dislocation-related luminescence is an important challenge from practical viewpoint. Recently, we have established that additional implantation of boron into silicon, in which the D1 luminescence was achieved by the self-ion implantation and annealing in oxidizing atmosphere, leads to the increase in luminescence intensity [Semiconductors 48, 199 (2014)]. This effect depends on the boron ion dose and is believed to be caused by the change in composition of the dislocation-related defect-impurity atmospheres. In this work, the effect of boron doping is studied in detail over a wide ranges of doses and annealing temperatures and analyzed taking into account the XTEM data and the depth-profiling data for the distribution of light-emitting centers obtained by step-by-step etching. The results are important for understanding the D1 line nature and can be used in the technology of optical and optoelectronic integrated circuits. Support in the frame of RFBR project (12-0200980) is gratefully acknowledged.

EP1 33

add to my program (close full abstract)

16:00 **Electronic Properties of Implanted Iodine Confined in Nanocages of C12A7**

Authors : Eduard Feldbach, Annika Pille, Eliko T?ldsepp, Raul Laasner, Sergey Omelkov, Marco Kirm
Affiliations : Institute of Physics, University of Tartu, Estonia

Resume : 12CaO?7Al2O3 (C12A7) is a highly radiation resistant compound due to its nanoporous crystal structure, which allows its modification by ion implantation. C12A7 is composed of a positively charged framework of nanocages, which can be filled with various negative ions. The aim of this work was to investigate the electronic properties of confined iodine ions using luminescence spectroscopy and theoretical DFT calculations. Iodine implantation at 300 keV, using fluences of 1015 and 1016 cm-2, at a target temperature of 600 ?C was carried out at the Ion Technology Centre in Uppsala. According to the measured RBS spectra the maximum of the concentration profile is at ~120

EP1 34

nm below the surface. Raman spectroscopy of the implanted samples has shown no evidence of the crystal lattice destruction, despite of the high fluence applied. Thermostimulated luminescence from the thin implanted layer, which provides information on defect states in solids, supports the result of Raman spectroscopy. The most significant implantation effects are detected in time-resolved cathodoluminescence spectra - two additional bands at ~2.4 eV and ~2.8 eV with decay times in microsecond range. According to the DFT calculations the confined iodine is negatively charged and its ground state is located ~0.5 eV above the top of the valence band. Possible interpretation of revealed luminescence bands as iodine related charge transfer transitions from triplet and singlet states will be discussed.

add to my program (close full abstract)

16:00 **Induced defects on graphene single layers by nanoelectrical discharges in room conditions**

Authors : Carmen Coya1, Miguel García-Vélez1, Carmen Munuera2, Alicia de Andrés2, Angel Luis Álvarez1
Affiliations : 1-Escuela Superior de Ciencias Experimentales y Tecnología (ESCET), Universidad Rey Juan Carlos, 28933 Madrid, Spain; 2-Instituto de Ciencia de Materiales de Madrid, CSIC, 28049 Madrid.

Resume : Electric arc lithography performed at low continuous voltages has been recently proven as a successful dry patterning technique for thin films of different conductive materials in room conditions [1]. In this work, we show an application of this procedure to graphene single layers on SiO2(90 nm) / Si-p+ substrates, proving an efficient large area and cost effective patterning procedure for electronic device development, which prevents photoresists and insolation steps.Resolution of this technique (which is currently 10 um, as determined by the used probe diameter), and the influence of critical parameters such as operating voltage (in the range 10 – 60 V) and probe speed, are discussed. We observe that Interesting defects, such as graphene oxide or nanographene domains may be induced during the patterning process. We discuss here, by means of Raman spectroscopy and AFM studies, including both topographic and electrostatic force measurements, the relation between the observed features and the operating conditions. Also, a depth study of the electrical discharge generation at submicron scale, which allows optimizing the procedure, is discussed. [1])J. Jimenez-Trillo,A. L. Alvarez,C. Coya,E. Céspedes,A. Espinosa, "The use of arc-erosion as a patterning technique for transparent conductive materials", Thin Solid Films, 520 (4), 1318-1322 (2011).

EP1 35

add to my program (close full abstract)

16:00 **Cristalline structure and optical properties of GaS-CdS nanocomposite**

Authors : Iuliana Caraman 1, Elmira Vatavu 2, Liviu Leontie 3, Marius Stamate 1
Affiliations : 1. Engineering Department, Vasile Alecsandri University of Bacau, 157 Calea Marasesti, Bacau, 600115 ROMANIA; 2 Faculty of Physics and Engineering, Moldova State University, 60 A. Mateevici str., Chisinau, MD-2009, MOLDOVA; 3 Faculty of Physics, Alexandru Ioan Cuza University of Iasi, 11 Carol I Blvd, Iasi, 700506, ROMANIA.

Resume : CdS-GaS nanocomposite has been obtained by thermal annealing of the single crystalline GaS plates in Cd vapors. The partial concentration of the nanocomposite's components can be changed by temperature and duration of their annealing. Cd vapors interact with sulfur from the atomic planes of the S-Ga-Ga-S packings resulting in formation of micro- and nano-cristallites of CdS. Photoluminescence (PL), XRD and AFM analyses have been carried out. CdS crystallites have pyramidal shape oriented predominantly along the C6 axis of GaS, both materials exhibiting a perfect crystalline structure. The edge of the absorption band of GaS plates is formed by indirect optical transitions, the bandgap being 2.52 eV at 80K. In the same spectral region, the fundamental absorption edge determined by direct transitions in CdS crystallites is situated. The absorption coefficient increases by 2 orders of magnitude as the photon's energy increases from 2.55 to 2.60 eV. The intercalation of the GaS crystals with Cd does not induce changes in the general structure of the PL spectrum of the primary (GaS) crystal but an increase of the blue band PL (at 2.43 eV) is observed. This band dominates the PL spectrum of the obtained composite at the annealing temperatures up to 600C and annealing time of 6 hours. An amplification of the PL in the A excitonic region of CdS takes place.

EP1 36

add to my program (close full abstract)

16:00 **Scale effects induced by imperfect interfaces in nanomaterials transport properties**

Authors : F. Pavanello(1), F. Manca(1), P-L. Palla(1,2), E. Lampin(1), F. Cleri(1,2), S. Giordano(1,3)

EP1 37

Affiliations : (1)Université des Sciences et Technologies de Lille, Cité Scientifique 59655 Villeneuve d'Ascq Cédex, France; (2)Institut d'Electronique de Microélectronique et de Nanotechnologie, Avenue Poincare, CS 60069, 59652 Villeneuve d'Ascq, France; (3)LICS, IEMN, UMR CNRS 8520, PRES Lille Nord de France, ECLille, Avenue Poincare, CS 60069, 59652 Villeneuve d'Ascq, France

Resume : One of the crucial factors governing the physical properties of nanomaterials is the complex behavior of the interfaces[1]. While at the macroscopic level their specific role is usually neglected, in nanostructured systems the properties of the contact between phases have to be carefully defined. The existing theoretical models of real interfaces can be ascribed to two main schemes, the low and the high conducting interfaces. In this work we present a generalized zero-thickness model[2][3] able to combine both the normal resistance of the low conducting scheme and the tangential conductance of the high conducting approach. The generality and the richness of such a model allows us to reproduce and to predict the effective electric, thermal, magnetic or dielectric behavior of imperfect and structured interfaces, which can be found in heterogeneous nanomaterials of technological interest[4]. As a first meaningful application we have applied the model to the analysis of the scale-effects in transport properties of nanocomposites. Moreover, such a model can be applied to the investigation of the thermal behavior of interfaces[5] which turn out to be crucial for heat dissipation in nanodevices. [1] P. L. Palla et al., Phys. Rev. B 80, 054105 (2009) [2] F. Pavanello et al., J. Appl. Phys. 112, 084306 (2012) [3] F. Pavanello et al., J. Appl. Phys. 113, 154310 (2013) [4] S. Yu et al., J. Appl. Phys. 110, 124302 (2011) [5] E. Lampin et al., Appl. Phys. Lett. 100, 131906 (2012)

add to my program (close full abstract)

16:00 **Preparation and characterization of doped and undoped nanoporous carbon for heavy metal removal from aqueous solution**

Authors : Imed Ghiloufi1,2; Lassaad El Mir1,2
Affiliations : 1- Al Imam Mohammad Ibn Saud Islamic University (IMSIU), College of Sciences, Riyadh, Saudi Arabia. 2- Laboratory of Physics of Materials and Nanomaterials Applied at Environment (LaPhyMNE), Faculty of Sciences, Gabes University, Tunisia.

Resume : Nanoporous carbons (NPCs), based on organic xerogel compounds, were synthesized by sol–gel method from pyrogallol and formaldehyde (PF) mixtures in water using perchloric acid as catalyst. These NPCs were prepared at different pyrolysis temperatures 650 ºC (PF-650), 700 ºC (PF-700) and 1000 ºC (PF-1000) and they are doped by different oxides CuO (PF-CuO) and NiO (PF-NiO). The obtained NPCs were characterized by scanning electron microscopy, transmission electron microscopy, X-ray diffraction and nitrogen porosimetry. These nanomaterials were used to study the effect of pyrolysis temperatures of NPCs on the uptake of Cr, Ni, Cd and Co from aqueous solution. In this work the effect of the presence of CuO and NiO in the NPCs on the adsorption of heavy metals from aqueous solution has been studied.

EP1 38

add to my program (close full abstract)

16:00 **Irradiation effects on the optical properties of silicon nanocrystals**

Authors : Benjamin Bruhn, Sidoeri Dekker, Bart van Dam, Tom Gregorkiewicz, Katerina Dohnalova
Affiliations : Van der Waals-Zeeman Institute, University of Amsterdam, 1098XH Amsterdam, The Netherlands

Resume : Highly energetic irradiation, be it electromagnetic waves or particles (e.g. electrons), can induce defects in luminescent materials, thereby introducing new efficient radiative and/or non-radiative pathways for exciton recombination. This is not only valid for bulk materials, but also low dimensional nanostructures. In porous silicon, for example, certain photoluminescence emission bands can be enhanced or quenched. How exactly the irradiation alters the optical properties of single nanocrystals, though, is unclear. In this study we investigate how emission properties of powders of porous silicon change upon exposure to an electron beam. We examine the two dominant emission bands: The F-band, that is observed in the blue and exhibits short PL lifetime (ns), and the red S-band with µs decays. Our study is performed on single emitter and ensemble level, and the results cross-correlated. . Special focus lies on the question whether light emission is quenched completely or gradually reduced, or whether it could even be enhanced.

EP1 39

add to my program (close full abstract)

16:00 **High Pressure Raman Study of Predominant Wurtzite InAs Nanowires**

Authors : Achintya Singha, Dipanwita Majumdar, Abhisek Basu, Goutam Dev Mukherjee, Daniele Ercolani, Lucia Sorba
Affiliations : Department of Physics, Bose Institute, 93/1, Acharya Prafulla Chandra

EP1 40

Road, Kolkata 700009, India; Department of Physics, Bose Institute, 93/1, Acharya Prafulla Chandra Road, Kolkata 700009, India; Department of Physical Sciences, IISER Kolkata 741252, India; Department of Physical Sciences, IISER Kolkata 741252, India; NEST-Istituto Nanoscienze-CNR and Scuola Normale Superiore, Piazza S. Silvestro 12, I-56127 Pisa, Italy; NEST-Istituto Nanoscienze-CNR and Scuola Normale Superiore, Piazza S. Silvestro 12, I-56127 Pisa, Italy

Resume : One dimensional semiconductor nanowires (NWs) of diameter in the range of few to several tens of nanometer find their potential as building blocks for the next generation of miniaturized electronic and optoelectronic devices.1-3Among them, InAs NWs are of particular interest for excellent electron transport property due to their small effective mass. As a thermodynamic parameter external pressure plays an important role to tune electronic and structural properties of a system. In low dimensional systems, number of factors like defects, confinement, and surface tension are important to understand the pressure induced electronic and structural transformations. Therefore, the studies of semiconductor NWs under pressure are particularly important for their technological applications. High pressure Raman scattering is a powerful technique for extracting information regarding vibrational properties and phase diagrams of both bulk and nanostructures.4-6 Here, we have investigated the hydrostatic pressure response (up to 58 GPa) of TO, LO and other optical modes of predominant wurtzite InAs NWs in a diamond anvil cell.7All the observed phonon frequencies increase linearly while the LO-TO splitting decreases with pressure. 7 The recorded Raman modes have been used to determine the mode Grüneisen parameters and also the value of Born's transverse effective charge ( ).7 The calculated exhibits a linear reduction with increasing pressure indicating an increase in covalency of NWs under compression.7A resonant Raman scattering is observed around 1.64 GPa due to increase of E1 band gap with applying pressure. A signature of structural phase transformation has been observed above pressure 10.87 GPa.7 We propose this transformation may be from wurtzite to rock salt phase although further experimental and theoretical confirmations are needed. References 1. W. Lu and C. M. Lieber, Nature Materials , 2007,6, 84. 2. S. W. Chung, J. Y. Yu, and J. R. Heath, Appl. Phys. Lett., 2000, 76, 2068. 3. P. J. Pauzauskie and P. Yang, Materials Today, 2006, 9, 36. 4. I. Zardo, S. Yazji, C. Marini, E. Uccelli, A. F. Morral, G. Abstreiter, and P. Postorino, ACS NANO, 2012, 6, 3284. 5. R. Trommer, E. Anastassakis, and M. Cardona, in Light Scattering in Solids, edited by M. Balkanski, R. C. C. Leite, and S. P. S. Porto, (Flammarion, Paris, 1976), p. 396. 6. D. Olego and M. Cardona Phys. Rev. B, 1982, 25, 1151. 7. D. Majumdar, A. Basu, G. D. Mukherjee, D. Ercolani, L. Sorba, A. Singha, arXiv:1401.2318[cond mat.mes-hall].

add to my program (close full abstract)

16:00 **UV-assisted room temperature gas sensing of GaN-core/ZnO shell nanowires**

Authors : Sunghoon Park, Hyunsung Ko, Jihwan Jung and Chongmu Lee
Affiliations : Department of Materials Science and Engineering, Inha University, Yonghyun-dong, Nam-gu, Incheon 402 - 751, Republic of Korea

Resume : GaN is highly sensitive to low concentrations of H2 in ambient air and are almost insensitive to most other common gases. However, it still remains a challenge to enhance their sensing performance and detection limit. This study examined the H2 gas sensing properties of GaN nanowires encapsulated with ZnO. GaN-core/ZnO-shell nanowires were fabricated by a two-step process comprising the thermal evaporation of GaN powders and atomic layer deposition of ZnO. The core-shell nanowires ranged from 80 to 120 nm in diameter and from a few tens to a few hundreds of micrometers in length with a mean shell layer thickness of ~8 nm. Multiple networked pristine GaN nanowire and GaN-core/ZnO-shell nanowire sensors showed the responses of 120 - 147% and 179 - 389%, respectively, to 500 - 2,500 ppm H2 at room temperature under UV (254 nm) illumination. The underlying mechanism of the enhanced response of GaN nanowire to H2 gas by ZnO encapsulation and UV irradiation is discussed.

EP1 41

add to my program (close full abstract)

16:00 **Lattice parameter of graphene on Ir(111) vs temperature : strain, commensurability and defects**

Authors : F. Jean,1 N. Blanc,1 T. Zhou,2 R. Felici,3 J. Coraux,1 G. Renaud 2
Affiliations : 1 Institut Néel (CNRS), Grenoble, France; 2 CEA INAC, Grenoble, France; 3 European Synchrotron Radiation Facility, Grenoble, France

EP1 42

Resume : The exceptional properties of graphene can be modified and hopefully tailored by strains. The origins of strain in epitaxial graphene are diverse: tendency to commensurability with the substrate, defects, and mismatch of thermal expansion coefficients. Isolated graphene was predicted to have a negative thermal expansion coefficient below room temperature. This could

account for recent observations made on exfoliated graphene on SiO2. Whether this effect should be expected also in epitaxial graphene remains unknown. We prepared high quality graphene on Ir(111) by chemical vapor deposition. The structural properties of the system were investigated in situ, as a function of sample temperature, in the ultra-high vacuum chamber where the samples were prepared, using synchrotron X-ray surface diffraction. At variance with the expectation for free-standing graphene, epitaxial graphene on Ir has a positive thermal expansion coefficient between 10 and 300 K that follows the expansion of iridium. Hence, despite the very high graphene stiffness, its weak but non-zero interaction with Ir is sufficient to strain it. Moreover, different commensurate states between the graphene and the substrate were observed during and after the growth as a function of temperature.

add to my program (close full abstract)

16:00 **Dielectric characterization of amorphous and disordered materials from temperature behavior of ac response**

Authors : Orest Fl'unt
Affiliations : Faculty of Electronics, Ivan Franko National University of Lviv, Ukraine

Resume : Low-frequency dielectric and impedance spectroscopy is powerful characterization method of amorphous and disordered materials, partly amorphous chalcogenide and pnictide thin films. The widely known models of low-frequency ac conductivity and dielectric loss explains fractional power shape of frequency spectra via wide distribution of localized levels in the forbidden gaps or by random distribution of localized centers. But expected temperature dependencies of ac response and their parameters strongly depend on the model, however a universality of temperature behavior of ac response of amorphous materials is often observed. The proposed model of frequency and temperature dependencies of ac response of amorphous and disordered materials consider the media as system of groups of elementary dipoles (charge carriers in double potential wells), polarization characteristics of which significantly differ from elementary ones. Relaxation time of dipole's formations may spread in wide temporal or frequency range, even if elementary dipoles are not temporally distributed. The model simultaneously explains fractional power shape of spectra and exponential temperature dependence of dielectric loss according to inverse Arrhenius law exp(T/T_0). According to model frequency exponent n linear decreases with increasing temperature. The frequency dependence of parameter T_0 has been explained and their correlation with other properties of amorphous materials has been analyzed.

EP1 43

add to my program (close full abstract)

16:00 **Surface composition, stoichiometry and photoluminescence properties of metal oxide nanoparticles**

Authors : Amir. R. Gheisi(1), Chris Neygandhi(1), Andreas Sternig(1), Daniel Thomele (2), Esther Carrasco Burgos(3), Hubertus Marbach(3), Oliver Diwald(2)
Affiliations : (1)Institute of Particle Technology, Friedrich-Alexander University Erlangen -Nürnberg, Erlangen, Germany; (2)Department of Materials Science & Physics, Paris-Lodron University of Salzburg, Salzburg, Austria; (3)Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander University Erlangen-Nürnberg, Erlangen, Germany

Resume : Optical properties of metal oxide nanoparticles are often subject to surface defects and impurities which originate form synthesis and sample storage in the ambient. Using Auger electron spectroscopy in conjunction with optical spectroscopies (UV diffuse reflectance and photoluminescence) we investigated the effect of annealing and oxygen adsorption on the optical properties resulted from different surface and subsurface defect concentration changes of vapor phase grown MgO and ZnO nanoparticles. The MgO nanoparticles show photoluminescence features which are related to excitons associated with surface defects at different levels of surface hydroxylation.[1] In the presence of molecular oxygen the radiative deactivation process becomes annihilated. Conversely, the as prepared ZnO nanoparticles exhibits an O2 induced increase in intensity of a broad emission feature with a maximum at □ = 600 nm. This effect is perfectly reversible with respect to oxygen pressure and attributed to adsorption induced band bending in the PL active subsurface region.[2] Annealing induced trends in the structural and optical properties of the two prototypical metal oxides MgO and ZnO will be discussed in the light of surface composition (surface defects and stoichiometry) as concluded from Auger electron spectroscopy measurements. Our results clearly underline that process induced changes at particle interfaces can determine nanoparticle luminescence. [1] A. Sternig et al., Nanoscale, 4, 2012, 7494 [2] Z. Zhang, J. T. Yates, Jr. Chem. Rev. 112, 2012, 5520.

EP1 44

add to my program (close full abstract)

16:00 **Theoretical modeling of HCl, HBr and HF adsorption on boron- and nitrogen-doped single-walled carbon nanotubes**

Authors : Nedilko S., Hizhnyi Yu., Chornii V., Borysiuk V., Gubanov V.
Affiliations : Taras Shevchenko National University of Kyiv, Volodymyrska Street 64/13, 01601, Kyiv, Ukraine

Resume : Boron- and nitrogen-doped carbon nanotubes (B-CNTs and N-CNTs) are actively studied at present as promising materials for gas sensors [1]. In such studies, theoretical modeling of adsorption of gas molecules on a CNTs allows prediction of several important physical and chemical properties of the sensor materials [2]. So far, adsorption of several types of molecules, in particular CO, NO, NH3, NO2, H2 and Cl2 was treated in the first-principles electronic structure calculations for B- and N-CNTs (see [2] and references therein). In our work we expand such theoretical studies of B- and N-CNTs considering adsorption of HCl, HBr and HF molecules. The electronic structures of B- and N-doped single-walled CNTs of different chilarity with adjacently placed HCl, HBr and HF molecules are calculated by the FLAPW method realized in Wien2k program package [3]. Changes of the dispersion curves and densities of states of the CNTs due to adsorption of the molecules are analyzed. Binding energies of the molecules to the CNTs and charge states of the molecules are obtained in geometry-optimized calculations. Results of calculations are analyzed in view of potential application of studied materials as gas sensors. [1] Battie Y., et al, Phys. Stat. Sol. B, 2011, 248, 2462–6. [2] J-J. Adjizian, at al, Carbon (2013), doi: http://dx.doi.org/10.1016/j.carbon.2013.09.064 [3] P. Blaha, et al, 2001. ISBN 3-9501031-1-2.

EP1 45

add to my program (close full abstract)

16:00 **Synthesis of nanocrystals of III-As alloys in silicon by ion implantation and rapid thermal annealing**

Authors : Rim Khelifi, Yann Le Gall, Dominique Muller and Daniel Mathiot
Affiliations : CNRS-Université de Strasbourg

Resume : Our goal is to use the versatility of ion beam synthesis to growth nanocrystals (NC) of GaInAs alloys of various compositions embedded in a silicon substrate. We studied first the annealing conditions necessary to grow well defined InAs and GaAs binary NC. High dose of As, Ga and In is implanted respectively at 130, 130 and 180 keV to have overlapping as-implanted profiles. The NC growth was then achieved by Rapid Thermal Annealing (RTA) at various temperature between 600 and 900°C for 1 min. RBS profiles shows that no significant impurity out-diffusion occurs below 900°C for both systems. In and As thermal redistribution leads to superposed profiles, but this cannot be checked for the Ga/As case because these impurities cannot be separated by RBS. Raman spectroscopy measurements prove that InAs NC are formed above 600°C, while 800°C annealing is necessary to obtain GaAs NC and show that these thermal budgets are enough to fully recrystallize the implanted layer. Grazing Incidence XRD patterns exhibits clear InAs and GaAs NC related peaks at depth of ~100 nm, consistent with the impurities projected range. Using Scherer formula, InAs and GaAs NC average diameter of 10 and 6 nm, respectively, is estimated. These results prove that GaAs and InAs NC can be grown in a common temperature range (700–800°C), opening the route to the growth of ternary GaInAs NC in the same conditions. Preliminary results on the characterization of these ternary NC will be given in our contribution.

EP1 46

add to my program (close full abstract)

16:00 **The excellent high-temperature dielectric properties of N-doped 3C-SiC: First-principles calculations and experiments**

Authors : Yan-Kun Dou, Hai-Bo Jin, Jing-Bo Li
Affiliations : Beijing Institute of Technology

Resume : The high-temperature dielectric properties of N-doped 3C-SiC nano-powders were evaluated in X-band at the temperature range of 293K-673K. Theory results imply that substitution of N in C sub-lattice is energetically more favorable than that in Si sub-lattice by using the first principles calculation. The electron density difference of N-doped 3C-SiC indicates the bond between Si and N has stronger ionic characteristics than that between Si and C. The doping of N can cause the band gap decreases by 225 meV, which can improve the dielectric properties of 3C-SiC. Intriguingly, the experiment results also prove that the complex permittivity and loss tangent of N-doped 3C-SiC obviously improved with temperature increasing. Compared to the undoped 3C-SiC, two additional dielectric relaxation peaks of imaginary permittivity were observed in the N-doped 3C-SiC. Two defect dipole models derived from the doped N and vacancy defects were proposed to understand the multiple dielectric relaxation in the N-doped 3C-SiC.

EP1 47

add to my program (close full abstract)

16:00 **Influence of the GR1 defect center on the SiV zero phonon line shape in nanocrystalline diamond films** EP1 48

Authors : S. Tóth1*, L. Himics1, M. Veres1, Z. Balogh2, P. Csíkvári3, M. Koós1
Affiliations : 1 Institute for Solid State Physics and Optics, Wigner Research Center for Physics, Hungarian Academy of Sciences, Hungary, H-1525 Budapest, P.O.Box 49., 2 Uzhhorod National University, 88000 Uzhhorod, Ukraine 3 Budapest University of Technology and Economics, Budapest, Hungary

Resume : Preparation and characterization of different light emitting centers constitutes an intensely studied field of nanodiamond research. The SiV center is of particular interest, since its stable, intense and narrow zero-phonon line (ZPL) at 738 nm can be utilized for in vivo biosensing. However, its emission can be affected by the neutral vacancy-related GR1 center, having doublet emission structure with ZPLs at 741 and 744 nm and being present in the top layer of CVD diamond films. This work aims at the clarification of the contribution of the GR1 center to the SiV PL emission. Excitation intensity dependent photoluminescence measurements were performed on nanocrystalline diamond films with different grain sizes (20-200 nm) grown by microwave CVD. The 488 nm line of an Ar-ion laser was used as excitation source and the laser power was changed in the 150-700 kW/cm2 region. Additionally, the variation of the SiV peak position, width and intensity was also studied with scanning PL measurements on a 10 x 10 microns area with excitation spot diameter of 1 micron. Presence of GR1 center in nanocrystalline films was proved by heat treatment process. Our results showed that there are at least two types of diamond structures having different spectral shape and behavior in the emission region of Si-V color center. Furthermore the contribution of the GR1 center depends on the average grain size, being higher in films with larger diamond crystallites.

add to my program (close full abstract)

16:00 **Ionic current rectification of graphene nanopore formed by irradiation** EP1 49

Authors : Huijun Yao, JianZeng, Dan Mo, Jinglai Duan, Jie Liu, Youmei Sun
Affiliations : Institute of Modern Physics, Chinese Academy of Sciences

Resume : The single layer graphene was irradiated by heavy ions and nanopore with diameter of 10 nm on graphene was formed. The ionic current rectification of graphene was observed. The influences of different KCl concentrations, pH values and different scanning speed were discussed in details. In our article, a new method for preparing graphene nanopore used for ionic current rectification was confirmed.

add to my program (close full abstract)

16:00 **Energy transfer in 2D and 3D packed silicon nanocrystals embedded in SiO2** EP1 50

Authors : Rens Limpens, Arnon Lesage & Tom Gregorkiewicz
Affiliations : University of Amsterdam (Institute of Physics) Science park 904, 1098 XH, Amsterdam

Resume : Silicon Nanocrystals (NCs) have been widely studied because of their interesting properties and enormous potential for applications in, e.g., photovoltaic industry. The biggest problem is the low emission (photoluminescence, PL) efficiency of Si NCs, which typically does not exceed 15%. This needs to be understood and then improved. In our recent study we have shown that a combination of the presence of a significant amount of defected NCs (termed as "dark" NCs due to the non-emitting character) and energy transfer towards these centers play the dominant role in the efficiency quenching. In the present study, we investigate this energy migration in specially prepared 2- and 3-dimensional (2D, 3D) ensembles of Si NCs where the energy transfer rate is expected to be different. By measuring effective lifetimes and calculating internal quantum efficiencies we are able to visualize and quantize the difference in magnitude of the energy transfer process in the two geometries. We conclude that energy migration is indeed quenched in the 2D system. Combining high-resolution microscopy with PL and spectrally resolved measurements of PL quantum yield, we demonstrate that also the percentage of dark NCs depends on the system's geometry and is smaller for the 2D packing. These findings vouch for a 2D packing of Si NCs in order to increase ensemble emission efficiencies, as in this way energy transfer to defected NCs is mitigated. R.Limpens and T. Gregorkiewicz, J.Appl.Phys, 114 (2013)

add to my program (close full abstract)

16:00 **Porous silicon irradiated in the electronic regime: modelling the damage cross-section.** EP1 51

Authors : B. Canut 1, J.M. Bluet 1, M. Massoud 1, P. Newby 1, V. Lysenko 1, I. Monnet 2
Affiliations : 1 Université de Lyon, Institut des Nanotechnologies de Lyon, CNRS, INSA de Lyon, France; 2 Centre de Recherche sur les Ions, les Matériaux et la Photonique, CEA -CNRS, Université de Caen, France
Resume : Mesoporous silicon (PS) samples of columnar morphology were processed by anodising p+ Si wafers in (1:1) HF-ethanol solution. Different current densities were used to obtain three different porosities (41%, 56% and 75%). The mean crystallite size varied between 12 nm (75% porosity) and 19 nm (41% porosity). These targets were irradiated at the GANIL accelerator, using different projectiles (129Xe ions in the 10 MeV-100 MeV energy range, 238U ions in the 100 MeV- 1 GeV energy range) in order to vary the incident electronic stopping power Se. Raman spectroscopy and cross sectional SEM observations evidenced a progressive amorphization of the nanocrystallites versus the irradiation fluence. The Se-dependences of the damage cross-sections (extracted from Raman results), exhibit linear behaviours above an electronic stopping power threshold which decreases with the sample porosity. These results, which cannot be obtained in bulk crystalline silicon irradiated at comparable Se, were ascribed to the low thermal conductivity of the PS targets and modelled in the framework of an analytical approach ("IDEA" model) which describes the relaxation of the prompt density of electronic energy received by the target.

16:00 **Simulations of electromechanical shape transformations of Au nanoparticles.**

Authors : V.Zadin, A. V. Krasheninnikov, F.Djurabekova, Long-Bing He , Bin-Jie Wang, Jun Sun, Li-Tao Sun, Scott X. Mao and Ze Zhang, K. Nordlund
Affiliations : Division of Materials Physics, Department of Physics and Helsinki Institute of Physics, P.O.Box 43 (Pietari Kalmink. 2)0001,4 University of Helsinki Intelligent Materials and Systems Lab, Institute of Technology, Tartu University, Nooruse 1, 50411 Tartu, Estonia; Department of Applied Physics, Aalto University, P.O. Box 11100, FI-00076 Aalto, Finland; Division of Materials Physics, Department of Physics and Helsinki Institute of Physics, P.O.Box 43 (Pietari Kalmink. 2)0001,4 University of Helsinki; SEU-FEI Nano-Pico Center, Key Lab of MEMS of Ministry of Education, Southeast University, Nanjing 210096, China FEI Company, Shanghai Nanoport, No.690 Bibo Road, Shanghai, 201203, PR China; SEU-FEI Nano-Pico Center, Key Lab of MEMS of Ministry of Education, Southeast University, Nanjing 210096, China; SEU-FEI Nano-Pico Center, Key Lab of MEMS of Ministry of Education, Southeast University, Nanjing 210096, China; Department of Mechanical Engineering and Materials Science, University of Pittsburgh, 3700 O'Hara Street, Pittsburgh, Pennsylvania 15261, USA; Department of Materials Science, State Key Lab of Si Materials, Zhejiang University, Hangzhou, Zhejiang, 310008, China; Division of Materials Physics, Department of Physics and Helsinki Institute of Physics, P.O.Box 43 (Pietari Kalmink. 2)0001,4 University of Helsinki;
EP1 52
Resume : Metallic nanocrystals can exhibit intriguing properties due to large surfaces specific for low-dimensional objects. Recently the experimental observation showed an interesting shape transformation of Au nanoparticle during simultaneous mechanical and electrical load. By applying the finite element methods, extended to include nanosize effects, we study the mechanisms of such trasformation. We utilize fully coupled electro-thermal calculations with nanoscale correction to the electric and thermal conductivities. The mechanical response of the material is simulated using the elastoplastic material model while the nanoscale mechanical interaction between gold and tungsten particles is simulated using adhesive contact modeling. We observe that Joule heating due to high electric currents increases the temperature of the nanoparticle to value close to the melting point. In combination with the mechanical stress, this causes significant plastic deformations within the nanoparticle, which can explain the observed shape modification of the latter.

16:00 **Photoluminescence from GaAs(1-x)N(x) dilute nitride achieved by nitrogen-implantation and flash lamp annealing**

Authors : Kun Gao, S. Prucnal, R. H?bner , W. Skorupa, M. Helm, Shengqiang Zhou
Affiliations : Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Institute of Ion Beam Physics and Materials Research, P.O. Box 510119, 01314 Dresden, Germany
EP1 53
Resume : Nitrogen atoms are isoelectronic substituents for arsenic in GaAs. A small amount of nitrogen doping can lead to a pronounced bandgap reduction. Therefore nitrogen-doping can be applied as a powerful technique to modify GaAs based materials for long wavelength optoelectronic devices. In this contribution we present the fabrication of dilute nitride material GaAs1-xNx by nitrogen-implantation and flash lamp annealing (FLA). N was implanted in to the commercial GaAs wafer to form a 0.2 ?m thick layer with atomic concentration

of about 0.76 % and 0.38 %. The as-implanted GaAs layer becomes amorphous due to the bombardment of nitrogen ions with high kinetic energy. The GaAs1-xNx layer with compressive strain is epitaxially regrown on GaAs during FLA treatment as confirmed by X-ray diffraction and micro-Raman spectroscopy. In the meantime the bandgap shrinkage is proven by photoluminescence spectroscopy. Based on the redshift of the GaAs1-xNx near band-edge emission, up to 60 % of the implanted N atoms are successfully incorporated into the lattice after FLA. According to our investigation, ion-implantation followed by ultrashort flash lamp treatment, which is quite efficient and low-cost, exhibits a promising prospect on bandgap engineering of GaAs based semiconductors.

add to my program (close full abstract)

16:00 **Electronic and magnetic properties of graphene nanoribbons with reconstructed zigzag edges** EP1 54

Authors : P. Vancsó1, 5, I. Hagymási2,3, Yong-Sung Kim4, 5, Chanyong Hwang4,5, L. Tapasztó1,5 and L. P. Biró1, 5
Affiliations : 1 Institute of Technical Physics and Materials Science, Research Centre for Natural Sciences, PO Box 49, H-1525 Budapest, Hungary, www.nanotechnology.hu 2 Strongly Correlated Systems "Lendület" Research Group, Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, PO Box 49, H-1525 Budapest, Hungary 3 Department of Theoretical Physics, University of Szeged, Tisza Lajos krt 84-86, H-6720 Szeged, Hungary 4 Center for Nano-characterization, Division of Industrial Metrology, Korea Research Institute of Standards and Science, Yuseong, Daejeon 305-340, Republic of Korea 5 Korean-Hungarian Joint Laboratory for Nanosciences, PO Box 49, H-1525 Budapest, Hungary

Resume : Graphene nanoribbons (GNR) with atomically perfect zigzag edges have a magnetic insulating ground state with antiparallel spin orientation between the two edges [1]. However, in real systems edge reconstructions and defects are always present. Ab-initio calculations have shown that under ambient conditions various edge reconstruction can be realized. One of the most preferable edge reconstruction is the extended pentagon-heptagon (5-7) reconstruction, which has also been recently observed by transmission electron microscopy [2]. In this work we have performed electronic structure and magnetic ordering calculations on GNRs with reconstructed and defective zigzag edges including the (5-7) reconstruction by applying the mean-field theory for the Hubbard model. Within the framework of this approximation we have also investigated the influence of the temperature, carrier density and the width of the GNRs on their electronic and magnetic properties. Our results indicate that these properties significantly depend on the type of the edge reconstruction and the external conditions. These predictions can be verified on GNRs which are fabricated by scanning tunneling lithography [3]. [1] Young-Woo Son, et al., PRL 97(2006) 216803 [2] Kwanpyo Kim, et al., Nat. Commun. 4(2013) 2723 [3] L. Tapasztó, et al., Nature Nanotech. 3(2008) 397-401

add to my program (close full abstract)

16:00 **Perspectives of enhancement of p-type conductivity in ZnO nanowires** EP1 55

Authors : Tamar Tchelidze, Tamaz Kereselidze, Teimuraz Nadareishvili
Affiliations : Ivane Javakhishvili Ybilisi State University, Faculty of Exact and Natural Sciences

Resume : Semiconductor nanowires, are believed to act as key elements in future nanoscaled optoelectronic devices, as they offer intriguing electrical and optoelectronic properties. However, the future of any semiconductor nanowire technology will essentially rely on their doping capability. The availability of both n- and p-type semiconductors is important for the realization of nanowire-based electronics. Wide band gap semiconductors, such as ZnO, suffer from doping polarity. They can be easily by doped n- (or p-type) to the expense of difficulties for doping of opposite type. Space confinement changes donor and acceptor ionization energies; The main factor that makes difficult to obtain n- or p-conductivity is formation of compensating defects. Compensating processes is strongly affected by electronic structure of system: band gap, ionization energies of donors, acceptors and their compensation centers. In the presented work we calculated energy levels of electron bound to Coulomb impurity that is incorporated in semiconductor nanowire. Effect of dielectric confinement on ionization energies are considered as well. For analyzing perspectives of suppressing processes of compensation and achieving high ohmic p-conductivity Kroger method of quasi-chemical equations is used.

add to my program (close full abstract)

16:00 **Catalytic effects of grain boundaries on hydrogen dissociation** EP1 56

Authors : Martin Panholzer, Markus Obermayr, Kurt Hingerl

Affiliations : Zentrum für Oberflächen und Nanoanalytik, Johannes Kepler University Linz, Altenberger Straße 69, 4040 Linz, Austria

Resume : Magnesium can effectively store hydrogen up to 7.6 wt%. This makes Mg an attractive material for hydrogen storage. However, there are two major drawbacks which hinder this storage technology from commercial, especially mobile usage, i) the high desorption energy and ii) the poor kinetics, limited by the low bulk diffusion coefficient of H in Mg/MgH2 (a tank has to be filled within minutes, as indicated in the DOE targets). The kinetics can be improved by addition of catalysts, reduction of particle size by e.g. high-energy ball milling (HEBM) and by the reduction of grain size to nanometer scale in the bulk material by severe plastic deformation (SPD). The improvement of the kinetics, by reduction of the particle size is a result of the increase of surface area (which increases the H2 dissociation rate) and reduction of the bulk diffusion length. In contrast the surface area for SPD processed material is not increased, but a similar kinetic enhancement compared to HEBM is reached. This shows that grain boundaries (GB) have a remarkable positive effect on the kinetics (100 x higher diffusion constant). Now the question arises, and there are hints in the literature [Jorge, A.M. et al. Int. J. Hydrogen Energy 38, (2013)], that GBs also reduce the activation energy of hydrogen dissociation. We investigate different reaction pathways by ab-initio methods. We especially investigate whether the H2 molecule penetrates the Mg GBs and if the H2 dissociation energy is lowered by a GB.

add to my program **(close full abstract)**

16:00 **Molecular dynamics simulations of MeV ion-induced craters in nanoscale polymer films**

Authors : Vivian M. de Menezes1, Leandro I. Gutierres1, Diego Tramontina2, Raquel S. Thomaz1, Ricardo M. Papaléo1,3, Eduardo M. Bringa2,4
Affiliations : 1PUCRS, Porto Alegre, Brazil 2Instituto de Ciencias Basicas, Universidad Nacional de Cuyo, Mendoza, Argentina 3UFRGS, Porto Alegre, Brazil 4CONICET, Mendoza, Argentina

Resume : Irradiation of polymers with fast ions is known to produce complex surface features: large craters surrounded by a rim, with sizes which depend on electronic stopping power. These induced craters have been previously studied in materials with thickness corresponding to bulk, but the mechanisms involved in the crater and rim formation in thin organic films is not fully understood up to now. In this context, molecular dynamics simulations, using a simple thermal spike model, were carried out to simulate ultra-thin layers of Lennard-Jones (LJ) molecular solids with binding energies mimicking polymeric compounds. LJ particles were modeled with sigma=0.5 nm, eps=0.5 eV, m=100 u, t_LJ=1.75 ps. To model the ion track within a cylinder of radius 2-8 σ, a temperature distribution with kT=3-25 eps for an effective stopping power of 300 eV/Å was used. In these simulations, crater size is mostly determined by evaporation and melt flow from the hot track, while the rim size is determined both by melt flow and coherent displacement of particles due to the large pressure developed in the excited track. As a consequence, it has been found a drop in sizes and its occurrence at different thickness for crater and rim. Our results were compared with experimental data of PMMA films and a qualitative agreement was found, indicating that electronic excitations in ion tracks do not diffuse significantly and that they couple rapidly to the ionic cores, even for the thinnest film considered here.

EP1 57

add to my program **(close full abstract)**

16:00 **Carbon and Hydrogen impurities in Silicon nanoparticles**

Authors : H. Ibadullaeva, A.O. Rahimova, A.P. Mukhtarov, M. Isakulova
Affiliations : H. Ibadullaeva, A.O. Rahimova, National University of Uzbekistan, 100214 Tashkent, Uzbekistan; A.P. Mukhtarov, Institute of Nuclear Physics AN RUz, 100214 Tashkent, Uzbekistan; M. Isakulova, Djizzakh State University, 130100 Djizzakh, Uzbekistan

Resume : Silicon nanoparticles have a great interest as a nanoelectronic materials. Impurities in Si has a big influence to his optoelectronic properties. The most undesireable impurities are carbon and hydrogen atoms. They play a key role in changing optoelectronic parameters of devices drastically changing their in overdoping semiconductor crystals. At the same time these impurities effect to nanoparticles characteristics has not yet been studied completely. We have studied spatial and electronic structure of the Si nanoparticles doped by carbon and hydrogen atoms by computer simulation in the frame of detalized tight-binding method combined with molecular dynamics simulation.

EP1 58

add to my program **(close full abstract)**

16:00 **Self-trapped excitons at the surface of Si nanocrystals in SiO2**
Authors : A.V. Gert, I.N. Yassievich
Affiliations : Ioffe Physical-Technical Institute of the Russian Academy of Sciences
Resume : The experimental data recently obtained by the femtosecond pump-probe spectroscopy technique have shown that the self-trapped exciton (STE) state plays a key role in the dynamics of hot excitons in the photoexcited silicon nanocrystals embedded in SiO2 matrix [W. D. A. M. de Boer, et al., Phys. Rev. B 85, 161409 (2012)]. We present the theoretical model of excitons self-trapped on Si-O bounds at the silicon nanocrystal surface. The capture of hot free excitons at self-trapped states as well as the reverse process have been studied. The nonradiative multiphonon recombination of the STE initiated by interaction with vibrations of local dipoles in amorphous SiO2 matrix has been considered, too [A.V. Gert, I.N. Yassievich, JETP Letters 97, 87 (2013)]. The relaxation process of "hot" carriers localized in Si nanocrystals has been modulated using Monte Carlo method. We demonstrate that effective exchange between the STE states and "hot" free exciton states leads to the wide energy distribution of "hot" carriers during 10-100 pcs after excitation.
EP1 59

add to my program (close full abstract)

16:00 **On the investigation of the chemical effects induced by ion bombardment in poly (methyl methacrylate) thin and ultra-thin films**
Authors : R. S. Thomaz1, D. Born1, L. I. Gutierres1, E. M. N. Oliveira1, J. Morais2, P. Louette3, R. M. Papaléo1, J. J. Pireaux3
Affiliations : 1Faculty of Physics, Pontifical Catholic University of Rio Grande do Sul, Brazil;2Physics Institute, Federal University of Rio Grande do Sul, Brazil;3Physics Department, University of Namur, Belgium
Resume : In this work, the influence of spatial confinement in one dimension on the chemical effects induced by 18 MeV Au ions in PMMA was investigated systematically, following bond breaking rates as a function of the thickness h of the layers (2
EP1 60

add to my program (close full abstract)

16:00 **Controlled Introduction of Point defects in Germanium Optoelectronic Structures through Gamma Irradiation - Influence on Device Performance**
Authors : Neil Patel* (1), Corentin Monmeyran* (1), Piotr Becla (2), Anuradha M. Agarwal (1), Lionel C. Kimerling (1) *Contributed equally to this work
Affiliations : 1) Microphotonics Center, Massachusetts Institute of Technology, Cambridge, MA 02139; 2) Capesym, 6 Huron Dr #1b, Natick, MA 01760
Resume : Monolithic integration of optoelectronics on a chip is a key solution to continue scaling processor performance. However, defects in germanium, a material of choice for optoelectronic circuits, and their impact on device performance have yet to be thoroughly studied. Gamma rays from a Co^{60} source are used for controlled introduction of defects that are characterized by DLTS. We find a primary state within the Ge bandgap (Ec - 0.35 eV) with an introduction rate of $7x10^{9}$ $cm^{-3}Mrad^{-1}$, which is used to model the performance of bulk Ge in waveguide-integrated (WIP) and free-space (FSP) photodetectors in radiation environments. The former are less sensitive. Our measurements predict that the dose required to create defects which increase the SRH current to a typical value of dark current for a FSP is only 4 Mrad, compared with $8x10^{6}$ Mrad for a WIP. Decrease of lifetime of carriers due to traps occurs at threshold γ doses of $5x10^{8}$ Mrad (FSP) and $7x10^{6}$ Mrad (WIP). Ge is also useful as a passive photonic component material for mid-IR applications in which changes in optical index (n,k) can cause circuit failure. A lower bound for the threshold γ dose which leads to a 0.001 index of refraction shift at λ = 3 μm due to carrier injection/compensation, is calculated to be $2x10^{7}$ Mrad. The lower bound for a γ dose leading to a 1 dB/cm increase in material loss at 3.54 μm due to absorption from the primary defect state (Ec - 0.35 eV) is calculated to be $3x10^{7}$ Mrad.
EP1 61

add to my program (close full abstract)

16:00 **Thermodynamic Analyses of Defect formation in BFO**
Authors : T. Tchelidze, T. Gagnidze, A. Shengelaya
Affiliations : Ivane Javakhishvili Tbilisi State University, Faculty of Exact and Natural Sciences
Resume : multiferroic materials, which simultaneously display magnetic and electric order have attracted interest because of their physical properties very promising for multifunctional device application. Among these properties the magnetoelectric coupling between the electric and magnetic degrees of freedom, where an electric (magnetic) polarization can be induced by a magnetic (electric field), is especially important. Bismuth ferrite (BFO) belongs to a class of single-
EP1 62

phase multiferroic materials. This compound has become recently subject of great interests due to room temperature multiferroic properties. A number of experiments have indicated that properties of BiFeO3, such as remnant polarization, dielectric constant, magnetization are very sensitive to defects. The presence of charged defects in ferroelectrics especially influences polarization and conductivity. Charged defects in ferroelectric material often combine into defect dipoles (DDs) or defect (donor-acceptor) complexes. In ferroelectrics the lowest energy configuration is satisfied when DDs align to spontaneous polarization We provide thermodynamic analyses of defect concentrational equilibrium in BFO, by means of Kroger method of quasi-chemical equations. We consider the system BFO (solid)-oxigen (gas) and calculate composition of defects at given temperature in dependence on oxygen partial pressure. Temperature and pressure ranges that coincide p-type, compensated, or n-type samples are defined. It is shown that for creation defect complexes, which strongly affects polarization properties of material, treatment in high oxygen pressure is needed. Calculation are carried out for BFO thin films and nanowires. The effect of reduction of dimensionality on DDs formation is discussed.

add to my program (close full abstract)

16:00 **Electrical and optical properties of sponge-like Ge embedded in dielectric matrix for solar cell applications**

Authors : M. Yilmaz2,4, B. Altuntas*1,2, S. Ilday2,3, R. Turan1,2 , S. Cosentino5, R. Raciti5, I. Crupi5, A. Mio5, G. Nicotra5, A. Terrasi5, S. Mirabella5
Affiliations : 1Department of Physics, Middle East Technical University, 06800, Ankara, TURKEY 2Center for Solar Cell Research and Applications (GÜNAM), Middle East Technical University, 06800, Ankara, TURKEY 3Department of Micro and Nanotechnology, Middle East Technical University, 06800, Ankara, TURKEY 4Department of Physics, Necmettin Erbakan University, 42090, Konya, TURKEY 5Dipartimento di Fisica e Astronomia and CNR-INFM, MATIS, Università di Catania, I-95123, Catania, ITALY

Resume : Ge nanocrystals is an attractive material for solar cell application due to quantum size effect, which makes it possible to tune the band gap and optical absorption properties. However, electronic transport between isolated nanocrystals should rely on the tunneling efficiency through the dielectric material in between them. It is highly desirable to have a system having both quantum confinement and easy transport channel. This is possible only in the case of interconnected nanostructures having a confinement in one or two dimensions. In this work we have prepared interconnected, sponge-like Ge nanostructures in SiO2 matrix using co-sputtering technique. We studied the electrical transport through this composite structure using I-V measurements in the vertical and lateral directions. Due to the differences in the vertical and lateral organization of the nanostructures we observed a difference in the carrier conductivity. This is particularly important for solar cells where the vertical transport is more crucial than the lateral transport. The optical response in these films is investigated by UV-VIS Spectroscopy. The results show that the band gap decreases with increasing substrate temperature as expected from the fact that at the size of Ge nanostructures increases with the substrate temperature. Photoresponse measurements, where the cut-off wavelength corresponds to the band gap of the material, confirm the variation of the band gap with increasing Ge size. We have also fabricated heterojunction device on Si substrate and observed a weak photovoltaic effect in the measured device.

EP1 63

add to my program (close full abstract)

16:00 **The inelastic thermal spike model applied to metal/insulator interfaces**

Authors : A. Chettah, H. Amekura, H. Kucal, Y. Takeda, M. Matsuda, A. Iwase
Affiliations : LRPCSI, University of Skikda, route d'ElHadaiek, BP 26, 21000 Skikda, Algeria; National Institute for Materials Science (NIMS), Tsukuba, Ibaraki 305-0003, Japan;CIMAP Laboratory, CEA-CNRS-ENSICAEN and Université of Caen, BP5133, 14070 Caen-cedex 5, France; National Institute for Materials Science (NIMS), Tsukuba, Ibaraki 305-0003, Japan; Japan Atomic Energy Agency (JAEA), Tokai-mura, Ibaraki 319-1195, Japan; Department of Materials Science, Osaka Prefecture University, Sakai, Osaka 599-8531, Japan

Resume : Recently,intermixing induced by 200 MeV Xe ion irradiation on metal-insulator interfaces (Bi/Al2O3and Au/Al2O3)was investigated experimentally via in-situ RBS measurements using 16 MeV C ions [1]. According to this study,atomic mixing could be observed in the Bi/Al2O3 bi-layer whereas no change has been found in the Au/ Al2O3 interface.In previous works, mixing induced by Swift Heavy Ions SHI wasascribed to inter-diffusion in liquid phases along the ion path.In the framework of the thermal spike model, the appearance of such molten phases could be predicted from the atomic temperature calculation. The present work is devoted to metal/insulator bi-layers.

EP1 64

Simulations were performed using known parameters for Au, Bi andAl2O3. Both bulk Bi and bulk Al2O3 are known to be sensitive to electronic stopping power (Se) and solid-liquid phase transition appears beyond a certain Se threshold values, while Au is insensitive.For the Bi/Al2O3 system,as expected,molten phase appearance was evidenced along the entire bi-layer. As for the Au/Al2O3system, the gold atomic temperature was kept below the melting temperature except for 2nm of width at the interface with Al2O3. While the mixing could be induced, the thickness of 2 nm would be below the detection limit of the in-situ RBS measurments [1]. [1] M. Hayashi, et al., Nucl. Instrum.Methods Phys. Res. B 314, 176 (2013).

add to my program **(close full abstract)**

Back

European Materials Research Society
23 Rue du Loess - BP 20 - 67037 Strasbourg Cedex 02 - France - Phone:+33-(0)3 88 10 63 72 - Fax:+33-(0)3 88 10 62 93 - emrs@emrs-strasbourg.com

PROGRAM VIEW : 2014 Spring
MY PROGRAM : 2014 Spring

Symposium : E

Defect-induced effects in nanomaterials

26 May 2014 | **27 May 2014** | 28 May 2014 | 29 May 2014 | 30 May 2014

hide a

start at	Subject	Num.
	Nanooxides I : Yanwen Zhang	
09:00	**Polarity driven defect formation in oxide nano-materials** **Authors :** Jacek Goniakowski, Claudine Noguera **Affiliations :** CNRS, INSP, Paris, France **Resume :** Extended polar objects present an electrostatic instability which requires substantial modifications of their surface charge density. The understanding of polarity-driven surface defects in oxides, such as surface non-stoichiometry, has been an active field of research in the last decades. It has extended more recently towards oxide/oxide interfaces due to their entirely new properties, such as a confined two-dimensional electron gas (2DEG), subject of enhanced correlation effects, magnetic, or even superconducting instabilities. On the other hand, it has been shown that the electrostatic forces driving polarity effects and the response they induce may by substantially different in oxide nano-objects. Below a critical size, these objects may sustain finite dipole moments which drive strongly size- and dimensionality- dependent properties. At small sizes, defects related to polarity may also extend beyond the surface region and drive structural transformations of the entire object, resulting in novel structures, with no bulk counterparts. Relying on first principles simulations, we will exemplify some of these effects at oxide/oxide interfaces and in nano-oxides of various dimensionalities. add to my program (close full abstract)	EO4 1
09:30	**The effect of oxygen vacancies in BaTiO3 and KNbO3.** **Authors :** Anna Kimmel, Peter Sushko, Markys Cain **Affiliations :** National Physical Laboratory; University College London; **Resume :** The effect of neutral oxygen vacancies on ferroelectric switching in tetragonal BaTiO3 and KNbO3 is investigated using density functional theory calculations. In both materials, stable axial oxygen vacancies and metastable equatorials vacancies are found to significantly but to different extent reduce the barrier for 180 degrees reorientation of the polar axis. We propose that the metastable equatorial vacancy can transform to the stable axial configuration via either oxygen vacancy diffusion or 90 degrees rotation of the polar axis near the vacancy site. We suggest that the latter mechanism is dominant in materials with slow oxygen vacancy diffusion and low formation energy of 90 degrees domain walls. add to my program (close full abstract)	EO4 2
09:45	**Small losses in heavily Ga-doped ZnO films at the telecommunication wavelength for plasmonic materials** **Authors :** T. Yamamoto, H. Song, J. Nomoto and H. Makino **Affiliations :** Kochi University of Technology **Resume :** We have investigated optical properties of heavily Ga-doped ZnO (GZO) polycrystalline films, which can be promising low-loss alternatives to metals at the telecommunication wavelength bands around 1300 nm and 1550 nm for plasmonics. Current plasmonic devices based on metals or metal alloys at the optical frequencies face significant challenges due to losses encountered in the materials. We deposited GZO films on glass substrates (200ºC) with various thicknesses ranging from 100 to 350 nm by ion-plating with dc arc discharge. Hall effect measurement results showed that 105- and 344-nm-thick GZO films have electrical resistivity of 2.5×10-4 Ωcm, carrier concentration of 1.08×1021 cm-3 and Hall mobility of 23 cm2/Vs and electrical resistivity of	EO4 3

1.8×10-4 Ωcm, carrier concentration of 1.23×1021 cm-3 and Hall mobility of 29 cm2/Vs, respectivley. Hall mobility increased with thicknesses up to 344 nm, whereas carrier concentration changed a little. Analysis based on Drude model shows that 105- and 344-nm-thick GZO films exhibited negative real permittivity at wavelenghth of more than 1256 nm and 1198 nm, respectively, which shows that the samples had a plasma frequency higher than the desired frequency of the application. Note that all the GZO films exhibited values of the imaginary part of the dielectric function of less than 0.6 in the range of wavelength smaller than 1500 nm. Those findings prove that the GZO films can be a promising material for the plasmonics.

add to my program (close full abstract)

10:00 **Break**

Nanooxides II : Eugene Kotomin

10:30 **Defect-induced effects in nanocrystalline oxides**

Authors : Yanwen Zhang (1,2), Dilpuneet S. Aidhy (1) , Tamas Varga (3), Sandra Moll (4), Philip D. Edmondson (5), Fereydoon Namavar (6), and William J. Weber (2,1)
Affiliations : (1) Materials Science & Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA; (2) Department of Materials Science & Engineering, University of Tennessee, Knoxville, TN 37996, USA; (3) Pacific Northwest National Laboratory, PO Box 999, Richland, WA 99352, USA; (4) TN International / AREVA, 1, rue des Hérons, 78182 Montigny Le Bretonneux, France; (5) Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, UK; (6) University of Nebraska Medical Center, Omaha, NE 68198, USA

Resume : Nanocrystalline oxides are of high interests for a wide range of applications due to their exceptional size-dependent materials properties, and nanostructured oxides are considered as potential candidates in advanced energy storage and production. Ever increasing energy needs have raised the demands for advanced fuels, and nanostructured oxides are considered as potential candidates with improved performance in advanced nuclear energy systems Understanding defect-induced effects in nanocrystalline oxides is important. Ion beam is an effective approach to tailor size-dependent material properties of oxide-based nanomaterials. Grain growth of nanocrystalline materials is generally thermally activated, but can also be driven by irradiation at much lower temperature. Cubic ceria and zirconia are well known ionic conductors that are also isostructural with urania, plutonia, and thoria-based nuclear fuels. Under ion irradiation, defect production and ionization effect lead to effective modification of interface volume in nanocrystalline ceria and zirconia. Experimental results have shown that both high electronic energy loss and nuclear energy loss lead to disorder and radiation-induced growth of the crystallite size is a function of total energy deposited. Atomistic simulations by adding high levels of disorder in the simulation cell have revealed fast grain boundary (GB) movements due to the present of high-level disorder in the close proximity to GBs, and the results is in good agreement with our the experimental results. The coupling of energy deposition to the electronic and lattice structures should both be taken into consideration when engineering nanostructural materials.

EO5 1

add to my program (close full abstract)

11:00 **Size-confinement effects in perovskite-like quantum paraelectric nanoparticles**

Authors : V. Trepakov1,2, M. Makarova1,3, Z. Potucek1, O. Stupakov1, E. Tereshina1 A. Dejneka1, L. Jastrabik1, and I. Bykov4.
Affiliations : 1Institute of Physics ASCR, 182 21 Prague 8, Czech Republic 2Ioffe Physical-Technical Institute of the RAS, 194 021 St.-Petersburg, Russia 3 NIMS, 1-1 Namiki, Tsukuba, Ibaraki, 305-0044 Japan 4 Institute for Problems of Material Science, NASc of Ukraine, Krjijanovskogo 3, 03680 Kiev, Ukraine

Resume : The interest in developing new approaches for fabrication of nanosized ABO3 highly polarizable perovskite-like oxides, establishment of the relationships between synthesis conditions, particles size and properties of these materials are steadily increasing. We report on recent development of high-efficiency methods of synthesis of nanoparticles (5–80 nm) of nominally pure and doped SrTiO3 and KTaO3 quantum paraelectrics, the analysis of their structure and properties evolution at different temperatures, particles size and correlations between their structural and physical properties depending on the concentration of intrinsic and impurity defects. The main attention is paid to: i)

EO5 2

the novel approach to the solvothermal synthesis and properties of the perovskite-type KTaO3 crystalline nanoparticles whose properties are turned out to be strongly controlled by magnitude of the solvent dielectric constant; ii) the noticeable lattice constant increasing was found for small SrTiO3 nanoparticles; iii) unusual temperature behavior of the R-line of photoluminescence of the Cr3+ impurity centers was treated as possible manifestation of low-temperature ferroelectric phase transition for the sufficiently small SrTiO3:Cr nanoparticles and iv) successive synthesis characterization and studies (X-ray, SEM, PIXE, Raman scattering, magnetization, EPR) of highly concentrated cubic perovskite-type SrTi1-xMnxO3 nanoparticles (x up to 0.5) revealing polar and magnetic ordering effects.

add to my program (close full abstract)

11:15 **Confinement effects for ionic carriers in ABO3 perovskite ultrathin films**

Authors : M. Arrigoni, D. Gryaznov, E.A. Kotomin, J. Maier
Affiliations : Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1 D-70569, Stuttgart, Germany; Institute of solid state physics, University of Latvia, Riga, Latvia; Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1 D-70569, Stuttgart, Germany; Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1 D-70569, Stuttgart, Germany

Resume : We discuss, how the one-dimensional confinement affects the electronic and energetic properties of point defects (color centers) in perovskite ultrathin films with respect to the bulk phase. Barium zirconate, BaZrO3, has a perovskite structure and serves as one of the constituent materials in electroceramic capacitors used in wireless communications, high temperature proton conductor and substrate for thin film growth. We have considered BaZrO3 as a model for a wide class of ABO3 perovskite-structured materials with partly covalent chemical bonding. Oxygen vacancies are common defects in perovskites responsible for transport properties. In ultrathin films, confinement effects arise due to the spatial restrictions of ionic relaxation around the defect sites, change of phonon spectra and expansion of the electronic wave function beyond the film boundaries. The study has been carried out performing ab initio simulations within the hybrid HF-DFT LCAO theory. Neutral and charged oxygen vacancies were considered in the bulk phase and in ultrathin films, where the defect was placed in the central layer of slabs with a thickness ranging from 3 to 13 crystalline planes along the [001] direction. As terminating layers of the films, both BaO and ZrO2 crystalline planes have been considered. We analyze the confinement effects through changes in the band structure, phonon spectra, electronic density distribution and the formation energies of defects in ultrathin films.

EO5 3

add to my program (close full abstract)

11:30 **The Nature of Intrinsic and Extrinsic Electron Trapping in SiO2**

Authors : Al-Moatasem El-Sayed, Matthew Watkins, Alexander Shluger
Affiliations : Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK

Resume : The mechanisms of electron and hole trapping in SiO2 and the nature of trapping sites are important for our understanding of a wide range of physical phenomena, such as radiation-induced damage and electrical breakdown, and for applications in fiber optics and micro-electronics. Hole trapping in silica has been relatively well understood with models of trapped holes and several hole trapping defects well established. Using classical and ab initio calculations we demonstrate that extra electrons can be also trapped in pure crystalline and amorphous SiO2 (a-SiO2) in deep band gap states. The structure of trapped electron sites in pure a-SiO2 is similar to that of Ge electron centers and so-called [SiO4/Li]0 centers in quartz. Classical potentials were used to generate amorphous silica models and density functional theory to characterize the geometrical and electronic structures of trapped electrons in crystalline and amorphous silica. The calculations demonstrate that an extra electron can be trapped at a Ge impurity in alpha-quartz in six different configurations. An electron in the [SiO4/Li]0 center is trapped on a regular Si ion with the Li ion residing nearby. Extra electrons can trap spontaneously on pre-existing structural precursors in amorphous SiO2. However, the electron self-trapping in quartz requires overcoming a barrier of about 0.57 eV and self-trapped polarons are unstable with respect to the delocalized state. The precursors for electron trapping in amorphous SiO2 comprise wide (>1320) {O--Si--O} angles and elongated Si--O bonds at the tails of corresponding distributions. Using this criterion we estimate the concentration of these electron trapping sites at ~ 4x1019 cm-3.

EO5 4

add to my program (close full abstract)

11:45 **Elemental and Strain Analysis of a La2/3Sr1/3MnO3/ZrO2 System**

Authors : Dan Zhou1, Yi Wang1, Wilfried Sigle1, Marion Kelsch1, Yuze Gao2, Hanns-Ulrich Habermeier2, Peter A. van Aken1
Affiliations : 1Max Planck Institute for Intelligent Systems, Stuttgart Center for Electron Microscopy, Heisenbergstraße 3, 70569 Stuttgart, Germany 2Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany

Resume : In this work, we studied the elemental distribution and strain in La2/3Sr1/3MnO3 (LSMO) doped with ZrO2 by analytical TEM techniques. ZrO2 forms non-magnetic nanoparticles which introduce anomalous magnetic anisotropy and modifications to the electric transport properties [1]. The spin, charge, and orbital ordering in LSMO are extremely sensitive to local structural and elemental changes. With the application of electron energy-loss spectroscopy (EELS) in a probe-aberration-corrected JEOL JEM-ARM200CF, atomic resolution elemental distribution, including La, Sr, Mn, Zr and O, and the Mn valence state variation at the interface between LSMO and ZrO2 were observed. Geometric phase analysis (GPA) of high-angle annular dark-field (HAADF) images allowed us to measure the strain around the interface. These results provide the basis for the understanding of the origins of transport anomalies. 1. Gao, Y.Z.; Zhang, J.C.; Fu, X.W.; Cao, G.X.; Habermeier, H.U.; Progress in Natural science: Materials International, 2013, 23(2), 127-132.

EO55

add to my program (close full abstract)

12:00 **Lunch**

Metallic nanostructures : Kai Nordlund

14:00 **Tailoring the thermal and superconducting properties of ion beam synthesized Pb nanoparticles in Si, Al and Cu matrices**

Authors : H. Wang (1), T. Picot (2), K. Houben (2), S. Bals (3), C. Detavernier (4), S.A. Brown (5), M.J. Van Bael (2), K. Temst (1) and A. Vantomme (1)
Affiliations : (1) Instituut voor Kern- en Stralingsfysica, KU Leuven, Celestijnenlaan 200D, B-3001 Leuven, Belgium (2) Laboratory of Solid State Physics and Magnetism, KU Leuven, Celestijnenlaan 200D, B-3001 Leuven, Belgium (3) EMAT, Dept. Fysica, Universiteit Antwerpen, Belgium (4) Department of Solid State Sciences, Ghent University, 9000 Gent, Belgium (5) The MacDiarmid Institute for Advanced Materials and Nanotechnology, Dept. of Physics and Astronomy, University of Canterbury, 8140, Christchurch, New Zealand

Resume : Epitaxial Pb nanoparticles (NPs) were synthesized by high-fluence ion implantation in single crystalline Si, Al and Cu, i.e. three matrices in which Pb has a limited solubility. By varying the fluence, implantation temperature or annealing conditions, the NP size (5-20 nm) and size distribution can be tuned. In combination with the selection of the matrix, the NP lattice parameters can be tuned. The melting/solidification of these Pb NPs reveals large superheating and supercooling effects. These thermal hysteresis effects, which drastically depend on the size of the NPs, are due to the (i) epitaxial alignment and (ii) different lattice mismatch between the Pb particles and the matrices, leading to a different pressure on the Pb NPs. Hence, this effect can be used to modify the melting behavior of the embedded Pb NPs. Pb NPs in Al (two superconductors with different critical parameters) exhibit a single superconducting transition with a critical temperature Tc, which increases linearly with the Pb/Al volume ratio. The good agreement with theoretical predictions of the proximity effect in the Cooper limit for strongly coupled superconductors, illustrates that the quality of the Pb/Al interface is excellent, which we attribute to the ion beam synthesis process. In this presentation, we will discuss the intimate interplay between the structural properties of the Pb NPs, e.g. the particle size, the matrix and the interface quality, and their thermal and superconducting response.

EO61

add to my program (close full abstract)

14:30 **Nano-size metallic oxide cluster formation in high-purity Fe-10%Cr alloy by ion implantation**

Authors : Ce Zheng (a), Aurelie Gentils (a), Joel Ribis (b), Odile Kaitasov (a), Vladimir A. Borodin (c)
Affiliations : (a) CSNSM, Univ Paris-Sud, CNRS, 91405 Orsay Campus, France ; (b) CEA, DEN, DMN, SRMA, F-91191 Gif sur Yvette, France ; (c) NRC Kurchatov Institute, Kurchatov Sq., 1, 123182 Moscow, Russia

EO62

Resume : Controlling the size, distribution and composition of nano-particles in a material is a fundamental problem for a broad variety of applications from

electronics and photonics to nuclear industry. Ion implantation is a powerful technique to synthesize nano-structures under well-controlled conditions. In this presentation we demonstrate that ion implantation can be successfully applied to create nano-size oxide precipitates in Fe-Cr steel. We report the results of an experiment on the metal-oxide particle formation in a high purity Fe-10wt.%Cr steel by ion implantation (using JANNuS-Orsay facility, where two accelerators are linked to a Transmission Electron Microscope), together with a structural characterization of these nano-oxide clusters. A dispersion of nano-size precipitates of metallic oxides is known to strongly improve mechanical properties of ferritic-martensitic steels. The Oxide Dispersion Strengthened (ODS) steels are promising candidates for structural components of future nuclear reactors. The broad application of these steels is however hindered by the relatively complicated and expensive production technology (powder co-grinding and high-pressure thermomechanical treatment) of ODS steels. Our experimental results indicate the feasibility of unconventional ways for nano-size oxide ensemble creation with high potential for control over the steel property amelioration by tailoring the parameters of oxide ensembles.

add to my program **(close full abstract)**

14:45 **Defect-induced stress development and defect stability in sputter-deposited refractory metal films**

Authors : G. Abadias(1), J.J. Colin (1), D. Magnfält (2), A. Michel (1), K. Sarakinos (2), C. Jaouen (2)
Affiliations : 1. Institut P', Dpt. Physique et Mécanique des Matériaux, Université de Poitiers-CNRS, France; 2. IFM-Linköping University, Plasma and Coatings Physics Division, Sweden

Resume : In the course of the past decade substantial progress has been made in understanding stress generation during thin film growth thanks to real-time and in situ diagnostics based on the measurement of the substrate curvature. Different archetypal stress behaviors have been reported based on the adatom mobility of the deposited material [1]. For deposition conditions that entail the use of hyperthermal species, e.g., magnetron sputtering, cathodic arc and ion beam assisted processes, the development of large compressive stresses is generally reported. For refractory metals, the stress level can reach up to several GPa, which can lead to premature failure by buckling at the film/substrate interface. It is well admitted that defect creation during film growth, as a consequence of the 'atomic peening' process, contributes to this compressive stress build-up. However, the intrinsic mechanisms of defect incorporation are not yet fully understood, especially for nanoscale thin films, where grain boundaries may play a significant role. The aim of the present work is to provide a comprehensive picture on the origin of defect-induced compressive stress development during sputter-deposition of low-mobility metals by combining situ wafer curvature (MOSS) and ex situ structural characterization (XRD, XRR, AFM, HRTEM). Examples will be given for Mo and Ta films, deposited in a large range of energetic bombardment conditions, by varying the working pressure, bias voltage and ionization degree of sputtered and buffer gas species (using the sputtering-based technique HIPIMS). The role of grain boundaries will be highlighted by growing films on template layers with controlled grain size. A linear dependence of the compressive stress magnitude with the grain boundary density is revealed from MOSS, suggesting preferential insertion of excess atoms at the grain boundary. This grain boundary densification [2] corresponds to a stress state which is predominantly of biaxial type, as confirmed by ex situ XRD. Above a certain energy threshold, which is material-dependent, incorporation of excess atoms in the grain bulk occurs (mostly as self-interstitials), leading to a hydrostatic stress component at the origin of a lattice expansion. The stability of the growth-induced defects is discussed based on the cohesion energy of the material (stable vs. metastable phases) and stress evolution after ion irradiation (up to 1 dpa). [1] G. Abadias, J.J. Colin, A Michel, C. Jaouen, Vacuum 100 (2014) 36 [2] D. Magnfält, G. Abadias, K. Sarakinos, Appl. Phys. Lett. 103 (2013) 051910

EO6 3

add to my program **(close full abstract)**

15:15 **Ion beam synthesis of the full spectrum of III-V:Mn ferromagnetic semiconductors**

Authors : Shengqiang Zhou
Affiliations : Helmholtz - Zentrum Dresden - Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstr. 400, 01328 Dresden, Germany

EO6 5

Resume : Ferromagnetic semiconductors have been under intensive investigation during the last decade. Until now, III-Mn-V based compound semiconductors are the only well accepted class of materials. The prototype

ferromagnetic semiconductor GaMnAs has revealed a variety of unique features induced by the combination of its magnetic and semiconducting properties. To prepare ferromagnetic semiconductors, one needs to dope the host with up to 5-10% Mn, which is far beyond the solid solubility of Mn in III-V compounds. As a non-equilibrium process, ion implantation can introduce enough dopants as required. However, the activation of dopants remains challenging due to the clustering of implanted ions during post-annealing. The solubility limit is a fundamental barrier for dopants incorporated into a specific semiconductor. On the other hand, one notes that the solubility limit in the liquid phase is generally much larger than that in the solid phase. Short-time annealing in the millisecond or nanosecond regime allows the epitaxial growth from a liquid phase. The mature development and commercialization of ion implantation promise the versatility. The approach combining ion implantation and pulsed laser melting allows us to prepare ferromagnetic semiconductors covering the full spectrum of III-V compound semiconductors. We have successfully synthesized ferromagnetic Mn doped III-V from InAs and GaAs to InP and GaP with different bandgaps. The results of magnetization, magnetic anisotropy, resistivity, anomalous Hall effect, magnetoresistance and x-ray magnetic circular dichroism obtained from the synthesized samples confirm the intrinsic origin and the carrier-mediated nature of the ferromagnetism. Moreover, in different III-V hosts we observe distinct differences regarding the magnetic anisotropy and conduction mechanism which are related with the intrinsic parameters such as the lattice mismatch, energy gap and the acceptor level of Mn. These results could allow a panorama-like understanding of III-V:Mn based ferromagnetic semiconductors. [1] D. Bürger, S. Zhou, et al., Phys. Rev. B 81, 115202 (2010). [2] S. Zhou, et al., Appl. Phys. Lett. 96, 202105 (2010). [3] S. Zhou, et al., Appl. Phys. Express 5, 093007 (2012). [4] M. Khalid et al., Phys. Rev. Lett., submitted (2013). [5] Y. Yuan, et al, unpublished results (2013).

add to my program (close full abstract)

15:45 **Break**

Nanowires : Nikolai Sobolev

16:15 **Radiation defects in low dimensional structures**

Authors : E. Alves1, K. Lorenz1, A. Redondo-Cubero1,T. Monteiro2, B. Daudin3, E. Wendler4

Affiliations : 1. Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico (IST), EN.10, P-2695-066 Bobadela, Portugal; 2. Departamento de Física e i3N, Universidade de Aveiro, 3810-193 Portugal; 3. CEA/CNRS Group,"Nanophysique et Semiconducteurs", INAC, CEA/Grenoble, 17 rue des Martyrs, Grenoble Cedex 9, 38054, France. 4. Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Max-Wien-Platz 1, 07743 Jena, Germany

Resume : In recent years the vast potential of low dimensional structures to develop new (opto)electronic devices is exploding and nanodevices such as lasers, transistors and sensors are already available. However, the scaling down poses several problems to obtain homogeneous doping and defect free structures. Indeed, even the presence of a reduced amount of defects could destroy or inhibit device operation. Homogeneous doping during the growth or by diffusion is difficult to achieve especially in compound materials. The well established ion implantation technique allows an excellentt control of the dopant distribution and has been successfully applied to dope nanostructures like nanowires (NWs) and multiple quantum wells (QWs). The problem posed by the implantation damage requires a clear understanding of defect production and recovery in these small structures. We will show and discuss results of NW and QW structures implanted with rare earth (RE) ions, correlating the damage role on the optical behavior of the implanted samples. The possibility to use defects to release interface strain in multiple QW through ion mixing will be also analyzed. The damage build-up and RE incorporation and activation in NWs and QWs were studied by Rutherford Backscattering/Channeling Spectrometry (RBS/C), high resolution X-ray diffraction (HRXRD) and photoluminescence (PL). The effect of subsequent annealing on the activation of the dopants and defect recovery will be discussed.

EO7 1

add to my program (close full abstract)

16:45 **Implantation damage and rare earth activation in GaN nanowires and thin films** EO7 2

Authors : M. Felizardo [a], N. Franco [a,b], M. Peres [a], E. Alves [a,b], K. Lorenz [a,b],

E. Nogales [c], B. Méndez [c], J. Rodrigues [d], T. Monteiro [d], M-P. Chauvat [e], P. Ruterana [e], T. Auzelle [f], B. Daudin [f]
Affiliations : [a] Instituto Superior Técnico (IST), Campus Tecnológico e Nuclear, Estrada Nacional 10, P-2695-066 Bobadela LRS, Portugal; [b] IPFN, IST, Portugal; [c] Dpto. Física de Materiales, Universidad Complutense de Madrid, 28040 Madrid, Spain; [d] Departamento de Física e i3N, Universidade de Aveiro, 3810-193 Portugal; [e] Centre de Recherche sur les ions les matériaux et la photonique (CIMAP) ENSICAEN, Boulevard Maréchal Juin 14050 Caen France [f] CEA/CNRS Group, "Nanophysique et Semiconducteurs", INAC, CEA/Grenoble, 17 rue des Martyrs, Grenoble Cedex 9, 38054, France.
Resume : GaN-based nanowires (NWs) are currently attracting considerable research interest as material for efficient light emitters and sensors. Ion implantation has been successfully applied to the doping of NWs with rare earth (RE) ions, however, the formation of implantation damage and defect removal is still largely unexplored [1]. Vertically aligned GaN NWs, grown on silicon substrates via molecular beam epitaxy, with an average density of 1E10 NW.cm-2, diameter of ~100 nm and ~1500 nm length have been implanted with 300 keV Europium ions, to fluences ranging from 1E13 to 3E15 at.cm-2. The damage build-up and Eu incorporation and activation in NWs and thin film reference samples were assessed by Rutherford Backscattering Spectrometry (RBS), X-ray diffraction (XRD), cathodoluminescence (CL) and photoluminescence (PL), as well as transmission electron microscopy. XRD 2Teta-Omega curves in several planes ([0002], [0004] and [0006]) reveal that implantation defects cause large strains in GaN thin films while strain in NWs remains much lower. Rapid thermal annealing efficiently recovers the crystal and activates the typical red Eu3+ light emission. CL measurements indicate a strong dependence of Eu emission intensity on the NW morphology with superior properties of non-coalesced NWs. In these regions NWs also show higher emission intensities than thin film reference samples and light emission is less affected by implantation defects.
[1] Ronning et al. Mat Sci Eng R 70 (2010) 30

add to my program **(close full abstract)**

17:00 **Band-offset driven efficiency of the doping of SiGe core-shell nanowires**

Authors : M. Amato (1), S. Ossicini (2) R. Rurali (3)
Affiliations : (1) Institut d'Electronique Fondamentale, UMR8622, CNRS, Université Paris -Sud, 91405 Orsay, France (2) Dipartimento di Scienze e Metodi dell'Ingegneria, Università di Modena e Reggio Emilia, Via Amendola 2 Pad. Morselli, I-42100 Reggio Emilia, Italy (3) Institut de Ciència de Materials de Barcelona (CSIC), Campus de la UAB, 08193 Bellaterra, Spain
Resume : One of the main limits of doping of pure silicon and pure germanium nanowires (Si and Ge NWs) is its inefficiency when the diameter is reduced, as a consequence of surface segregation of impurities, strong quantum confinement and dielectric mismatch [1]. In the case of doping with boron or phosphorus impurities of Si and Ge NWs the impurity state is deep into the band gap and cannot be electrically activated at typical device temperatures. This phenomenon is responsible of several problems about the real applications of these types of materials for electronic devices. Results of our ab-initio DFT calculations on core-shell silicon-germanium NWs [2] (with diameter of 2.4 nm) show how this limit can be easily overcome by opportune doping with boron and phosphorus impurities. In these nanostructures, in fact, the band offset between the two materials causes localization of the valence states on germanium and of conduction states on silicon. As a consequence of this property, with particular doping conditions, a one-dimensional electron (hole) gas at the band edge is created and the carrier density is uniquely controlled by the impurity concentration without no need of thermal activation. Additionally, SiGe core-shell nanowires, providing naturally the separation between the different types of carriers, electron and holes, are ideally suited for photovoltaic applications.
[1] M. T. Bjork, et al. Nat. Nanotech. 4, 103 (2008). [2] M. Amato, et al. Nano Letters, 11, 594, (2011).

EO7 3

add to my program **(close full abstract)**

17:15 **Interplay between defects in metallic nanowire networks and their physical properties: a modeling and experimental approach**

Authors : M. Lagrange1, D. P. Langley1,2, D. Munoz-Rojas1, C. Jimenez1, N. D. Nguyen2, Y. Bréchet3, D.Bellet1
Affiliations : 1Laboratoire des Matériaux et du Génie Physique CNRS - Grenoble INP, 3 parvis Louis Néel CS 50257, 38016 Grenoble, France. 2 Laboratoire de Physique des Solides, Interfaces et Nanostructures Département de Physique, Université de Liège Allée du 6 Août 17, B-4000 Liège, Belgique. 3 Laboratoire de Science et Ingénierie des

EO7 4

Matériaux et des Procédés CNRS - Grenoble INP, 1130 rue de la piscine 38042 Saint-Martin d'Hères, France.

Resume : The use of random metallic nanowire networks as transparent conductive materials (TCMs) is increasing rapidly. These materials can be used in flexible/stretchable electronics, flexible displays, touch screens, photovoltaics or as transparent heaters. Metallic nanowire networks can be deposited by using low-cost and scalable deposition techniques and exhibit very interesting electrical, optical, thermal and mechanical properties. In addition to usual material defects (such as grain-boundaries) any deviation from a "perfect" infinite network (i.e. nanowire length distributions, finite device size or nanowire curvature for instance) play a prominent role in the physical properties of the resulting percolating network. Using Monte Carlo simulations, and based on experimental available wires the effects of these defects are explored. Experimental work is focused on the influence of nanowire density as well as defects within the nanostructured network such as the inhomogeneity of the network, the grain-boundary along a nanowire, the morphological nanowire instabilities… The influence of these defects on the physical properties of this promising nanostructured network will be presented. References: D.P. Langley, G. Giusti, C. Mayousse, C. Celle, D. Bellet, J.P. Simonato. Nanotechnology 24 (2013) 452001. D.P. Langley, G. Giusti, M. Lagrange, R. Collins, C. Jiménez, Y. Bréchet, D. Bellet. Solar Energy Materials and Solar Cells (2013),http://dx.doi.org/10.1016/j.solmat.2013.09.015

add to my program **(close full abstract)**

17:30 **Inducing and Engineering Defects in Ge Nanowires**

Authors : Subhajit Biswas ?, Michael A. Morris?, and Justin D. Holmes?,*
Affiliations : ?Materials Chemistry & Analysis Group, Department of Chemistry and the Tyndall National Institute, University College Cork, Cork, Ireland. Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Dublin 2, Ireland.

Resume : Considerable research effort was applied to tune the crystal structure and defect formation in nanowires by influencing the thermodynamic, kinetic and energetic limits in widely popular bottom-up nanowire growth paradigms. In this research, we present a novel fundamental concept to intrinsically tune basic thermodynamics and kinetics at the growth interfaces during catalytic germanium (Ge) nanowire growth for defect engineering in nanowires. An epitaxial defect transfer mechanism has been utilized to induce axial stacking faults from twinned catalytic materials to the Ge nanowire body. These stacking faults occur mainly in the form of twins, where twin boundary separates two neighbouring crystal domains with very specific relative crystallographic orientations without any dangling bonds at their interface. Manipulation of twinning probabilities in the catalytic particles enabled successful modification of twinning densities in the nanowires. Coherent twinning phenomenon perpendicular to the nanowire growth axis was also induced utilizing the interfacial tensions at the growth interfaces from the fluctuation in the mass transport by using metal germanide alloy catalysts. Defined twinning events in nanowires directs to interesting physical properties such as mini-band formation and the opening of zero energy gaps at the superlattice Brillioun zone boundary, induction of a direct bandgap in germanium, and phonon backscattering from the modulated side facets of the nanowires leading to interesting thermoelectrical property.

EO7
5

add to my program **(close full abstract)**

Back

PROGRAM VIEW : 2014 Spring
MY PROGRAM : 2014 Spring

Symposium : E

Defect-induced effects in nanomaterials

26 May 2014 | 27 May 2014 | **28 May 2014** | 29 May 2014 | 30 May 2014

hide a

start at	Subject	Num.
	Defect-induced effects : Eduardo Alves	
09:00	**Formation of nanoscale radiation defects in graphite and diamond by energetic argon clusters** **Authors :** V.N. Popok (1), M. Hanif (1), J. Samela (2), K. Nordlund (2), V.P. Popov (3) **Affiliations :** (1) Aalborg University, 9210 Aalborg, Denmark; (2) University of Helsinki, 00014, Helsinki, Finland; (3) Institute of Semiconductor Physics, 630090 Novosibirsk, Russia **Resume :** Cluster ion implantation is a powerful tool for engineering of surfaces and thin layers on the nanoscale. Cluster consisting of many atoms generates multiple collisions, thus, transferring locally a significant amount of energy causing a number of specific phenomena. In the current work, keV-energy argon cluster ions of a few tens of atoms in size were implanted in graphite and diamond. Radiation damage areas formed by individual clusters were studied experimentally using atomic force and scanning tunneling microscopy for as implanted samples and after thermal and chemical treatments. The experimental part was corroborated by molecular dynamics simulations that allowed grounding several conclusions relevant for the development of cluster stopping theory and practical applications of cluster beams. It is found that (i) cluster implantation shows a clear presence of size effect, larger clusters have lower stopping power and produce deeper damage; (ii) there is no crater formation on graphite due to elastic response of graphene planes to cluster impact while craters on diamond are formed by direct sputtering, there is no liquid flow effect found; (iii) threshold displacement energy for cluster impact on diamond is estimated; (iv) stopping of clusters in diamond shows a strong similarity to the stopping in graphite, thus, demonstrating the same scaling law in which both depth of radiation damage and projected range of cluster constituents linearly depend on cluster momentum.	EO81
	add to my program (close full abstract)	
09:15	**Doped TiO2 and SrTiO3 nanotubes for photocatalytic applications: Predictions from first principles** **Authors :** Yu.F. Zhukovskii(1), S. Piskunov(1), O. Lisovskii(1), J. Begens(1) and E.Spohr (2) **Affiliations :** (1) Institute of Solid State Physics, University of Latvia, 8 Kengaraga str., LV-1083, Riga, Latvia; (2) Lehrstuhl für theoretische Chemie, Universität Duisburg-Essen, Universitätstr. 2, 45141 Essen, Germany **Resume :** Titania and strontium titanate are well-known semiconductors comprehensively studied in materials science, thanks to their widespread technological applications. Doped TiO2 and SrTiO3 nanotubes (NTs) are known to be potentially promising electrodes for visible-light-driven photocatalytic applications. In this study, ab initio calculations have been performed to study the ground state properties of monoperiodic TiO2 and SrTiO3 nanotubes containing extrinsic point defects. The hybrid exchange-correlation functionals B3LYP and B3PW within the framework of density functional theory have been applied for calculations on NTs with the following substitute impurities: C(O), N (O), S(O), and Fe(Ti). The variations in formation energies obtained for these doped nanotubes have allowed us to predict the most stable compositions, irrespective of the changes in growth conditions. The changes in the electronic structure have been analyzed to show the extent of localization of the in-gap states induced by defect. The mid-gap levels positioned inside the band gaps of	EO82

defective nanotubes make them attractive for numerous applications. Moreover, inspecting the electronic charge isodensity plots, we have concluded that increased covalency in impurity-host interatomic bonds may enhance adsorption properties of defective NTs. According to obtained results, S-doped TiO2 NT and N-doped SrTiO3 NT make these nanotubes to be good candidates for efficient photocatalyst working under daylight irradiation.

add to my program (close full abstract)

09:30 **Structural Phase Transformation in TiO2 nanoparticles induced by visible light**

Authors : Luigi Stagi, Pier Carlo Ricci,Carlo Maria Carbonaro, Marcello Salis, Alberto Casu, Francesco Delogu, Stefano Enzo

Affiliations : Dipartimento di Fisica, Università degli Studi di Cagliari, S.P. Monserrato-Sestu Km 0,700, 09042 Monserrato (CA), Italy;Dipartimento di Fisica, Università degli Studi di Cagliari, S.P. Monserrato-Sestu Km 0,700, 09042 Monserrato (CA), Italy;Dipartimento di Fisica, Università degli Studi di Cagliari, S.P. Monserrato-Sestu Km 0,700, 09042 Monserrato (CA), Italy;Dipartimento di Fisica, Università degli Studi di Cagliari, S.P. Monserrato-Sestu Km 0,700, 09042 Monserrato (CA), Italy; Istituto Italiano di Tecnologia (IIT), via Morego 30, 16163 Genova, Italy;Dipartimento di Ingegneria Meccanica, Chimica, e dei Materiali, Università degli Studi di Cagliari, via Marengo 2, 09123 Cagliari, Italy;Dipartimento di Chimica e Farmacia, Università degli Studi di Sassari, via Vienna 2, 07100 Sassari, Italy

Resume : Titanium dioxide (TiO2) is a strategic material for a very wide range of applications encompassing pigments, nonlinear optics devices, gas sensor and Dye-Sensitized solar cells. Some mixed-phase TiO2 nanoparticles with coexisting polymorph (anatase + rutile, anatase+brookite) exhibit enhanced photoactivity, possibly due to the separation of charge carriers in different phases that suppresses electron−hole recombination. Hence, much research has been performed to elucidate and control the phase transformation between these two phases. Within this framework, achieving a suitable control of the phase transition behavior of nanometer-sized TiO2 materials would represent a significant progress on the way of their full exploitation in different areas of science and engineering. In this work we report visible light induced anatase to rutile structural phase transformation mechanism depending on the surrounding environment and power laser density on the samples. Thermal origin of the process was excluded by in situ Raman measurements that permit the estimation of the local temperature. The mechanism was attributed to surface defects induced by oxygen desorption involving F color centers. The kinetic of desorption process were also studied through intragap excited photoluminescence measurements. Transmission Electron Microscopy images revealed the presence of small polycrystalline aggregates suggesting the coalescence among neighbouring nanoparticles. Finally, a mechanism to promote or inhibit the transformation acting on the concentration and depth of color centers is presented.

EO8 3

add to my program (close full abstract)

09:45 **Lithium ion dynamics in micro- and nanocrystalline layer-structured insertion materials as seen via 7Li nuclear magnetic resonance**

Authors : Julia Langer, Viktor Epp, Martin Wilkening

Affiliations : Institute for Chemistry and Technoloy of Materials, Graz University of Technology, Stremayrgasse 9, 8010 Graz, Austria DFG Research Unit 1277

Resume : Solid-state nuclear magnetic resonance (NMR) spectroscopy can be a very powerful tool to study lithium ion motion from an atomic-scale point of view. Here, we report on 7Li NMR relaxometry measurements on the stage-1 graphite intercalation compound, LiC6, the most prominent anode material for lithium ion batteries. Li diffusion is anticipated to be two-dimensional, i.e., it occurs along the buried interfaces composed by the commensurate layers of carbon. Quantitative information of the in-plane diffusion process were obtained by SLR NMR measurements carried out in the so-called rotating frame of reference. Fortunately, by making use of the spin-locking technique we were able to probe the characteristic diffusion-induced rate peak entailing valuable information on Li self-diffusion in LiC6 around ambient temperature. In addition, results of comparative study of Li motion in chemically-intercalated tin disulfide (Li0.17SnS2) will be presented. 7Li NMR spectra of nanostructured, defect-rich Li0.17SnS2, crystallizing also with a layer structure, point to two spin reservoirs with distinct Li ion dynamics. Complementary NMR measurements on Li diffusion in nanostructured SnS2, which was prepared by mechanical treatment, might help identify the origin of the dynamic heterogeneity found in nano-LixSnS2. Such a comparison turned out to be useful to correlate the dynamic properties with the defects introduced via high-energy ball milling.

EO8 4

add to my program (close full abstract)

10:00 **Break**

Properties of SiC : Harry Bernas

10:30 **Irradiation Response of Nano-Engineered SiC**

Authors : C.-H. Chen (1), Y. Zhang (2,1), M. L. Crespillo (1), S. Shannon (3), M. Ishimaru (4), and W. J. Weber (1,2)
Affiliations : (1) Department of Materials Science & Engineering, University of Tennessee, Knoxville, TN 37996, USA; (2) Materials Science & Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA; (3) Nuclear Engineering Dept., North Carolina State University, Raleigh, NC 27695, USA; (4) Institute of Scientific and Industrial Research, Osaka University, Osaka 567-0047, Japan

Resume : Nano-engineered silicon carbide (NE-SiC) thin films have been grown on Si (100) wafers by low-pressure chemical vapor deposition. These NE-SiC films predominantly exhibit the 3C cubic structure with nanosized columnar grains grown along the [111] direction. A unique feature of these NE-SiC films is the high density of (111) of stacking faults and twins (planar defects) perpendicular to the growth direction that create a nanolayered structure within each grain. The response of the NE-SiC to electron and ion irradiation, as well as helium implantation and subsequent ion irradiation, has been investigated. The results from electron and ion irradiation studies suggest that defect migration is primarily two-dimensional and limited between the planar defects, which increases the resistance of the NE-SiC to irradiation-induced amorphization. Such two dimensional diffusion is supported by density functional theory calculations. The NE-SiC films have also been implanted with helium ions (up to 8000 appm) at 275°C to avoid irradiation-induced amorphization, and no bubble formation is observed. Subsequent irradiation of the helium implanted samples with 9 MeV Au ions at 700°C to 10 dpa revealed preferential bubble growth at grain boundaries, suggesting that helium migration may also be limited by two-dimensional diffusion. The nanolayered structure exhibits surprising stability under irradiation to 10 dpa at 700°C.

EO9 1

add to my program (close full abstract)

11:00 **Micro-Raman spectroscopy and in-situ TEM annealing of ion-irradiated SiC fibers: influence of the microstructure on radiation tolerance and recrystallization**

Authors : J. Huguet-Garcia1*, A. Jankowiak2, S. Miro3, D. Gosset4, Y. Serruys3, J.M. Costantini4
Affiliations : 1. CEA, DEN, SRMA, LC2M, F-91191 Gif-sur-Yvette, France. 2. CEA, DEN, SRMA, LTMEX, F-91191 Gif-sur-Yvette, France. 3. CEA, DEN, SRMP, Laboratoire JANNUS, F-91191 Gif-sur-Yvette, France. 4. CEA, DEN, SRMA, LA2M, F-91191 Gif-sur-Yvette, France.

Resume : Two third-generation SiC fibers, Hi Nicalon S (HNS) and Tyranno SA3 (TSA3), were irradiated with 4-MeV Au3+ at different temperatures up to a dose higher than the dose to amorphization (DTA) at room temperature (RT) for SiC (~ 0.4 displacement per atom). Both fibers present a unique microstructure consisting in faulted 3C-SiC grains and free carbon at grain boundaries and triple points, with clearly different grain sizes (~ 20 nm for HNS, and ~ 200 nm for TSA3). Micro-Raman spectroscopy data reveal that fibers with a refined grain size are less radiation resistant since they present a higher critical amorphization temperature. In light of these results, HNS fibers were thermally annealed to increase their grain size and irradiated in the same conditions. It is found that annealed HNS fibers have a TSA3-like behavior under irradiation. Moreover, in-situ TEM annealing of the ion-amorphized fibers was conducted to cross-check the Raman data. The annealing process triggers an epitaxial recrystallization of the amorphous layer from the amorphous-crystalline interphase for temperatures higher than ~ 930 ºC. This threshold temperature is higher than those for ion-amorphized SiC single crystals, i.e. 875 ºC. Finally, TEM images and electron diffraction patterns show that the recrystallized layer consists in randomly oriented 3C-SiC grains. SEM reveal that no structural damage of the SiC foils occurred during the test.

EO9 2

add to my program (close full abstract)

11:15 **In situ evolution of helium bubbles in SiC under irradiation**

Authors : M.F. Beaufort1, M. Vallet1, E. Oliviero2, J.F. Barbot1
Affiliations : 1Institut Pprime, CNRS - Université de Poitiers - ENSMA - UPR 3346, Département Physique et Mécanique des Matériaux, SP2MI, Bd M. et P. Curie - BP 30179,

EO9 3

86962 Futuroscope, Chasseneuil Cedex, France 2CSNSM - IN2P3 - CNRS, Université Paris -Sud, 91405 Orsay Campus France
Resume : In-situ transmission electron microscopy (TEM) investigations were performed in order to follow the evolution of helium bubbles under heavy ion irradiation (Au, 1.5MeV) in 4H-SiC as a function of fluence. 4H-SiC thin foils containing well-characterized bubble populations consisting of a layer of bubbles with a mean radius of 3nm were used. The SiC / He bubble specimens were then observed and irradiated in-situ in a transmission electron microscope at the JANNuS-Orsay facility*. Results indicated that the effects of displacing irradiation (1.5MeV Au ions) resulted in the gradually decrease of the bubble diameter with dose. A 1-D model showed that half of the ejected–He is re-trapped during the displacing irradiation. At high dose, the excess of vacancies due the combined effects of bubble shrinkage and displacing irradiation concomitant with a large concentration of free-He-atoms leads to the formation of satellite tiny-bubbles. The system evolves toward a steady state of bubble size keeping all the helium atoms in the matrix

add to my program (close full abstract)

11:30 **Experimental and computational investigation of the defects involved in ion-beam-induced amorphization and recrystallization phenomena in SiC**

Authors : A. Debelle1, M. Backman2,4, A. Boulle3, F. Djurabekova4, A. Chartier5, B. Weber2,6, L. Thomé1, K. Nordlund4, F. Garrido1
Affiliations : 1. CSNSM, Univ. Paris-Sud/CNRS/IN2P3, Orsay, France 2. DMSE, University of Tennessee, Knoxville, USA 3. SPCTS, Univ. Limoges/CNRS, Limoges, France 4. University of Helsinki, Helsinki, Finland 5. CEA-Saclay, DEN, DPC, SCCME, Gif-Sur-Yvette, France 6. MST Division, ORNL, Oak Ridge, Tennessee, USA
Resume : Silicon carbide (SiC) has been attracting an increasing interest for many applications in extreme environments such as structural components in fission and fusion reactors or for microelectronics devices. For all these applications, a comprehensive understanding of its behaviour under ion irradiation appears as a major fundamental issue. In this work, we present a combined experimental and computational study of both the amorphization and recrystallization processes that can take place in SiC under ion irradiation. For the amorphization process, 3C-SiC single crystals have been irradiated with 100 keV Fe ions at different fluences and characterized using RBS/C and XRD. Strain and damage levels have been monitored and compared to values obtained from molecular dynamics simulations that simulated controlled, defective SiC cells and a good agreement has been obtained. Furthermore, the well-known stimulation of the amorphization process has been confirmed and was attributed to the elastic energy stored in the defective layer that contains irradiation defects. Regarding the recrystallization phenomenon, damaged 3C-SiC single crystals have been submitted to swift heavy ion irradiation (870 MeV Pb ions) and a healing effect has been evidenced. The recovery has been observed experimentally using RBS/C and TEM and confirmed by MD calculations combined with thermal spike modelling.

EO9 4

add to my program (close full abstract)

12:00 **Lunch**

Poster session II : Ricardo Papaléo and Feng Ding

13:30 **Strain status and interdiffusion of epitaxial Pr0.7Sr0.3MnO3/La0.5Ca0.5MnO3 bilayer structure**

Authors : H.O.Wang, P.Dai, W.S.Tan
Affiliations : Key Laboratory of Soft Chemistry and Functional Materials, Ministry of Education, Department of Applied Physics, Nanjing University of Science and Technology, Nanjing, 210094, P. R. China
Resume : Epitaxial bilayer structure consisting of Pr0.7Sr0.3MnO3 (PSMO) and La0.5Ca0.5MnO3 (LCMO) was grown on (001)-oriented SrTiO3 substrate by pulsed laser deposition technique. Grazing incident x-ray reflectivity (GIXRR) and atomic force microscope (AFM) were applied to characterize the surface morphology and interdiffusion of Pr0.7Sr0.3MnO3/La0.5Ca0.5MnO3 (PSMO/LCMO) bilayer. A structural model including five layers was presented to theoretically simulate GIXRR data. The perfect GIXRR data fitting result indicated that interdiffusion at PSMO/LCMO interface could not be negligible; there was a large interdiffusion zone at the interface with a thickness of about 7 nm. High resolution synchrotron x-ray diffraction (HRXRD) patterns were also

EP2 1

employed to investigate the average structure and strain status. Besides PSMO and LCMO layer diffraction peaks, we observed another additional peak, which might stem from the large transient zone resulting from interdiffusion. This implied that the variation of crystalline structure of PSMO/LCMO bilayer occurred due to interdiffusion. Strain status was decided by Jahn-Teller (JT) strain and bulk strain together. The mechanism for strain relaxation state was different from that of tetragonal distortion.

add to my program (close full abstract)

13:30 **TRANSMISSION PROPERTIES IN DIMER FIBONACCI GaAs/Ga1-XAlXAs SUPERLATTICES**

Authors : Aziz Zoubir* , Sefir Yamina, Djelti redouan and Bentata Samir
Affiliations : Laboratory of Technology and Properties of solid

Resume : The effect of a uniform electric field across multibarrier systems (GaAs/AlxGa1-xAs) is exhaustively explored by a computational model using exact Airy function formalism and the transfer-matrix technique. In the case of biased DFHBSL structure a strong reduction in transmission properties was observed and the width of the miniband structure linearly decreases with the increase of the applied bias. This is due to the confinement of the states in the miniband structure, which becomes increasingly important (Wannier-Stark effect).

EP2 2

add to my program (close full abstract)

13:30 **A study on the microscopic damages of Cyanoacrylate/SiO2 nanocomposites due to scratch test**

Authors : A. Abbasi Eliyaderani, S. M. Zebarjad, M. Kashefi Torbati
Affiliations : Atefeh Abbasi Eliyaderani' Seyed Mojtaba Zebarjad' Mehrdad Kashefi Torbati

Resume : One of the main limitations in application of Cyanoacrylate (CA) groups is their mechanical properties such as scratch resistance that is not clearly defined. Based on literature survey done by the authors, there are not any papers concentrated on role of nano-size particles on scratch behavior of Cyanoacrylate glue. Thus the main goal of the current research is focused on the role of nano-size SiO2 on scratch behavior of Cyanoacrylate. For this purpose Alkoxyethyl Cyanoacrylate and silicon dioxide nano powders were used as matrix and reinforcement respectively. Para-toluene solfunic acid and caffeine were added to the glue. All samples were scratched under different loads and the scratch velocity was kept constant. The scratch behaviors of Cyanoacrylate nanocomposites were evaluated using scanning electron microscopy. The results indicated that Cyanoacrylate nanocomposites exhibit a more brittle damage mode, which is evidenced by the regular plastic drawing and crack lines. Various scratch induced damage features, such as mar, pseudo fish-scale, parabolic crack, and material removal, observed in the studied nanocomposites. Microscopic evaluation showed that with addition of nano size SiO2, the Cyanoacrylate scratch mechanism changed.

EP2 3

add to my program (close full abstract)

13:30 **Numerical Investigation of nanoscale SiGe DG MOSFET performance against the interfacial defects**

Authors : T. Bentrcia, F. Djeffal, M. Meguellati and D. Arar
Affiliations : 1) Department of Physics, University of Batna,Batna 05000, Algeria. 2)LEA, Department of Electronics, University of Batna, Batna 05000, Algeria. E-mail: faycal.djeffal@univ-batna.dz, faycaldzdz@hotmail.com, Tel/Fax: 0021333805494

Resume : The SiGe-based alloy is considered as one of the most promising materials for reliable and high performance microelectronic devices. The use of a lower band-gap material in the channel region of the MOSFET, such as SiGe, is a potential candidate given their compatibility with the process developed for pure Si-based devices. Moreover, the important increasing in the drain current due to the increased electrons mobility in SiGe material is expected. However, the growth of this material is not totally controlled, and the presence of defects is more than expected after a growth run of this material. Therefore, in order to obtain a global view of SiGe-based nanoscale Double Gate (DG) MOSFET performance under critical conditions, numerical modeling of nanoscale SiGe DG MOSFET including Interfacial defect effects (SiGe/Si) is indispensable for the comprehension of the fundamentals of such device characteristics. Based on numerical investigation of a nanoscale SiGe DG MOSFET including the defects in the interface region, in the present paper a numerical model for I-V and small signal characteristics by including the interfacial defects, after considering the uniform function approximation for the interface defects distribution at the drain said, is developed to explain the immunity behavior of the nanoscale SiGe-based transistor against the defect densities. In this context, DC and RF characteristics

EP2 4

of the proposed design are analyzed by 2-D numerical simulation and compared with conventional Si DG MOSFET characteristics.

add to my program (close full abstract)

13:30 **SEGREGATION ON THE SURFACE OF TITANIUM STEEL 12Cr18Ni10Ti EXPOSED ELECTRON BEAM**

Authors : Sergey Plotnikov, Nazgul Yerdybayeva

Affiliations : East Kazakhstan State Technical University, Ust-Kamenogorsk, the Republic of Kazakhstan; Sergey Plotnikov, Nazgul Yerdybayeva

Resume : SEGREGATION ON THE SURFACE OF TITANIUM STEEL 12Cr18Ni10Ti EXPOSED ELECTRON BEAM Sergey Plotnikov, Nazgul Yerdybayeva East Kazakhstan State Technical University, Ust-Kamenogorsk, the Republic of Kazakhstan In support of the research program in Kazakhstan material TOKAMAK KTM created the stand of simulation tests (FIC). Generator working on the beam-plasma discharge is used to generate plasma. At the moment gas puffing installation is being mounted. The irradiation of samples by continuous electron beam was carried out in this installation[1]. The aim of the work on the simulation stand is to obtain data of the degree degradation of construction materials samples surface under the influence of the electron beam exposure and plasma discharge[2]. The work objective is to study the structural and phase changes of the surface under the influence of the continuous electron beam on construction steel 12Cr18Ni10Ti. Plasma generator based on a beam-plasma discharge (BPD) of low pressure at which the electron beam along the magnetic field is injected into the drift chamber interaction used in the simulation KTM stand. When irradiated steel sample maximum power of the electron beam is 75 W at the heating power of the cathode-heated unit of 130W. Maximum temperature of steel sample registered by thermocouple reached 920 ? C. Study of the structural and phase changes of the samples surface after exposure of continuous electron beam is performed on a scanning electron microscope JEOL JSM-6390LV with energy dispersive microanalysis attachment INSA Energy. Electron beam irradiation of materials leads to abnormal redistribution of elements in alloys. That allows are used to create pre-defined profile of the impurity distribution and provide the necessary performance characteristics of products. Structural and phase changes in the sample surfaces is the result of thermal effects of the electron beam Literature. 1 S. V. Plotnikov, N. K. Yerdybaeva, A. A. Kolodeshnikov, V. A. Zuev, V. I. Ignashev, T. R. Tulenbergenov, and I. A. Sokolov Titanium Segregation on the Surface of 12Kh18N10T Steel under the Action of an Electron Beam//Technical Physics, 2013, Vol. 58, No. 12, pp. 1817?1821 2. S.V.Plotnikov, D.V. Postnikov The Influence of Electron Beam Irradiation on Impurity Redistribution of Binary Metallic Systems / Izv.Vuz. Physics, № 8, 2002, P.124-129

EP2 5

add to my program (close full abstract)

13:30 **Thickness dependence of magnetic properties in FeCoB-O soft magnetic films**

Authors : Huaping Zuo, Shihui Ge, Feng Zhang, Guowei Wang, Min Xu

Affiliations : Huaping Zuo, Min Xu Science and Technology on Surface Engineering Laboratory, Lanzhou Institute of Physics, Lanzhou 730000, China; Shihui Ge, Feng Zhang, Guowei Wang Key Laboratory for Magnetism and Magnetic Materials of Ministry of Education, Lanzhou University, Lanzhou 730000, China

Resume : Thin films of FeCoB-O with various thicknesses were deposited by reactive magnetron sputtering in a Ar + O2 atmosphere. The dependence of soft magnetic properties and high frequency characteristics on film thickness were investigated systematically. It was found that the films exhibit small coercivity Hc not exceeding 10 Oe for the film thickness range between 148 nm to 374 nm. Relatively high values of the real part of complex permeability and ferromagnetic resonance frequency were obtained and they can be adjusted by changing the film thickness. A largest Hk value of 78 Oe was obtained for the film with a thickness of 148 nm, a saturation magnetization 4πMs = 10.2 kG and a resistivity ρ = 3638 μΩ•cm were consistently obtained. Such good soft magnetic properties are ascribed to the exchange coupling among magnetic particles.

EP2 6

add to my program (close full abstract)

13:30 **Manipulating anisotropic superconducting usingi ferroelectric domain wall engineering**

Authors : Yen-Lin Huang1, Vu- ThanhTra2, Heng-Jui Liu1, Long-Yi Chen3, Shih-Ting Guo4, Wei-Li Lee4, Chih-Wei Luo3, Jiunn-Yuan Lin2, and Ying-Hao Chu1

Affiliations : 1. Department of Materials Science and Engineering, National Chiao Tung University, HsinChu, 300, Taiwan, 2. Institute of Physic, National Chiao Tung University, HsinChu, 300, Taiwan,3. Department of Electrophysics, National Chiao Tung University, HsinChu, 300, Taiwan, 4. Institute of Physics, Academia Sinica, Nankang, Taipei, Taiwan

EP2 7

Resume : In this work, we use two different kinds of periodically domain patterns (71 and 109) in a model multiferroic, BiFeO3 (BFO), to manipulate the critical temperature of high temperature superconductor, YBa2Cu3O7-σ (YBCO). In 109 domain pattern, each neighboring domain has contrary out-plane polarization which generates a regularity of up-down electric fields. On the other hand, in 71 domain pattern, each neighboring domain has opposite in-plane polarization, leading to the periodically compressive and tensile strain fields. Moreover, within these nanometer-scale domain walls (~2 nm), there are uncompensated spins corresponding to local magnetic fields. In contrast to normal YBCO, the transport and optical porperties observed here are significantly different in two orthogonal in-plane directions. Based on our results, we can estimate the local magnetic field, the perturbing effect to superconductivity, is about 7 Tesla from the domain walls in BFO. In summary, we have demonstrated a unique superconducting behavior through the domain structures of BFO at nanometer-scale. By controlling these two different domain structures, we intrigue more insights of superconducting mechanism and the functionality of complex oxide heterostructure for next-generation devices.

add to my program (close full abstract)

13:30 **Effects of morphology and RE doping on emission of La1-xRExVO4 powders**

Authors : O. Chukova, S.G. Nedilko, S.A. Nedilko, T. Voitenko
Affiliations : Taras Shevchenko National University of Kyiv, 4-b acad. Hlushkova Ave, 03680 Kyiv, Ukraine

Resume : Light emitting materials based on RE-activated vanadates are widely used in optical technologies. Their luminescence characteristics and related properties depend on various factors, and grain structure of powders as well as influence of RE dopants on the host lattice are among them. The morphology of synthesized micro and nanosized materials may be different for various methods of synthesis. In the present work, series of the La1 xRExVO4 (RE = Eu, Sm) powders were synthesized by solid state, co-precipitation and sol gel methods. Phase compositions and crystal lattice parameters of un-doped and RE-doped samples were determined by XRD. The microstructure of the obtained compounds was studied with SEM. Average grain sizes of powders synthesized by co-precipitation method is several times smaller than average grain sizes of powders synthesized by solid state and sol gel methods. Measured emission spectra consist of wide bands of the matrix emission and narrow spectral lines caused by inner f-f electron transitions in the impurity ions. We have observed differences in emission and excitation spectra for samples obtained by different methods and for samples with low and high activator concentrations. These results were discussed in connection with structure of the nearest surrounding of emission centers. The differences are explained by increasing of grain boundaries effects under decreasing of grains sizes. The investigation was supported by DFFD of Ukraine (Project # F54.1/040).

EP2 8

add to my program (close full abstract)

13:30 **STUDY THE THERMAL DIFFUSION, SEGREGATION AND DISTRIBUTION OF NIOBIUM ATOMS IN DEPTH OF DILUTED ALLOY OF MOLYBDENUM WITH NIOBIUM**

Authors : N.A.Nurmatov, Y.S.Ergashov
Affiliations : National University of Uzbekistan

Resume : Study the penetration depth of niobium atoms in Mo (110) and (100), the construction of high-quality model of the niobium atoms near the surface of alloy. Using the low-energy ion implantation method of niobium atoms, monocrystalline samples were obtained from the niobium-molybdenum alloys . Concentration distribution of niobium atoms in a depth monocrystalline molybdenum were determined. Change of the atomic concentration on the subsurface of the alloy has been experimentally shown based on the heat treatment and prolonged heating of the crystal. A maximum concentration of niobium atoms is observed at approx. 4 atomic layer depth of the diluted alloy at a temperature close to 1400 K. A maximum atomic concentration of the niobium atoms on the subsurface of the alloy reaches to approx. 3%. Auger - spectra, spectral dependent quantum yield, and energy dependent photoelectron distribution [1] indicate that the obtained alloys are clean. Analyzing the results obtained are the following experimental facts. When a crystal surface is bombarded by ions of the alloying element, occurs a spraying of surface layer atoms of the crystal, atoms of the impurity element and the atoms of the doping component. The last one give a limit on the number of elements implemented into the surface layer of the target. On the other hand, in the process play role the atomic structure of the crystallographic orientation, the atomic ratio of the sizes niobium and molybdenum, and surface coupling ma

EP2 9

add to my program (close full abstract)

13:30 **INVESTIGATION OF ALGAINP HETEROSTRUCTURES UNDER GAMMA-IRRADIATION IN THE FIELD OF RESTRUCTURING DEFECT STRUCTURE**

Authors : Orlova Ksenia Nikolaevna, Gradoboev Alexandr Vasilievich
Affiliations : National Research Tomsk Polytechnic University

Resume : The results of research of resistance AlGaInP heterostructures with multiple quantum wells to irradiation of 60Co gamma rays are presented. Investigations were performed on the LEDs (λ = 630 nm). Irradiation was performed in the passive mode, i.e. without the application of an electric field, and the level of exposure was characterized by the absorbed dose. It is established that the reduction of the light output power during irradiation by gamma rays occurs in the three stages. At the first stage light output power reduction is a consequence of radiation-induced restructuring initial defects, and the second stage - due to the introduction of radiation defects. In the extreme case, the second stage proceeds to the third stage (the mode of low electron injection). On the boundary between the first and second stages relaxation processes - a partial recovery of the light output power on its overall decline are observed. Heterostructures with a pronounced effect of small doses - restoring light output power due to radiation-induced strain relaxation without the formation of additional structural defects are identified. These process precedes the first stage of light output reduction under irradiation by gamma rays.

EP2 10

add to my program (close full abstract)

13:30 **Atomistic study of martensitic transformation on ω to α phase transformation in Ti-15Mo alloy**

Authors : Sung Jin Kang(1), Sung-Hwan Kim(1), Hu-Chul Lee(2), Yoon-UkHeo(2),Jae-HyeokShim(3), Heung Nam Han(1) and Miyoung Kim(1)*
Affiliations : (1) Department of Materials Science & Engineering, Seoul National University,151-744 South. Korea (2) Graduate Institute of Ferrous Technology(GIFT), Pohang University of Science and Technology, 790-784, South Korea (3) High Temperature Energy Materials Research Center, Korea Institute of Science and Technology, 136-791, South Korea *Corresponding author: mkim@snu.ac.kr

Resume : The β-Titanium alloysare inherently ductile due to its bcc crystal structure and havemore application potentials compared to the brittle α-Titanium alloys1. To stabilize the metastable β-Ti alloy upon quenching to room temperature, V, Mo, Fe and Ta are commonly added1.The β-Ti alloy could be further hardened by heat treatment, precipitating finely dispersed round shaped α-Ti phase. Interestingly,this α-Ti phase is not formed directly from the β-Ti alloy but from the nucleation sites provided by ωphase. While there have been intensive studies on the phase transformation of pure Ti2, Ti alloys, especially detailed atomistic dynamics of Ti alloys, haverarely been investigated during the phase transformation. Mo is commercially used as β-Ti stabilizer as well as α phase formatting element from the core of the ω phase precipitates. We investigate Ti-Mo(15 wt%) alloy for the phenomena of martensitic α-Ti phase formation from ω phase using aberration corrected high annular angle dark field scanning electron transmission microscopy and electron energy loss spectroscopy which are highly capable of chemical information as well as atomic structural information. We show the atomically resolved images ofextremely early stage of ω→αtransition state mediated by defects and compositional variations. We further investigated the atomistic dynamics by ab-initio calculations based on the experimental results. 1. S. Nag et.al, ActaMaterialia 57 (2009), 2136-2147 2. Richard G. Henning et.al, Nature materials 4 (2005), 129-133

EP2 11

add to my program (close full abstract)

13:30 **Investigation of the processes of nanodimensional structure formation in the surface area Pd and PdBa under ionic bombing**

Authors : B.E.Umirzakov, S.B.Donaev
Affiliations : Tashkent state technical university

Resume : Works carried out showed in recent years that in case of semiconductor and dielectric films in the course of ionic implantation and the subsequent annealing in blankets is formed two - and three- component nanocrystals and nanofilms. Similar researches for metals and metalfloatables weren't carried out so far. This work is devoted to research of change of topography, structure and properties of a surface of Pd and PdBa (Ba-1,5 of %) at ionic bombing and the subsequent annealing. Technological processing (ionic implantation, a thermal activation) and researches of structure, electronic structure, issue properties, degree of a covering of a surface decided by Ba atoms on use by the AES, EELS and UES methods in the conditions of ultrahigh vacuum (P ≤ 10-6 Pa). The technique of experiment is described in [1]. The

EP2 12

topography of a surface was studied by the SEM method in standard Camabax installation. Bombing carried out Ba+ ions with energy of E0 = 0,5-5 keV and a dose of radiation of D = 1014-1017 cm-2. Since a dose of D = 1015 cm-2 on a surface of Pd were formed separate cluster phases enriched with atoms of barium with superficial diameters to 50-60 nanometers. With increase in a dose to D ≈ 5÷6•1015 cm-2 the sizes of these phases increased and formed islands, and at a dose of D ≥ 1016 cm-2 are formed the continuous uniform alloyed layer. After warming up at T=100-1100 K in all above specified cases connections like Pd-Ba, with thickness from 3-4 nanometers (were formed at E0=0,5 keV) to 10-12 nanometers (E0=5 keV). In work the analysis of the received results is given.

add to my program (close full abstract)

13:30 **Unusual surface morphology of porous silicon passivated by Fe3 electrochemical deposition: Micro structural and Photoluminescence studies**

Authors : A. Mabrouk, N. Lorrain, M. L. Haji and M. Oueslati
Affiliations : Asma Mabrouk

Resume : In this paper, we analyze photoluminescence spectra (PL) of porous silicon (PS) layer elaborated by electrochemical etching and passivated by Fe3 ions (PSF), via current density electro-deposition and temperature measurements. We observe unusual surface morphology of PSF surface and anomalous emission behavior. The PSF surface shows regular distributions of cracks, leaving isolated regions or ?platelets? of nearly uniform thickness. These cracks become more pronounced for high current densities. The temperature dependence of the PL pic energy (EPL) present anomalous behaviors, i:e., the PL peak energy shows a successive red/blue/redshift (S-shaped behavior) with increasing temperature that we attribute to the existence of strong potential fluctuations induced by the electrochemical etching of PS layers. A competition process between localized and delocalized excitons is used to discuss these PL properties. In this case, the confinement potential plays a key role on the enhancement of PL intensity in PSF. To explain the temperature dependence of the PL intensity, we have proposed a recombination model based on tunneling and dissociation of excitons.

EP2 13

add to my program (close full abstract)

13:30 **Effect of proton irradiation H (2.5 MeV) on the critical parameters of composite HTS tapes**

Authors : Antonova L.Kh.1, Demikhov T.E.2, Troitskii A.V.1, Didyk A.Yu.3 , Kobzev A.P.3, Kulikauskas V.S.4, Mikhailova G.N.1
Affiliations : 1 A.M. Prokhorov General Physics Institute of RAS; 2 Lebedev Physical Institute of RAS; 3 Joint Institute for Nuclear Research; 4 Skobeltsyn Institute Nuclear Physics of MSU (Moscow State University)

Resume : Proton irradiation H (2.5 MeV) have been conducted of the 2-G composite HTS (high temperature superconducting) tapes YBCO(123) to increase the current-carrying capacity and determine the radiation resistance. The HTS tapes have complex multilayer architecture, wherein the superconducting layer takes only 1% in the thickness. TRIM Model calculations have shown that the energy of protons should be about 2.5 MeV so that the path length within the tape was more than 20 microns, and protons could achieve the superconductor layer. Irradiation was carried out on the Dubna accelerator (AG-5) and in MSU. The sample temperature did not exceed 100C during the irradiation. Measurements of Tc and Ic were carried out by the resistive method. The dependence of the critical current on the magnetic field studied in fields up to 8T at 77 K. Critical current increasing was observed at the fluence range 2x10^15 - 6x10^15 ions/cm^2. This fact arises from generation of radiation defects in the superconductor during H irradiation. A threshold was defined: 6x10^16 ion/cm^2 for radiation damage of the 2-G YBCO tape. Since protons do not cause tracks in the material, as in the case of heavy-ion irradiation, therefore the generation of pinning centers have to go through the other mechanism.

EP2 14

add to my program (close full abstract)

13:30 **Surface Effects under Visible Irradiation and Heat Treatment on the Phase Stability of γ-Fe2O3 Nanoparticles and γ-Fe2O3 –SiO2 Core-Shell Nanostructures**

Authors : Luigi Stagi , Jose A. De Toro, Andrea Ardu, Carla Cannas, Alberto Casu, Pier Carlo Ricci
Affiliations : Dipartimento di Fisica, Universitá degli Studi di Cagliari, S.P. Monserrato-Sestu Km 0,700, 09042 Monserrato (CA), Italy;Instituto Regional de Investigación Científica Aplicada (IRICA), Departamento de Física Aplicada, Universidad de Castilla-La Mancha, 13071 Ciudad Real, Spain; Department of Chemical and Geological Sciences,

EP2 15

University of Cagliari, Monserrato Campus, SS 554 bivio Sestu, I-09042 Monserrato (CA), Italy;Department of Chemical and Geological Sciences, University of Cagliari, Monserrato Campus, SS 554 bivio Sestu, I-09042 Monserrato (CA), Italy; Nanochemistry Department, Istituto Italiano di Tecnologia, via Morego 30, 16163 Genova, Italy;Dipartimento di Fisica, Universitá degli Studi di Cagliari, S.P. Monserrato-Sestu Km 0,700, 09042 Monserrato (CA), Italy

Resume : Iron oxides are characterized by a wide variety of compounds, which differ by structural and magnetic properties. The continuing interest for this kind of materials is mainly due to the ability to take advantage of their diversity to find new important applications in several research field. Among iron oxides, γ-Fe2O3 has attracted a growing attention because its use as catalyst, pigment, gas sensitive material. Its potential applications also concern the realization of high density magnetic storage device and in vivo biological studies. In this work we report the structural evolution of □-Fe2O3 (maghemite) in bare nanoparticles and in core/shell □-Fe2O3/SiO2 systems as a function of laser irradiation and heat treatment by the combined use of Raman spectroscopy, Transmission Electron Microscopy, X-ray Diffraction. In the bare system, □- to α- Fe2O3(hematite) phase transformation was obtained with very low beam density powers (less than 2 mW at 632.8 nm focalised with a conventional 10X microscope objective). Phase transformation cannot be obtained by light irradiation in a □-Fe2O3/SiO2 core/shell system, but it can be induced by heat treatment at very high temperature (1100°C). Fe2O3 nanoparticles at high temperature can diffuse inside the silica matrix forming aggregates with the □ phase and increased size. The key role of the particle surface is discussed and a physical mechanism for the nucleation of hematite crystallites from the bonding of neighbouring maghemite nanoparticles through hydrate defect states is proposed.

add to my program (close full abstract)

13:30 **Defect modes in a magnonic crystal and their applications in energy-efficient spin-wave devices**

Authors : K. Di, H. S. Lim, S. C. Ng, V. L. Zhang, and M. H. Kuok
Affiliations : Department of Physics, National University of Singapore

Resume : Magnonic crystals, the magnetic analogue of photonic crystals, enable magnonic band engineering and hold great promise for the field of magnonics which employs spin waves as information carriers. We investigate the defect-induced effects on the band structure and spin-wave propagation properties of a magnonic crystal, as well as the coupling between defect modes. The defect states in magnonic crystals are found to induce many novel properties. We demonstrate that defect magnonic crystals in magnonic devices, such as spin-wave filters and switches, could be used as building blocks in integrated magnonic nanocircuits. Furthermore, the control magnetic field applied in the proposed devices is very low, thus ensuring energy-efficient magnonic nanocircuits.

EP2 16

add to my program (close full abstract)

13:30 **Formation of nanodimensional structures on the surface of GaAs by ion implantation**

Authors : S.B.Donaev(a), A.K.Tashatov(b), B.E.Umirzakov(a)
Affiliations : a) Tashkent state technical univercity b) Karshi state univercity

Resume : In this work we studied the effect of ion implantation on the surface topography of single-crystal film GaAs. Were obtained electron microscopic image of a GaAs surface after various stages of ion bombardment of Ba+ with energy E0 = 0,5 keV. The surface of the " pure " GaAs has a relatively smooth microtopography. Implantation of barium ions from the dose D=4·1014 cm-2, leads to a change of surface microrelief. At a dose of D=8·1014 cm-2 in the surface region of GaAs appear separate molecular complexes - clusters with modified structure and composition. They arise due to sharp thermal heterogeneity and in some cases reach a diameter of 10-15 nm. Since the dose D=6·1015 cm-2, there is a union of separate sections (clusters) with each other. Increasing the dose of Ba+ ions to 6·1016 cm-2 leads to the complete unification of clusters and surface layers of GaAs completely amorphized. Postimplantation annealing at T=900 K for 30 min causes recrystallization of the surface layer and the formation of ternary compounds such as Ba+Ga+As. In this annealing sample implanted dose D=8·1014 cm-2, results in the formation island film, and annealing the sample implanted with D=6•1016 cm-2, - a continuous film. In both cases, the formed compound with an exemplary ternary composition Ga0.4Ba0.6As.

EP2 17

add to my program (close full abstract)

13:30 **Thermal annealing effects in Mn-doped heterostructures with GaAs/InGaAs/GaAs quantum wells**

Authors : I.L. Kalentyeva, O.V. Vikhrova, Yu.A. Danilov, B.N. Zvonkov, M.N. Drozdov, A.V. Kudrin

Affiliations : Lobachevsky State University of Nizhni Novgorod, Russia; Institute for Physics of Microstructures, Russian Academy of Sciences

Resume : III-V compound heterostructures doped by Mn are a basis for semiconductor spintronics devices, for example, spin LEDs. The greatest technological difficulty is associated with intricate interaction of Mn atoms with heterostructure materials. Among these Mn-related effects are formation of MnAs clusters and rapid diffusion of Mn atoms. We studied consequences of isochronal (30 min) thermal annealing on 77 K photoluminescence (PL) and composition of heterostructures with three InxGa1-xAs quantum wells (QWs) and delta-doped layer. The delta-layer is separated from upper QW-1 by GaAs spacer with thickness of ds. The delta-layer and GaAs cap layer were grown at 400°C by laser ablation, while formation of the QWs and spacer was carried out at 600°C by MOCVD. The quantum wells had the same thickness (≈ 9 nm) and recognized by indium content from x = 0.11 to 0.26. This expedient made possible to identify the position of PL peaks on spectra with depth location of quantum well. We observed quenching emission and "blue" shift of the PL peak for the QW-1 nearest to delta-layer. The annealing temperature, at which the marked changes in the PL spectra occur, decreases from 625 to 425°C when ds value changes from 12 to 4 nm. As shown by SIMS, at elevated temperatures there are simultaneously Mn redistribution and mixing QW-1 at the upper boundary. Processes are due to diffusion of gallium vacancies, the main supplier of which is the low-temperature GaAs cap layer.

EP2 18

add to my program (close full abstract)

13:30 **Stark effect in GaNAsBi/GaAs quantum wells operating at 1.55 µm**

Authors : C. Bilel*, M. M. Habchi, A. Rebey, and B. El Jani

Affiliations : University of Monastir, Faculty of Sciences Unité de Recherche sur les Hétéro-Epitaxies et Applications (URHEA), 5019 Monastir, Tunisia E-mail: * chakroun_bilel01@yahoo.fr

Resume : The effect of an applied stationary electric field on the band structures of GaNAsBi/GaAs quantum wells has been investigated using self-consistent calculations. Such study based on the optimization of N and Bi contents can be useful to improve physical proprieties of emitters or photodetectors devices operating at 1.55 µm. We have examined the quantum confined Stark effect on the shape of the confining potential, the Fermi level, the subband energies and their corresponding wave functions as well as their occupations, and the charge density distributions. We have also determined the oscillator strength and the absorption coefficient of the inter-subband transitions and their dependences on the applied perturbation. Keywords: Stark effect; GaNAsBi/GaAs QWs; band structures; self-consistent calculations.

EP2 19

add to my program (close full abstract)

13:30 **Possible defect-induced ferromagnetism in Cr doped SiC single crystals**

Authors : Yu Liu, Shengqiang Zhou, Gang Wang, Shunchong Wang, Wei Sun, Xiaolong Chen

Affiliations : Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), P.O. Box 510119, 01314 Dresden, Germany Yu Liu, Shengqiang Zhou; Research & Development Center for Functional Crystals, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China Yu Liu, Gang Wang, Shunchong Wang, Wei Sun, Xiaolong Chen; Collaborative Innovation Center of Quantum Matter, Beijing, China Xiaolong Chen

Resume : Defect-induced ferromagnetism (FM) was realized in non-magnetic materials, such as highly oriented pyrolytic graphite (HOPG), HfO2, and Li doped ZnO. Recently, such FM was also found in SiC by doping, neutron bombardment and ion implantation. As now SiC crystals are available in microelectronic grade, the good crystallinity makes SiC a kind of potential materials for spin electronics. However, one problem in defect-induced FM in bulk SiC crystals is that the magnetization induced by defects is not strong, which might increase the difficulty for the further study. Here, we demonstrate the enhanced defect-induced FM in Cr doped SiC. The 4H-SiC single crystals were grown by physical vapor transport method. The SiC sample is diamagnetic when the nominal doping density of Cr is below 0.5%, whereas the room-temperature FM reaching 1.5 x 10-3 emu/g is observed in SiC with 1% Cr doping. However, the actual Cr concentrations in magnetic SiC measured by secondary ion mass spectroscopy are nearly equal in both the nominal 0.5% and 1% samples, so Cr doping is not

EP2 20

the origin of the FM. After annealing, the decreased magnetization suggests that the FM is closely associated with defects. However, we can not distinguish the defect types by positron annihilation lifetime spectroscopy or photoluminescence. The defects with higher dimensions rather than divacancies are proposed to induce the FM in Cr doped SiC. More efforts are needed to clarify this puzzling phenomenon.

add to my program (close full abstract)

13:30 **The parameters of localized states in Er-doped TlInSe2 single crystals**

Authors : S.N.Mustafaeva 1, M.M.Asadov 2
Affiliations : 1Institute of Physics, National Academy of Sciences of Azerbaijan, 2Institute of Chemical Problems, National Academy of Sciences of Azerbaijan

Resume : TlInSe2 single crystals are typical representatives of chain-layered semiconductors and attract a lot of attention due to their interesting physical properties. These properties include strong anisotropy of the electric parameters related to special features in the crystalline structure. Chain and layered crystals usually contain structural defects, such as vacancies and dislocations. The presence of these defects results in a high density of localized states near the Fermi level. The states localized in the band gap are responsible for most electronic processes occurring in semiconductors. The large anisotropy in chemical bonding (strong, ionic-covalent bonds within the chains and weak, van der Waals forces between the chains) enables effective doping of TlInSe2 single crystals. The concentration and nature of dopants have a significant effect on the electrical properties of TlInSe2 single crystals. The electrical properties (loss tangent, real and imaginary parts of complex dielectric permittivity, and ac conductivity of Er-doped (1 mol % Er) p-type TlInSe2 single crystals have been studied in the frequency range from 50 kHz to 35 MHz. The results demonstrate that the dielectric dispersion in the studied crystals has a relaxation nature. The experimental frequency dependence of the dissipation factor for TlInSe2:Er single crystals is characterized with a monotonic descending with frequency, which is evidence of the fact, that conductivity loss becomes the main dielectric loss mechanism at studied frequency range. At all studied frequencies the ac conductivity of the crystals varies according the law, characteristic of hopping conduction through localized states near the Fermi level. The Fermi-level density of states, the spread of their energies, and the mean hop distance and time have been estimated.

EP2 21

add to my program (close full abstract)

13:30 **Modification and Decreasing Defects of Thin Gate Dielectric of MIS Devices by Injection-Thermal and Irradiation Treatments**

Authors : V.V.Andreev1, G.G.Bondarenko2, V.M.Maslovsky3, A.A.Stolyarov1, D.V.Andreev1
Affiliations : 1) Bauman Moscow State Technical University, Kaluga Branch. 4, Bazhenov St., Kaluga, 248600, Russia 2) National Research University Higher School of Economics, 20, Myasnitskaya Ulitsa, Moscow 101000, Russia 3) The state unitary enterprise of a city of Moscow Research-and-production centre "SPURT", Zelenograd, West of the 1-st proezd 4, 124460, Russia

Resume : The effect of high-field injection–thermal and irradiation treatments on MIS structure reliability and decrease defects of the nanothin gate dielectric have been investigated. Injection-thermal treatment (ITT) of MIS structures was the high-field electron injection given the charge in gate dielectric and then the restoration of parameters of MIS structures by means of thermal annealing. MIS structures have been studied using the new techniques of control current stress. The study showed that the ITT can improve the MIS structures reliability, leading to an increase in the charge injected to breakdown and identify structures with defects. This result was attributed to a structural modification of SiO2 and its interfaces as a result of ITT. It is shown that the ITT at elevated temperatures can lead to poor reliability characteristics of MIS devices. This phenomenon seems to be associated with obstruction of the activation of electron and hole traps at elevated temperatures. It has been shown that the irradiation treatment allows to reduce the density of defects in thermal SiO2 films, SiO2 films doped phosphorus and oxynitride films and as a result is increased the reliability of MIS devices.

EP2 22

add to my program (close full abstract)

13:30 **Axial Strain controlled electrical conduction in 2D transition metal oxides and dichalcogenides**

Authors : Sumeet Walia, Hussein Nili, Sivacarendran Balendhran, Sharath Sriram, Madhu Bhaskaran
Affiliations : Functional Materials and Microsystems Research Group, School of Electrical and Computer Engineering, RMIT University, Melbourne, Victoria 3001, Australia

EP2 23

Resume : Two-dimensional (2D) transition metal dichalcogenides and oxides (TMDs) are attracting tremendous interest due to their fascinating electronic and optical properties. The presence of an intrinsic bandgap and the possibility to engineer their electronic energy states makes these materials highly desirable. Molybdenum disulphide (MoS2) and molybdenum trioxide (MoO3) are the most popular 2D transition metal dichalcogenide and oxide, respectively. So far, doping and intercalation techniques have been widely employed for tuning the electronic band structures of TMD monolayers, however a precise control over such manipulations is yet to be achieved. The application of localised strain is an attractive approach for tuning the band gaps and electronic transport properties of TMD monolayers due to the metal–semiconductor transitions that are known to occur due to strain effects. In this work, we analyse the effect of axial strain on the electronic properties of the most commonly used TMDs (MoS2 and MoO3). We perform mechanical nanoindentation on the monolayers by applying highly localised axial strain. In situ current–voltage (I–V) characteristics are acquired at varying strain levels. A time based correlation between the applied strain and current is also obtained. It is shown that electronic transitions in TMDs can be engineered using highly localised strains. Such strain effects offer a potential tool for controllably tuning transport properties and adding to the operational versatility of TMDs opening new horizon for prospective applications in electronics, optoelectronics, and NEMS.

add to my program **(close full abstract)**

13:30 **LEED-STUDY OF LAYER EPITAXY DURING GROWTH INITIAL STAGE**

Authors : S.J.Nimatov, D.S.Rumi
Affiliations : Tashkent state technical university

Resume : The investigation of the initial stage of the epitaxial growth of nanocrustals is needed to get the information on the layer structure and to identify the mechanism of the growth. With the development of the surface sensitive method of low and mean energy electron diffraction and technology tendency to nanofilm systems, the estimations of the degree of the surface perfection at the qualitatively new quasi-two-dimensional level, obtained during the epitaxial growth of real surface are needed. While investigating the ultrafine layers the sensitivity of the diffraction methods to the characteristic manifestations of growth initial stages rises, connected with the growth velocity change. Both the selective deposition with the following island coalescecence and defect annealing on substrate surface and also the development of proper nanofilm defects define the contrast of the structural and hence the electrophysical properties of the transition layers and phase boundaries. An apparatus has been made which allowed to measure the contrast of the diffraction and background intensities of low energy electron diffraction (LEED) patterns and to estimate the structural surface perfection. The initial stage of Bi layer growth on Si(111) and solid-phase epitaxy for Ge on Si(111) have been investigated. The conditions which allow to choose the production processing for atomically smooth Bi surfaces on Si(111) have been determined. The influence of heat treatment conditions for Si(111) sample on the preepitaxial preparation and structure of Ge film during annealing and evaporation stages have been studied.

EP2 24

add to my program **(close full abstract)**

13:30 **DISTRIBUTION PROFILES OF ATOMS AT THE BOUNDARY OF CoSi2/CaF2/Si (111) NANOFILM SYSTEM**

Authors : B.E.Umirzakov, S.J.Nimatov
Affiliations : Tashkent state technical university

Resume : Ion-electron technology coupled with atomic-sensitive diagnostic methods is widely used in modern thin film nanoelectronics. In recent years there is an increasing interest in the study of thin films of metal silicides and epitaxial films like CoSi2, CaF2 due primarily uniqueness of their physical properties. On the basis of such silicide films the new of multi-layer systems like silicide -insulator-semiconductor can be created, which are the basic elements of highly complex devices of solid state electronics (LSI, ULSI, radiation detectors, solar elements, electronic storage devices etc.). Although these films have the same crystal structure, they must be in agreement with certain requirements: the presence of strong chemical bonds and low diffuse of atoms of contacting surfaces, the proximity of the lattice constants and of the thermal expansion coefficients. The main optical parameters are the refractive index n, the reflection coefficient r, and the dielectric permittivity. All of these parameters are directly connected with the microscopic parameters of the crystal and depend on the temperature and in some cases on the thickness of the dielectric film. In this paper, the chemical composition and the distribution profile of the

EP2 25

impurity atoms in depth of nanofilm CoSi2/SaF2 system grown on the Si (111) by molecular beam epitaxy (MBE) method under ultrahigh vacuum conditions have been studied by use of the Auger Electron Spectroscopy (AES) and by Secondary Ion Mass Spectr

add to my program (close full abstract)

13:30 **Enhancing electrical properties of transparent Er-doped ZnO films**

Authors : Y. Kafadaryan (a), N. Aghamalyan (a), A. Igityan (a), S. Petrosyan (a), N. Aramyan (b), R. Hovsepyan (a)
Affiliations : a-Institute for Physical Research, NAS of Armenia, Ashtarak, Armenia; b-Institute of Radiophysics & Electronics, NAS of Armenia, Ashtarak, Armenia

Resume : Er (0.48-1.2 at.%)-doped ZnO thin films were prepared by e-beam evaporation and electrical and optical properties characterized using optical transmission and far-infrared reflectivity spectroscopy. The optical conductivity s (□), dielectric e1(□),e2(□), effective mass, meff (□), and electron loss energy ? Im[1/e(□)] functions of Er-doped ZnO films have been calculated via Kramers-Kronig transformation of the reflectivity spectra and analyzed by the generalized Drude (one-component) and Drude-Lorentz (two-component) models. Lorentz oscillator is necessary to simulate the spectroscopic data, revealing the presence of bound optically active electrons, whereas one-component Drude model leads to a frequency dependent scattering rate (□) and enhanced low-frequency effective mass (meff). Absorption edge, band-gap energy shift (□E), and free charge concentration (N) depending on Er concentration have been obtained by optical transmission spectra. Carrier transport properties (N/m, meff, mopt, rDr) determined from Drude analysis and optical transmission spectra (N, □E) have been compared with data obtained by Hall measurements. The electron concentration (N/m) and electron mobility in Er-doped ZnO films are achieved up to 1021 cm-3 and ~ 10-3 m2/Vs. The carrier transport properties including doping mechanism and carriers origin is discussed.

EP2 26

add to my program (close full abstract)

13:30 **Magnetic resonance in ion-beam synthesized Fe3Si films (computer simulation)**

Authors : N.A.Balakirev, V.A.Zhikharev
Affiliations : Kazan National Research Technological University

Resume : High dose Fe+ ion implantation into Si assisted by an external magnetic field results in the formation of granular magnetic film with pronounced uniaxial magnetic anisotropy in the film plane[1]. In [2] it was supposed that the anisotropy is caused by the growth of elongated clusters of magnetic silicide Fe3Si and computer simulation of this process was made. Magnetic (ferromagnetic) resonance is one of the methods sensitive both to the shape of ferromagnetic particles and to their spatial arrangement. In the present work, the features of magnetic resonance signals for synthesized Fe3Si films are numerically studied. Shape anisotropy of the clusters leads to large shift of resonance signal depending on the magnetic field orientation. Dipole-dipole interaction between clusters also results in the signal shift, but, more important, strongly influences the absorption line shape (for example, at 10% concentration of clusters in the film the absorption line is bimodal). The results are due to the peculiarities of dipole field distribution over the granular film which are discussed. [1] G.G.Gumarov,V.Yu.Petukhov,V.A.Zhikharev et al. Nucl.Instr.Meth.Phys.Res.B, 267 (2009) 1600 [2] N.A.Balakirev,G.G.Gumarov,V.A.Zhikharev et al. Comp.Material Science, 50 (2011) 2925

EP2 27

add to my program (close full abstract)

13:30 **Reduction of Contribution of Grain Boundary Scattering to Carrier Transport Using Critical Layers for Polycrystalline Al-Doped ZnO Films Prepared by Magnetron Sputtering**

Authors : J. Nomoto1), H. Song1), H. Makino1), S. Kishimoto1), 2) , T. Yamamoto1)
Affiliations : 1) Materials Design Center, Research Institute, Kochi University of Technology, Japan ; 2) Kochi National College of Technology, Japan

Resume : We will clarify the effects of critical layers (CLs) on the improvement of carrier transport of highly transparent Al-doped ZnO (AZO) polycrystalline films. In this work, our aim is to establish the roles of the CLs prepared at the beginning of the film growth on control of properties of the AZO films. To achieve low-electrical resistive (ρ) AZO films, it is necessary to develop a deposition technology to realize (1) an increase in carrier mobility in grain bulk (Mig), and (2) reduction of the contribution of grain boundary (GB) scattering to carrier mobility, which can be defined by a ratio of Mig to carrier mobility at the GB (Mgb). We deposited AZO films on glass substrates at a substrate temperature of 200 ºC using magnetron sputtering (MS) technique with Al2O3 contents of 2.0 wt.% in the sputtering target. Firstly, we deposited the AZO

EP2 28

films as CLs with various thicknesses ranging from 2 to 30 nm by a rf-MS (rf power of 200 W). Then, we deposited AZO films by a dc-MS (dc power of 200 W) to obtain 500-nm-thick AZO films. Analysis of the data obtained Hall effect measurements combined with the analysis based on Drude model shows the distinct role of the 10-nm-thick CLs on the drastic reduction in Mig / Mgb from 29.3 % of the CLs-free AZO films to 7.1% of the AZO films with the CLs together with an increase in carrier concentration. As a result, the ρ decreased significantly from 3.59×10-4 Ωcm of the CLs-free AZO films to 2.89×10-4 Ωcm of the AZO films with the CLs.

add to my program (close full abstract)

13:30 **Transport and magnetic properties of proton-irradiated ferromagnetic InMnAs layers with MnAs inclusions**

Authors : A.V. Kudrin, Yu.A. Danilov, A.V. Shvetsov, H. Boudinov
Affiliations : University of Nizhny Novgorod, Nizhny Novgorod 603950, Russia; Instituto de Física, Universidade Federal do Rio Grande do Sul, Porto Alegre 91501-970, Brazil

Resume : Ion irradiation can vary the carrier concentration in semiconductors due to formation of radiation defects. We investigated the influence of proton implantation on transport and magnetic properties of InMnAs layers. The layers were grown by laser deposition technique and contain MnAs clusters of 20-50 nm in size. We have shown that the MnAs clusters determine magnetic and magnetortansport properties of as-grown InMnAs layers. In particular, the anomalous Hall effect (AHE) is related to presence of the MnAs clusters. To change the carrier concentration in the layers and the type of majority carriers, the proton implantation was carried out with an energy of 100 keV and a fluence in the range 1e11 – 2e15 cm-2. Proton implantations with fluences up to 1e14 cm-2 lead to a decrease in the concentration of carriers (holes) as a result of the partial compensation of the Mn acceptor impurity by radiation-induced donor-type defects. We observed that for InMnAs layers with different Mn content the conversion of the conductivity type from p to n occurs for a fluence about 2e14 cm-2. For this fluence the hump on the resistivity dependence on the fluence was observed for all samples. We have found that the magnetic property of irradiated and as-grown layers is practically unchangeable. It should be noted that the AHE was observed also in layers irradiated to n-type. For p and n-type layers the hysteresis part of the AHE keeps its sign while the linear part of the AHE changes it.

EP2 29

add to my program (close full abstract)

13:30 **Spin-Dependent Domain Wall Scattering Effect in Magnetoresistance of Metal-Polymer Composites Prepared by Implantation of Transition Metal Ions**

Authors : Y.A. Bumai1, A.A. Kharchenko2, R.I. Khaibullin3, M. G. Lukashevich2, V.B. Odzhaev1
Affiliations : 1 Belarussian national technical university, 220030, Minsk, Belarus; 2 Belarusian State University, 220030, Minsk, Belarus; 3 Kazan Physical-Technical Institute, RAS, 420029, Kazan, Russian Federation

Resume : Metal-Polymer composites have been formed in thin (40μm) films of polyimide (PI) and polyethyleneterephthalate (PET) by implantation of 40 keV Co+, Cu+, Ag+ and Fe+ ions with high fluences (2.5•10^16–1.5•10^17cm^-2). Magnetoresistance (MR) and magnetic hysteresis loops have been measured at 4.2 K and magnetic fields up to 5 T. After implantation an increase of conductivity of the near-surface layers for all composites have been observed. Insulator to metal transition (IMT) at critical fluences 5•10^16 and 1•10^17 cm^-2 has been detected correspondingly for PI(Co) and PET(Fe) only. Negative magnetoresistive effect on both sides of the IMT for these composites has been observed. On the insulating side of the IMT magnetoresistance is characterized by non-monotonic dependence on magnetic field and hysteresis with sharp minima at magnetic fields of 0.1 T. The MR value at these fields is of about 2% and twice as large as the MR at 5 T. The MR peak disappears after magnetic field increasing in the same direction. Magnetic hysteresis loops at low temperatures are open, but coercive force is smaller (~0.03 T). It allows to conclude, that in spite of insulating regime of conductivity MR of metal-polymer composites is not caused by electron tunneling between magnetic clusters. Spin-dependent scattering of electrons by domain walls in agglomerates of magnetic inclusions is supposed to be responsible for the effect.

EP2 30

add to my program (close full abstract)

13:30 **Cathodoluminescence analysis of damage accumulation in irradiated Gd2Zr2O7**

Authors : Iwona Jozwik-Biala 1). Jacek Jagielski 1,2). Grzegorz Gawlik 1). Urszula Brykala 1). Gerard Panczer 3). Xiaochun Wang 3). Nathalie Moncoffre 4). Aurelien Debelle 5). Lionel Thomé 5)
Affiliations : 1) Institute of Electronic Materials Technology, Wolczynska 133, 01-919

EP2 31

Warszawa, Poland; 2) National Center for Nuclear Research, A. Soltana 7, 05-400 Otwock, Poland; 3) Institut Lumière Matière, UMR5306 Université Lyon 1-CNRS, Université de Lyon 69622 Villeurbanne cedex, France; 4) Institute de Physique Nucléaire Lyon, UMR5822, 69622 Villeurbanne Cedex, France; 5) Centre de Sciences Nucléaires et de Sciences de la Matière, IN2P3-CNRS, Université Paris-Sud, 91405 Orsay Cédex;
Resume : Pyrochlores with general formula A2B2O7 exhibit many interesting structural, physical, and electrical properties related to their various chemical compositions allowing for technological applications in various domains, such as catalysis, sensors, ionic conductors, or thermal barrier coatings. They also belong to the group of materials expected to be used as immobilization matrices for nuclear wastes. Polycrystalline Gd2Zr2O7 samples prepared by hot pressing technique were irradiated with 320-keV Ar ions at fluences ranging from 1x1011 to 2x1016 cm-2. A cathodoluminescence (CL) spectra consisting of six peaks positioned at ~493, 547, 593, 619, 698 and 730 nm were recorded for virgin and irradiated samples. The changes of peaks areas related to the increasing irradiation fluences were registered and the data analyzed in the frames of Multi -Step Damage Accumulation (MSDA) model. That allowed for the determination of kinetics and cross-section for radiation damage build-up. The direct correlation between the defects formation and the rapid decrease of the luminescence signal was observed, which mostly occurs in the first stage of the defects accumulation and is probably caused by creation of small defects clusters. The results point out to the possible use of luminescence techniques for quantitative analysis of damage accumulation in polycrystalline materials, thus offering interesting practical applications.

13:30 **Resistivity Changes Associated with Grain Coarsening in Nanocrystalline Nickel**

Authors : J E Danbrough(1), B Roebuck(2), PEJ Flewitt(1)
Affiliations : (1)Interface Analysis Centre, School of Physics, University of Bristol, Bristol, UK; (2)National Physical Laboratory, Teddington, UK
Resume : Samples of nanocrystalline nickel of ~50nm grain size have been subjected to a range of isochronal and isothermal heat treatments in the temperature range 300°C to 600°C. Resistivity measurements have been made on all heat treated specimens resulting in a range of grain size specimens containing different dislocation densities. These measurements have been made at room temperature and 77K. This allows the contribution of electron scattering from temperature and crystal defects, imperfections and grain boundaries on the changes in resistivity to be explored. The changes in resistivity have been correlated with grain size measurements made post testing by focused gallium ion beam milled section and imaging subsurface. In addition grain coarsening at temperature has been monitored for the isochronal heat treatments using a dedicated resistivity system at the National Physical Laboratory. It is observed that the initial nanocrystalline nickel of grain size ~50nm coarsens to ~550nm and then stabilizes but at temperatures above 485°C this is followed by the onset of abnormal grain growth. The results are discussed with respect to the grain size dependency of resistivity and the role of grain boundary volume together with the ability of the resistivity technique to provide a dynamic measure of grain coarsening.

EP2 32

13:30 **Ion-induced degradation of phase stability and hardness of TiZrSiN nanocomposite thin films**

Authors : V.V. Uglov1, G. Abadias2, S.N. Dub3, G. N. Tolmachova4, S.V. Zlotski1, I.A. Saladukhin1, S.S. Leshkevich1
Affiliations : 1Belarusian State University, Minsk, Belarus; 2University of Poitiers, Poitiers, France; 3Institute for Superhard Materials NAS, Kiev, Ukraine; 4Kharkov Institute of Physics and Technology, Kharkov, Ukraine
Resume : Structure and phase composition of the coatings based on transition metal nitrides can be signifi-cantly improved by addition of silicon. Such thin films are potential candidates for radiation-tolerant materials due to high density of interfaces which act as efficient sinks and recombination sites for radiation-induced point defects. The effects of the irradiation (180 keV Xe2+, doses 1•10^16 cm-2 and 5•10^16 cm-2) on the structure, phase composition and hardness of nanocomposite (TiZr)1-xSixN thin (300 nm) films deposited by magnetron sputtering (silicon concentration x≤0.22) were studied. It was found that the increase in Si content results in the transformation of structure from nanocrystalline (x ≤ 0.06, grain size of 10-18 nm) to nanocomposite (0.09 ≤ x ≤ 0.13, grain size of 4-8 nm) and then to amorphous (x ≤ 0.22) state. The phase composition of the films changes from two-phase (crystalline c-TiZr(Si)N + amorphous a-SiNy) to the amorphous system: a-TiZrSiN. Nanocomposite

EP2 33

TiZrSN film is a composite based on c-TiZr(Si)N grains with the size of 4-8 nm surrounded by an amorphous a-SiNy phase. Ion irradiation with Xe ions triggers the crystallization of TiZrN-rich grains for nanocomposite ($0.09 \leq x \leq 0.13$) and amorphous films ($x \leq 0.22$). It was found that irradiation leads to a decrease in nanoindentation hardness, due to the accumulation of Xe ion in the coating, as well as the elemental redistribution of solid solution constituents in the area of collisions cascades.

add to my program (close full abstract)

13:30 **Study on γ-ray irradiation resistance of novel telluride glasses**

Authors : S.Baccaro, A.Cemmi, Y. Zhou, Y. Yang, G.Chen
Affiliations : ENEA, Roma (Italy): S.Baccaro; A.Cemmi ECUST, Shanghai (China): Y. Zhou; Y. Yang; G.Chen

Resume : Compared with traditional silicate and phosphate glasses, heavy metal oxide telluride glasses possess special properties, such as high density, refractive index and dielectric constant, notable nonlinear optical effects, good corrosion resistance and high thermal and chemical stability. Tellurite glasses are also interesting for their high electrical conductivity for potential application in solar cells and low-current, long life batteries. There are significant progresses in variety of heavy metal oxide telluride glasses but their irradiation resistance is less reported. In this work, effects of γ-ray irradiation on series of novel telluride glasses in TeO2-B2O3-Bi2O3-PbO system are studied. In particular, the γ-ray irradiation induced formation of different defect centers in telluride glasses is characterized by UV and visible transmission spectra and calculated with Radiation Induced Absorption Coefficient (RIAC) formula. The influences of different dopants (Ag2O, Li2O, WO3, Cr2O3, CeO2, NiO) on the γ-ray irradiation effect are compared and discussed with respect to structural variation between undoped and doped tellurate glasses with the help of FTIR spectra.

EP2 34

add to my program (close full abstract)

13:30 **Modification of the interface defect composition of GaN epitaxial layers for HEMT structures by weak magnetic fields**

Authors : Red'ko R.A., Konakova R.V., Milenin V.V., Shvalagin V.V., Red'ko S.M.
Affiliations : V. Lashkaryov Institute of Semiconductor Physics of the National Academy of Sciences of Ukraine, 41 Nauky Pr., 03028 Kyiv, Ukraine

Resume : Epitaxial layers of GaN under investigation were MOCVD-grown on Al2O3 substrate and doped with Si up to 1.6·1019 cm-3 carriers concentration. The width of films was 2.0-2.5 μm varied. Photoluminescence measurements were carried out at room temperature in the 350–650 nm wavelength range using a Perkin-Elmer LS55 PL spectrometer. The spectral dependencies of the optical density of epitaxial structures were measured at 300 K with a spectrophotometer Specord 210 in the 350–1100 nm wavelength range. The treatment in pulse weak magnetic field was at regime with B = 60 mT, f = 10 Hz, τ = 1.2 ms, t=1, 3, 5 and 8 min. All measurements were repeated during the time that was needed to reaching some equilibrium state with non-changed OD and PL spectra. Usually, it was near the month. WMF treatment with different duration leads to different features in OD spectra. The influence of WMF on GaN/Al2O3 device structures leads to the reduction of defects, which exist at the interface film-substrate due to destruction of the metastable complexes. The study of the evolutionary features of GaN/Al2O3 structures OD spectra have shown an exponential dependence of the maximum of WMF-induced effect on the duration of magnetic-field treatment. Such WMF action can be used as a cost-effective method for modification of the structural parameters and decrease of non-equilibrium centres in semiconductor materials and devices

EP2 35

add to my program (close full abstract)

13:30 **Structural and optical characterization of AlxGa1-xN alloys doped with Rare Earth ions**

Authors : M. Fialho a, K. Lorenz a, S. Magalhães a, J. Rodrigues b, A. J. Neves b, T. Monteiro b, E. Alves a
Affiliations : a Campus Tecnológico e Nuclear, IPFN, Instituto Superior Técnico, Universidade de Lisboa, EN10, 2695-066 Bobadela LRS , Portugal; b Departamento de Física e i3N, Universidade de Aveiro, 3810-193 Aveiro, Portugal

Resume : Light emission from rare earth (RE) doped III-N semiconductors presents great promise for applications in electroluminescence devices. RE exhibit sharp optical emission lines due to the intra-4fn shell transitions making the tuning of light emission from the ultraviolet to the infrared in the AlGaN host realized by an appropriated choice of the dopant ion. This work study AlxGa1-xN samples grown by halide vapour phase epitaxy on (0001) sapphire substrate. Ion implantation was performed with RE ions emitting in the red (Pr3+), blue

EP2 36

(Tm3+) and green (Tb3+) region of the wavelength spectrum. The fluences range between 1x1014 at/cm2 and 1x1015 ion/cm2 and the implantations were performed with the beam tilted (10º) or aligned with the c-axis. Two energies, 150 and 300 keV, were selected to investigate the surface effects. The damage accumulation and the RE lattice site location was investigated by Rutherford Backscattering/Channeling Spectrometry (RBS/C) and High Resolution X-ray Diffraction. Rapid Thermal Annealing treatments at 1200 ºC were performed to remove damage and promote optical activation of the rare earth ions. Results show that RE ions occupy two preferential sites, the high symmetry substitutional Ga/Al site and a site displaced along the c-axis from this regular site. In order to establish models for the observed recombination centres, temperature and excitation intensity dependent Photoluminescence measurements were performed for selected samples.

add to my program (close full abstract)

13:30 **Investigation of 'memory effect' of RADIATION EXPOSURE in AlGaAs heterostructures**

Authors : Gradoboev Alexander Vasilievich, Sednev Vyacheslav Vladimirovich
Affiliations : National Research Tomsk Polytechnic University

Resume : Radiation influence leads to the degradation of the parameters of semiconductor structures and various manufactured on their basis semiconductor devices. Purpose is researching of "memory effect" under irradiation by fast neutrons in AlGaAs heterostructures. Objects of study - LEDs infrared range based on double heterostructures AlGaAs. Previously we irradiated the LEDs by fast neutrons and performed annealing of radiation defects in the current mode workout. Then radiation power reduction was studied under irradiation by fast neutrons. A result of researches the existence of "memory effect" established. The appearance of "memory effect" leads to an increase in radiation resistance under subsequent irradiation. The possible mechanisms of "memory effect"are considered.

EP2 38

add to my program (close full abstract)

13:30 **Defect-enhanced F ion conductivity in layer-structured BaSnF4 prepared by high -energy ball milling combined with soft annealing**

Authors : Florian Preishuber-Pflügl, Martin Wilkening
Affiliations : Institute for Chemistry and Technology of Materials, Graz University of Technology, DFG SPP 1415, Stremayrgasse 9, A-8010 Graz, Austria

Resume : The demand for alternative battery concepts other than conventional lithium ion technologies has revived research activities on all-solid- state batteries based on fast fluorine ion conductors. Tetragonal BaSnF4 exhibits high ion conductivity due to the highly mobile F-ions in the Ba-Sn sublattice of the double-layered crystal structure. Commonly, the ternary fluoride is obtained via conventional high temperature solid-state reactions leading to good ionic conduction. Here, we employed high-energy ball milling combined with a subsequent soft annealing step to prepare BaSnF4 from the binary fluorides BaF2 and SnF2. This approach yields a defect-rich non-layered primary product which can be transformed into the desired layer-structured modification by annealing at a temperature as low as 573 K. The large amount of defects, expected to be partially preserved also in the tetragonal form, originates from the input of stress and strain due to the initial milling process. It might be the key to understand the enhanced ionic conductivity observed in our case, which is in competition with that of powdered PbSnF4 being the fastest fluorine ion conductor known so far. Here, we report on conductivity values of 1.13 · 10-3 S/cm (300 K) measured in situ by employing broadband impedance spectroscopy, which was carried out over a large frequency range (10–3 Hz to 10 MHz). Finally, first conductivity results on the influence of non-isovalent cation doping of BaSnF4 will also be presented.

EP2 39

add to my program (close full abstract)

13:30 **Charged Defects and Defect-induced Processes in Nitrogen Films**

Authors : E.V. Savchenko1*, I.V. Khyzhniy1, S.A. Uyutnov1, G.B. Gumenchuk2, A.N. Ponomaryov3, V.E. Bondybey2
Affiliations : 1Institute for Low Temperature Physics and Engineering NASU, 61103 Kharkov, Ukraine 2Lehrstuhl für Physikalische Chemie II TUM, 85747 Garching, Germany 3Helmholtz Zentrum Dresden-Rossendorf, Dresden 01328, Germany

Resume : Radiation effects in solid N2 attract much attention in diverse fields such as material and surface sciences, physics and chemistry of interstellar and solar systems, particle physics. Radiation-induced phenomena were discussed principally in terms of neutral species reactions. The experiments [1] revealed thermally stimulated exoelectron emission (TSEE) from pre-irradiated N2 films. Creation of ionic species N3+ in electron-bombarded solid N2 was reported

EP2 40

recently [2]. Charged defect creation and defect-induced effects in electron-bombarded films of solid N2 were studied employing cathodoluminescence (CL), nonstationary luminescence NsL and activation spectroscopy. Recording the CL spectra sequences on exposure time enabled us to monitor defect production, excited particle ejection and fragmentation of molecules. Surface- and bulk-related species were discriminated by varying electron energy, i.e. the penetration depth. Creation and accumulation of N3+, N4+ and trapped electrons (up to 10^15 cm-3) as well as N radicals was detected especially in the nanostructured films. Spectroscopic evidence of excited N2* (C3Πu) molecule desorption was obtained for the first time. Charge recombination reaction N4+ + e → N2 + N2* → N2 + N2 + hv) is supposed to be the stimulating factor for desorption observed. Dynamics of post-irradiation processes was probed with TSL and TSEE. Comparative study of the NsL with dynamics of the TSL spectra and the TSEE yield elucidated the contribution of neutralization and recombination reactions. [1] I. Khyzhniy, E. Savchenko, S. Uyutnov, G. Gumenchuk, A. Ponomaryov, V. Bondybey, Radiation Measurements, 45 (2010) 353. [2] Y-J. Wu, H-F. Chen, S-J. Chuang, T-P. Huang, Astrophys. J. 768: 83 (2013).

add to my program (close full abstract)

13:30 **Process of hole capture in Ge/Si heterostructure with Ge quantum dots.**

Authors : A. A. Bloshkin*,**, A. I. Yakimov*, V. A. Timofeev*, A. V. Dvurechenskii*,**, A. A. Kirakosyan***

Affiliations : *Institute of Semiconductor Physics SB RAS, 630090 Novosibirsk, Russia. ** Novosibirsk State University, Novosibirsk, Russia *** Yerevan State University, Yerevan, Armenia.

Resume : We report an admittance spectroscopy of Ge/Si heterostructures with Ge quantum dots, grown by molecular beam epitaxy. The holes energy levels and cross sections for hole capture to the bound states in Ge quantum dot, are determined by admittance spectroscopy. We found that for heterostructures with quantum dots, grown at temperatures Tg≤450°C hole capture cross sections σ_p and activation energy E_h related to each other by exponential dependence (Meyer-Neldel rule): σ_p = σ_p0 exp(E_h/E_0) with unified parameters E_0 = 23,7±11,3 meV and σ_p0=1.67×10-17±3.74×10-16 cm2. For heterostructures with quantum dots grown at higher temperatures we found that hole capture cross section does not depend on activation energy. It was shown that Meyer-Neldel rule is violated in heterostructures treated in hydrogen plasma. The sample treated in hydrogen plasma with temperature of 100°C in 30 minutes does not show any difference with as grown sample. With increasing of plasma treatment temperature to the 150°C the characteristic energy E_0 was increased to the value of 87 meV. The sample, threaded in hydrogen plasma with the temperature 200°C show quite different behavior of σ_p(E_h): hole capture cross section is exponentially decreased with increasing of hole activation energy. For the nanonoclusters synthesized by low temperature epitaxy the experimental data are evidence of electron-phonon interaction mechanism for hole capture into Ge quantum dots assisted by structural defects.

EP2 41

add to my program (close full abstract)

13:30 **Defect evolution and precipitation in carbon implanted strained SiGe and SiSn layers**

Authors : P.I. Gaiduk, A.Nylandsted Larsen,F.L. Bregolin, W. Skorupa

Affiliations : Department of Physics and Astronomy/iNANO, Aarhus University, Denmark; Department of Semiconductor Materials, Helmholtz-Zentrum Dresden-Rossendorf

Resume : We will report on carbon segregation and precipitation, and on structural transformations in strained layered Si/SiGe/Si and Si/SiSn/Si structures after molecular-beam epitaxial (MBE) growth, carbon ion implantation, and thermal treatment. The idea behind this study is that due to their specific strain distribution, pseudomorphic layers of Si/SiGe and Si/SiSn promote spatial separation of vacancies and interstitials followed by segregation of foreign dopant atoms. Both radiation damage and strain are supposed to have impact on the precipitation of poorly soluble dopants. Based on SIMS data we will demonstrate that the redistribution of the implanted carbon atoms around the strained Si/SiGe layers results in their accumulation on the Si side and depletion on the SiGe side. On the contrary, uphill (ascending) diffusion of carbon into the SiSn layer takes place in the case of the Si/SiSn structure. The TEM study demonstrates formation of plate-like defects, stacking faults and thin carbon-precipitated flakes in the Si/SiGe layers. Raman spectra reveal peaks at 1600 and 2700 cm-1 which might be associated with carbon-related phases, and graphene-like nanoflakes. No such defects are found in the Si/SiSn layers;

EP2 42

instead, a very strong effect of retardation of tin precipitation is seen. The concepts of strain-enhanced separation of point defects and dopant precipitation will be discussed.

add to my program (close full abstract)

13:30 **An interatomic potential for Fe-Cr-C: modeling stainless steels**

Authors : K.O.E. Henriksson, C. Björkas, K. Nordlund
Affiliations : Department of Physics P.O.Box 43 (Pietari Kalmin katu 2) FIN-00014 University of Helsinki Finland

Resume : Stainless steel is an affordable and corrosion-resistant multipurpose material used in many forms in many venues of modern society. When used in nuclear power production construction steels in the vicinity of the core develop a microstructure that changes the mechanical properties of the steel. Investigation of these effects with atomistic accuracy requires an interatomic potential (force model) for the Fe-Cr-C system, which constitutes the most basic stainless steel. In this report, a potential in the Abell-Brenner-Tersoff form for the entire Fe-Cr-C system is presented to enable such calculations. The potential reproduces e.g. the lattice parameters, formation energies and elastic properties of the principal Fe and Cr carbides, especially cementite (Fe3 C), the Fe-Cr mixing energy curve, formation energies of simple C point defects in Fe and Cr, and the martensite lattice anisotropy --- all results with fair to excellent agreement with empirical data. Tests of the predictive power of the potential show that e.g. Fe-Cr nanowires and bulk samples become elastically stiffer with increasing Cr and C concentrations. Also, tests with Fe3 C inclusions show that these act as obstacles for edge dislocations moving through otherwise pure Fe.

EP2 43

add to my program (close full abstract)

13:30 **Fe-ion implantation induced defects in TiO2 thin films**

Authors : V. Scuderi (a), G. Impellizzeri (a), L. Romano (a), P. Sberna (a), E. Arcadipane (a), R. Sanz (a), F. Simone (a), V. Privitera (a)
Affiliations : (a) CNR-IMM MATIS and Department of Physics and Astronomy, University of Catania, Via S. Sofia 64, I-95123 Catania, Italy

Resume : TiO2 is the most promising material for photocatalytic applications because of its high efficiency, low cost, chemical inertness, and photostability. However, the widespread technology use of TiO2 is impaired by its wide band gap (about 3 eV) which absorbs only the UV part of the solar spectrum. Here we originally report the positive effect of Fe+ ion implantation on the photocatalytic activation of TiO2 thin films. We implanted TiO2 films (100 nm in thickness) with Fe+ ions at 80 keV with ion fluence in the range 5x1015 - 20x1015 ion/cm2. The samples were afterwards annealed for 1 h at 450, 550 or 650 °C. The materials were structurally characterized by: x-ray diffraction to reveal the effects of the ion implantation on the crystalline structure, Rutherford backscattering spectrometry to obtain information on the induced defects. The optical band gap of TiO2 film, eventually doped, was evaluated by transmittance and reflectance measurements. The doped materials show a remarkable optical absorption band in the VIS, the intensity decreases with increasing the annealing temperature. A band gap narrowing from 3.2 to 1.9 eV was determined for the samples annealed at 450 °C. These results were correlated to the presence of defects induced by the ion implantation process, which is responsible for new energy levels inside the band gap of the TiO2. The photocatalytic activity of the doped TiO2 films were also studied under UV-VIS light.

EP2 44

add to my program (close full abstract)

13:30 **Irreversible change in the conductivity of 2-dimensional electron gas at LaAlO3/SrTiO3**

Authors : Shin Ik Kim,1,2 Hyungkwang Lim,1,3 Doo Seok Jeong,1 Seung-Hyub Baek,1 Jin-Sang Kim1, and Seong Keun Kim,1
Affiliations : 1Electronic Materials Research Center, Korea Institute of Science and Technology, Seoul 136-791, South Korea 2Department of Nanomaterials, University of Science and Technology, Daejeon, 305-333, South Korea 3Department of Materials Science and Engineering, Seoul National University, Seoul, 151-744, South Korea

Resume : Since the discovery of two-dimensional electron gas (2DEG) at the interface between two band insulating oxides, LaAlO3 (LAO) and SrTiO3 (STO), considerable efforts have been dedicated to the development of novel electronic devices utilizing such a 2DEG. In particular, it was recently reported that the conductivity can be controlled using an external stimulus such as electric field, polar adsorbate, and light illumination. The tunability of the conductivity usually results from the variation in the accumulation/depletion of surface (or interface) charge under an external stimulus. It is believed that the formation of oxygen vacancies near the interface between STO and LAO is one of the reasons for

EP2 45

2DEG at the interface. Under an external stimulus such as the electric field, the oxygen vacancies at the interface can significantly influence the performance of the devices utilizing 2DEG. In this study, we examined the transport behavior of epitaxially grown LAO thin films on (100) STO substrate. We found that under the application of negative bias, the transport of 2DEG at the LAO/STO interface was irreversibly changed. The irreversible change is attributed to the migration of oxygen vacancies at the interface by the electric field.

add to my program (close full abstract)

13:30 **Rare-Earths Orthoniobates – Structural, Optical and Electrical Properties**

Authors : Cláudio Nico, F. Costa, Teresa Monteiro, Manuel P.F. Graça
Affiliations : Department of Physics & i3N, University of Aveiro, Portugal

Resume : Rare-earths Orthoniobates (RENbO4) constitutes a material class that have been exploited due to their interesting physical properties and its dependence with the lanthanide element. Besides paramagnetism and ferroelasticity, negative compressibility and interesting optical properties, these materials are known by the mixed types of conduction processes (protonic, ionic and electronic). Powders were prepared by sol-gel route, using the Pechini method, and single crystalline fibres by laser floating zone (LFZ). These samples were analysed by powder and single-crystal XRD, respectively, SEM and Raman spectroscopy. XRD measurements reveal the fibres single crystalline nature with monoclinic structure. Photoluminescence studies were performed as a function of temperature and very sharp and intense lines from the RE3+ ions were observed. Particularly for the ErNbO4, besides the fingerprint transition of the Er3+ at 1.54 um the samples exhibit strong red upconversion under 980 nm wavelength excitation. Furthermore, impedance spectroscopic studies with different atmospheres, with different hydrogen contents, were performed as a function of temperature to demonstrate the potentiality of these materials for application in fuel-cells.

EP2 46

add to my program (close full abstract)

13:30 **Defect-tailored ZnO with the Exceptional Photocatalytic Activity**

Authors : Ting-Ting Chen,1 I-Chun Chang,1 Ping-Yen Hsieh,1 Hsin-Tien Chiu,2 and Chi-Young Lee1*
Affiliations : 1Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu 30013, Taiwan, R. O. C.;2Department of Applied Chemistry, National Chiao Tung University, Hsinchu 30010, Taiwan, R.O.C.

Resume : Defects engineering on ZnO is a paramount issue in the high-efficiency photocatalysis for the next generation. Here, graphene oxide (GO) was employed to create VZn- acceptor and VO+ donor defects in ZnO lattice via a simple solvothermal reaction. Because of the oxygen release from GO thermal reduction, Schottcky and Frenkel reaction became prominent defect formation pathway to create diamagnetic defects in ZnO. Meanwhile, the Both GO and reduced graphene oxide (rGO) further catalyzed the defect ionization to create paramagnetic defects. ZnO/rGO nanocomposites with many zinc and oxygen vacancies exhibit significant photocatalytic activity due to the effective charge separation in the photodegradation of methyl orange. The photo-induced charges, holes and electrons were trapped by VZn acceptor and VO donor, respectively. The Electron paramagnetic resonance (EPR) measurements and scavenger-assisted photocatalytic reactions further show that h+ and •OH enhanced the photoactivity of ZnO/rGO as the photocatalyst.

EP2 47

add to my program (close full abstract)

13:30 **Complex diffusion behaviour of oxygen in nanocrystalline BaTiO3 ceramics**

Authors : Roger A. De Souza
Affiliations : Institute of Physical Chemistry, RWTH Aachen University and JARA-FIT, Landoltweg 2, 52056 Aachen, Germany

Resume : 18O/16O exchange annealing and subsequent Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) analysis is used to investigate oxygen transport in dense, nanocrystalline (average grain size d ≈ 300 nm) ceramics of nominally un-doped BaTiO3. All isotope profiles show the same unusual shape: a flattened profile over the first ~100 nm, followed by a short, conventional diffusion profile. We demonstrate that the entire isotope profile can be described quantitatively by a numerical solution to the diffusion equation based on an increase in the local oxygen diffusion coefficient close to the surface. This position-dependent increase is attributed to additional oxygen vacancies that are generated by diffusion of chlorine impurities out of the ceramics. The presence of chlorine derives from the chemical route necessary to produce nanometric powders: it thus indicates a new manner in which nanocrystalline ceramics may differ from their microcrystalline counterparts.

EP2 48

add to my program (close full abstract)

13:30 **RADIATION EFFECTS IN Si-Ge SUPERLATTICE p-n JUNCTIONS**

Authors : A.I. Siahlo 1), N.A. Poklonski 1), S.B. Lastovskii 2), H. Presting 3), N.A. Sobolev 4,5)
Affiliations : 1) Belarusian State University, 220030 Minsk, Belarus; 2) Scientific-Practical Materials Research Centre, NAS of Belarus, 220072 Minsk, Belarus; 3) Daimler Research & Development Ulm, 89081 Ulm, Germany; 4) Departamento de Física and I3N, Universidade de Aveiro, 3810-193 Aveiro, Portugal 5) National University of Science and Technology "MISiS", 119049 Moscow, Russia

Resume : We studied the influence of 3–4 MeV electron irradiation on the electrical properties of p-n junctions formed inside Si_6/Ge_4 superlattices (SL; The lower indices are the numbers of the Si and Ge monolayers in a SL period). I-V characteristics, C-V profiles and admittance were measured at T = 4.2–300 K. At 300 K, the forward branch of the I-V characteristics (IVC) monotonously shifts with increasing electron fluence, Φ, to lower voltages. On the contrary, at 77 K it shifts to higher voltages. At Φ ≥ 1.5*10^17 cm 2, negative differential conductivity (S-type IVC) is observed. Charge carrier and compensating impurity concentration profiles were calculated from the C-V measurements. The charge carrier concentration monotonously decreases with increasing electron fluence in all sample layers. Its relative change is equal in the SL and buffer. The barrier capacitance and conductance of the structures monotonously decrease with increasing fluence at 4.2–300 K as a consequence of the charge carrier removal in both SL and buffer. Admittance measurements at f = 1 MHz show a steep decrease of the capacitance C in the as-grown sample below 30 K, accompanied by a peak in the G(T) dependence. Upon irradiation, the peak shifts to higher temperatures. From these measurements we obtained the activation energy of the level, whose recharging produces the observed behaviour, to be equal to 44 meV. Most probably it belongs to Sb that was used as a surfactant during the sample growth.

EP2 49

add to my program (close full abstract)

13:30 **AMORPHIZATION OF SYMMETRIC AlAs/GaAs SUPERLATTICES UPON ION IMPLANTATION**

Authors : N.A. Sobolev 1), B. Breeger 2), H.T. Grahn 3), W. Wesch 2), E. Wendler 2)
Affiliations : 1) Departamento de F?sica and I3N, Universidade de Aveiro, 3810-193 Aveiro, Portugal; 2) Institut f?r Festk?rperphysik, Friedrich-Schiller-Universit?t, 07743 Jena, Germany; 3) Paul-Drude-Institut f?r Festk?rperelektronik, 10117 Berlin, Germany

Resume : AlAs/GaAs symmetric superlattices (SLs) with periods of 2.8, 20 and 150 nm grown on SI-GaAs(001) substrates were implanted with 200 keV Ar ions at 20 K with fluences in the range from 1*10^12 to 5*10^15 cm?2. The whole damage profile was placed inside the SL. Defect production was studied in situ by means of Rutherford backscattering/channeling (RBS/C) spectrometry and after warm-up to 300 K by RBS/C and cross-sectional transmission electron microscopy (XTEM). The results were compared to those obtained on a series of Al(x)Ga(1-x)As alloy samples with x ranging from 0 to 1. With respect to the amount of damage, the thinnest-period SL behaved like an alloy of the corresponding composition, whereas the behavior of that with a period of 20 nm was already quite peculiar with no coherent amorphization of the different layers. Finally, for the AlAs/GaAs SL with a period of 150 nm, a selective damage and amorphization behaviour was clearly visible in the RBS spectra. A strong defect annealing occurred following a warm-up to 300 K, whereupon the damage profile became narrower. We found a strong dependence of the recovery on the damage level produced during the low-temperature irradiation. The amorphization mechanism of the SLs and its relation to the compositional intermixing, defect diffusion etc. are discussed from the viewpoint of the current models for amorphization in the (Al,Ga)As system.

EP2 50

add to my program (close full abstract)

13:30 **ENHANCED RADIATION HARDNESS OF InAs/InP QUANTUM WIRES**

Authors : N.M. Santos 1), N.A. Sobolev 1), J.P. Leitão 1), M.C. Carmo 1), D. Fuster 2), L. González 2), Y. González 2), W. Wesch 3)
Affiliations : 1) Departamento de Física & I3N, Universidade de Aveiro, 3810-193 Aveiro, Portugal; 2) IMM-Instituto de Microelectrónica de Madrid (CNM-CSIC), 28760 Tres Cantos, Madrid, Spain; 3) Institut für Festkörperphysik, Friedrich-Schiller Universität, 07743 Jena, Germany

Resume : The photoluminescence (PL) of InAs/InP quantum wires (QWRs) is observed between 1300–1550 nm, an important region for the optoelectronic industry. The resistance of optoelectronic devices to particle irradiation is crucial in space-based telecommunication applications. In this work, we report on the influence of 2.4 MeV proton irradiation on the PL of self-assembled InAs/InP

EP2 51

QWRs and InAs/InP quantum wells (QWs) that show PL emission at similar wavelengths. The PL spectra of the QWRs consist of three main bands corresponding to families of QWRs of different height. The study of the temperature dependence of the PL reveals several excitation and transport processes of charge carriers between the wires of different heights. The proton irradiation leads to a quenching of the PL intensity both in QWR and QW samples. At the highest proton fluence used (1*10^15 cm−2) the intensity is reduced by somewhat more than an order of magnitude. This fact proves an extremely high radiation hardness of the InAs/InP QWRs because the PL in quantum size structures of other materials systems is completely quenched at such a high dose. The thermal stability of the PL is deteriorated upon irradiation, obviously due to the competition for the capture of photoexcited carriers between the QWRs and irradiation-induced defects. Another possible mechanism is tunnel escape of the captured carriers from the QWRs to neighboring defects.

add to my program (close full abstract)

13:30 **Electrical Modulation of Local Conduction at BiFeO3-CoFe2O4 Tubular Interfaces**

Authors : Ying-Hui Hsieh1, Evgheni Strelcov2, Jia-Ming Liou3, Yi-Chun Chen3, Sergei V. Kalinin2, Ying-Hao Chu1

Affiliations : 1 Department of Materials Science and Engineering, National Chiao Tung University, Hsinchu 30010, Taiwan; 2 Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, United States; 3 Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan

Resume : The plentiful physical properties arise from the interactions between degrees of freedom - charge, orbital, spin, as well as lattice, and these interactions can be modified through the effects of local symmetry breaking, charge transfer, electrostatic coupling, strain, and frustration at the oxide interfaces, producing intriguing phenomena and providing the possibility for next -generation devices. The oxide interface can be classified into 3 types- heterointerface, homointerface and tubular interface through composition or structure. Some observations such as 2D electron gas at the LaAlO3-SrTiO3 heterointerface or local conductivity at the BiFeO3 domain wall (homointerface) have been found. These complex oxide interfaces create an arena to discover novel phenomena. This study presents the origin and the electrical modulation of conduction at tubular interfaces in the self-assembled BiFeO3-CoFe2O4 system through scanning probe microscopy. The origin of the conduction is the accumulation of oxygen vacancies at interfaces, and the conduction at tubular interfaces can be controlled by applied bias to drive the movement of oxygen vacancies. Our findings suggest that the tubular oxide interface can not only be the medium of the coupling between phases, but also be a new state of the matter, providing a novel concept on oxide interface design and opening a pathway alternative for the explorations of diverse functionalities in complex oxide interfaces.

EP2 52

add to my program (close full abstract)

13:30 **Modelling Y2O3 in ODS steels: initial result for yttrium**

Authors : Morten Nagel, Krister O. E. Henriksson

Affiliations : Department of Physics, P.O. Box 43 (Pietari Kalmin katu 2), FI-00014 University of Helsinki, Finland

Resume : Oxide-Dispersion Strengthened (ODS) steels are promising construction materials for future fission and fusion reactors where the amount of radiation damage is expected to be larger than in contemporary constructions. These steels will contain oxide particles (e.g. Y2 O3). Atomistic modelling of these materials require a reliable interatomic potential for the Fe-Y-O ternary system. In this work we present results for the pure Y interaction: ab initio calculations of several yttrium phases as well as simple defects to create fitting database and a parametrization of the pure Y potential with its performance against this database.

EP2 53

add to my program (close full abstract)

13:30 **Luminescence of Macro and Nanocrystalline MgO excited by VUV synchrotron radiation**

Authors : A.I. Popov (1,2), L. Shirmane (1), V. Pankratov (1), A. Lushchik (3), V.E. Serga (4), A. Kotlov (5), J. Zimmermann (6)

Affiliations : (1) Institute of Solid State Physics, Univ of Latvia, Riga, LV-1063, Latvia; (2) Institute Laue-Langevin, F-38042 Grenoble, France; (3) Institute of Physics, Univ of Tartu, Tartu, 51014, Estonia; (4) Riga Tech Univ, Inst Inorganic Chemistry, LV-2169 Salaspils, Latvia; (5) HASYLAB, DESY, Hamburg, D-22761, Germany; (6) TU Darmstadt, D-64287 Darmstadt, Germany;

Resume : Comparative analysis of the luminescent properties of nanocrystalline MgO with macrocrystalline powder analogues and a single crystal has been

EP2 54

performed under excitation by pulsed VUV synchrotron radiation. Special attention was paid to VUV spectral range, which is not reachable with commonly used lamp and laser sources. The nanopowder with average crystallite size of nanoparticles (10-15 nm) of MgO was prepared by the extractive-pyrolytic method, while single crystal of MgO was grown by the arc-fusion method. Luminescence spectra and the excitation spectra for different emissions have been studied at the Superlumi station of HASYLAB at DESY using synchrotron radiation of 3.6-25 eV from the DORIS III storage ring in a wide temperature range of 10-293 K. Results obtained show clearly a distinct difference in the excitation spectra for nano- and macrocrystalline samples. A considerable blue shift of about 0.3 eV of the luminescence excitation band caused by deformation -induced defects/vacancy complexes is revealed in nanocrystalline samples.

add to my program (close full abstract)

13:30 **Defect-induced red emission in Y2O3-ZrO2 nanopowders**

Authors : N. Korsunska1, V. Papusha1, O. Kolomys1, V. Strelchuk1, A. Kuchuk1, V. Kladko1, Yu. Bacherikov1, T. Konstantinova2, L. Khomenkova1
Affiliations : 1) V. Lashkaryov Institute of Semiconductor Physics, 45 Pr. Nauky, Kyiv 03028, Ukraine 2) Donetsk Institute for Physics and Engineering named after O.O. Galkin of the NASU, 72 R. Luxemburg str., Donetsk 83114, Ukraine

Resume : ZrO2 offers diverse applications such as catalysts, high temperature and corrosion resistant coatings, sensors, radiation detectors, etc. Present work deals with the study of luminescence and structural properties of Y2O3-ZrO2 nanopowders with different Y2O3 content. The powders were sintered by co-precipitation of Zr and Y nitrates at different calcination temperatures. The structural and light emitting properties were controlled by XRD, TEM and Raman scattering, photo- (PL) and cathodoluminescence (CL) methods. At the same calcinations temperature, the increase of Y2O3 content stimulates the decrease of the sizes of ZrO2 nanograins and the transformation of crystalline phase from monoclinic through the tetragonal to cubic. Generally, room temperature PL spectra showed several bands in UV-orange range, whose shape depends on the excitation light wavelength. Along with this, CL spectra demonstrate additional "red" emission, which intensity exceeds that of other CL bands. At lower temperatures, preferable enhancement of "red" CL band, its narrowing and peak position shift to the longer wavelengths were found. This behaviour testifies to the non-elementary nature of "red" CL band. Its nature and mechanism of its excitation are discussed. It is supposed that complex defects, containing oxygen vacancies and impurities, are responsible for this emission appeared under high-energy excitation only. The dominant contribution of red emission into CL spectra opens some perspectives for its application as a marker for high-energy radiation.

EP2 55

add to my program (close full abstract)

13:30 **The role of grain boundaries on light species behavior in nanostrutured W**

Authors : M. Panizo-Laiz 1, N. Gordillo 1, E. Tejado 2, J. Y. Pastor 2, F. Munnik 3 J. M. Perlado 1, R. Gonzalez-Arrabal 1
Affiliations : 1-Instituto de Fusi?n Nuclear, ETSI de Industriales, Universidad Polit?cnica de Madrid, C/ Jos? Gutierrez Abascal, 2, E-28006 Madrid, Spain. 2-Departamento de Ciencia de Materiales CISDEM, ETSI de Caminos, Universidad Polit?cnica de Madrid, E-28040 Madrid, Spain. 3-Forschungszentrum Dresden-Rossendorf, PO.Box 10119, D-01314 Dresden, Germany.

Resume : One of the challenges in the design of future nuclear power plant is to develop materials capable to resist in the hostile environment of a fusion reactor. Because of its low sputtering yield, low-activation, high melting point, high thermal conductivity and low thermal expansion, tungsten is one of the most attractive materials proposed for first wall applications in nuclear fusion reactors. Even when W is assumed to be the best candidate as plasma facing material (PFM), some limitations have been identified that have to be defeated in order to fulfil specifications i.e. an important point of concern to the light species behavior (H, D, T and He). Nowadays some strategies to overcome these limitations are being investigated. In this work we study the influence of sample microstructure and of irradiation conditions on the hydrogen behavior in Tungsten (W). For this purpose, commercial coarse grained (CGW) and nanostructured W (NW) samples were implanted with (i) H at room temperature (RT), (ii) sequentially with C and H at RT, and (iii) simultaneously (co-implanted) with C and H at RT. To study the possible effect of implantation temperature on H behavior, a CGW and a NW samples were sequentially implanted with C at RT and with H at 400?C. Scanning electron microscopy images show that nanostructured samples consist on columns with an average diameter of about 100 nm. These nanocolumns are stable under the studied

EP2 56

implantations conditions. Moreover, blistering is absent in all studied samples. X -ray diffraction data illustrate that all samples are mono-phase (α-W phase) and that none of the implantations led to the appearance of secondary phases. Resonant nuclear reaction analysis data show that the H behaviour in NW samples is mostly dominated by the presence of intrinsic defects (i. e. grain boundaries).

add to my program (close full abstract)

13:30 **Van der Waals surface evolutions in III-VI layered crystals under neutron irradiation**

Authors : O.M.Sydor, Z.D.Kovalyuk
Affiliations : Chernivtsi Department of the Institute of Materials Science Problems, the National Academy of Sciences of Ukraine, Iryna Vilde St., 5, Chernivtsi, 58001, Ukraine

Resume : Layered A3B6 crystals, in particular InSe and GaSe, have unique physical properties. So, their cleaved surface (0001) is atomically perfect and also inert in environment. Therefore, InSe and GaSe can be used for creation and investigation of nanosized objects, including high-energy irradiations. In this work, the effect of bremsstrahlung neutron irradiation (Eeff=8 MeV) on surface changes in A3B6 crystals is investigated by AFM method. The used fluences are: F1=10^13, F2=10^14 and F3=10^15 n/cm^2. For initial InSe and GaSe surfaces the roughness average (Ra) was about of 0.053 and 0.059 nm, respectively, and the maximum height difference of the relief did not exceed 0.36 and 0.56 nm, respectively. The formations on the surface of irradiated crystals are, in fact, vacancies which have a form of wells or pits. Their planar distribution is comparatively homogeneous. For GaSe the Ra value increased to 0.83 and 1.29 nm at fluences F1 and F3, respectively, the density of nanoformations (NF) decreased from ~6x10^9 cm^-2 to 2x10^9 cm^-2. Their vertical dimensions did not exceed 1 nm for the fluence F1, but increased by 2–3 times for F3. In the case of InSe, at fluence F1 density of NF was ~2x10^8 cm^-2 and their vertical dimensions did not exceed 2 nm but at fluence F3 these values became ~4x10^7 cm^-2 and ~10 nm, respectively. Note that for the sample subjected to the maximum irradiation the broadening of separate pits and their coalescence into clusters of a bigger size take place.

EP2 57

add to my program (close full abstract)

13:30 **Influence of strontium titanate antiferrodistortive phase transition on the magnetic properties of La0.7Sr0.3MnO3 thin films**

Authors : D. A. Mota1, Y. Romaguera Barcelay1, A. M. R. Senos2, C. M. Fernandes2, P. B. Tavares3, I. T. Gomes4, P. Sá4, L. Fernandes4, B. G. Almeida4, F. Figueiras5, P. Mirzadeh Vaghefi5, V. S. Amaral5, J. Fontcuberta6, A. Almeida1 and J. Agostinho Moreira1
Affiliations : 1. IFIMUP and IN-Institute of Nanoscience and Nanotechnology, Departamento de Física e Astronomia da Faculdade de Ciências da Universidade do Porto. Rua do Campo Alegre, 687, 4169-007 Porto, Portugal. 2. Department of Materials and Ceramics Engineering, CICECO, University of Aveiro, 3810-193 Aveiro, Portugal. 3. Centro de Química – Vila Real. Universidade de Trás-os-Montes e Alto Douro. Apartado 1013, 5001-801. Vila Real. Portugal. 4. Centro de Física. Universidade do Minho, P-4710-057 Braga, Portugal. 5. Department of Physics & CICECO, University of Aveiro, 3810-193 Aveiro, Portugal. 6. Institut de Ciència de Materials de Barcelona (ICMAB–CSIC) Campus UAB, Bellaterra 08193, Spain.

Resume : The manganites are materials with an extremely strong coupling between three degrees of freedom: electronic, spin and lattice order [1]. Of particular interest is La0.7Sr0.3MnO3 (LSMO), showing a Curie temperature of 360K and an almost full spin polarization. LSMO thin films grown coherently on cubic substrates are subjected not only to a biaxial strain, due to lattice mismatch, but also to an angular distortion which induce strain and consequently changes on magnetic properties. Epitaxial LSMO thin films, with thicknesses ranging from 20 up to 330 nm, were deposited on (100)-oriented strontium titanate (STO) substrates by laser ablation. Magnetic properties of the as-processed thin films were characterized with a SQUID magnetometer in the vicinity of the antiferrodistortive STO phase transition (TSTO). This work shows that antiferrodistortive ordering emerging in STO below 105K, induces significant changes on the magnetic properties of LSMO thin films. For LSMO films thinner than 100 nm, the pinning of the magnetic domains of LSMO film to the substrate domain pattern, explains the increase of both the coercivity and magnetization, observed below TSTO through the interface-mediated magnetoelastic coupling. Contrarily, the in-defect magnetization observed for thicker films can be understood by the formation of randomly oriented magnetic domain reconstructions associated with film relaxations confirmed by both XRD and HR-TEM. [1] A. J. Millis, Nature (London) 392, 147 (1998).

EP2 58

add to my program (close full abstract)

13:30 **Defect-induced magnetism in V-doped titanium dioxide**

Authors : A. Smekhova*,1, O. Yildirim2,4, M. Butterling2, S. Cornelius2, Yu. Mikhailovskiy1, A.Novikov1, A. Semisalova1,5, A. Orlov3, E. Gan'shina1, N. Perov1, W. Anwand2, A.Wagner2, K. Potzger2, A.B. Granovsky1

Affiliations : 1 M.V. Lomonosov Moscow State University, Leninskie Gori 1, 119991 Moscow, Russia; 2 Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstrasse 400, 01328 Dresden, Germany; 3 Federal State Research and Design Institute of Rare Metal Industry, B. Tolmachevsky lane 5-1, 119017 Moscow, Russia; 4 Institute for Physics of Solids, Technical University Dresden, Zellescher Weg 16, 01069 Dresden, Germany; 5 Lappeenranta University of Technology, Skinnarilankatu 34, 53850 Lappeenranta, Finland

Resume : Since the pioneering paper of Y. Matsumoto et al. [Y. Matsumoto et al., Science 291, 854 (2001)], the number of publications on TiO2 films doped by different 3d impurities, such as cobalt, iron, vanadium or manganese, is steadily increased. Up to now the most popular but competitive points of view on origin of ferromagnetism at RT are carrier-mediated and defect-induced models. We report recent experimental results about room-temperature ferromagnetism in V-doped TiO2- δ thin films with different electric conductivities. Films were prepared on LaAlO3 (001) substrates by RF magnetron sputtering in reduced argon–oxygen atmosphere, while the V to Ti metal ratio was fixed at 1at.% or 3at%. For Ti0.99V0.01O2-δ the direct relation between saturated magnetization probed by SQUID and the concentration of negatively charged structural defects probed by Positron Annihilation Spectroscopy (PAS) has been established [O. Yildirim et al., accepted to PSS]. The absence of magneto-optical transversal Kerr effect signal and the anomalous Hall effect supports the assumption of defect-induced origin of magnetism in the studied films without involvement of free charge carriers or the local magnetic moment of the V ion. For Ti0.97V0.03O2-δ the strong magneto-optical signal has been found with a huge difference in spectral shapes for films with different conductivities. The results of PAS are discussed. The work was supported by a joint German-Russian project HRJRG-314 & RFBR 12-02-91321-SIGa

EP2 59

add to my program (close full abstract)

13:30 **Adeshion and mechanical properties of implanted nanostructured tungsten**

Authors : N. Gordillo 1, E. Tejado 2, M. Panizo-Laiz 1, J. Y. Pastor 2, J. M. Perlado 1, and R. Gonzalez-Arrabal 1

Affiliations : 1 Instituto de Fusión Nuclear, ETSI de Industriales, Universidad Politécnica de Madrid, C/ José Gutierrez Abascal, 2, E-28006 Madrid, Spain; 2 Department of Materials Science- Research Centre on Safety and Durability of Structures and Materials (CISDEM) , UPM-CSIC, C/ Profesor Aranguren s/n,E- 28040, Madrid, Spain

Resume : Owing to its properties: high melting point, low vapor pressure, low physical and chemical sputtering yields, low thermal expansion, electrical conductive properties and relative chemical inertness, tungsten seems to be one of the best candidates to be used as shielding material in plasma facing materials (PFM) for future nuclear fusion reactors. Nowadays, the capabilities of nanostructured materials for such applications are being attracted much attention due to their radiation-resistant and self-healing behavior. In this work, the capacity of the nanostructured W (nW) as protective role in PFM is studied and the radiation-induced changes in the structure and mechanical properties have been investigated. For this purpose, high density coatings made of nanometric tungsten columns (nW) were prepared by direct current (DC) magnetron sputtering and later were implanted under different conditions: (i) single implanted with H, (ii) sequentially with C and H, and (iii) simultaneously (co-implanted) with C and H at room temperature. The stress state was analyzed by X-ray diffraction, while the mechanical properties and adhesion to the substrate have been characterized using the nanoindentation and the nanoscratch techniques respectively.

EP2 60

add to my program (close full abstract)

13:30 **DFT calculations of charge states on rough Si and Cu surfaces**

Authors : Avaz Ruzibaev, Flyura Djurabekova

Affiliations : Department of Physics and Helsinki Institute of Physics, University of Physics

Resume : In many modern applications which employ electric fields of significant strength, such as the Atom Probe Tomography (APT) technique, a successor of field ion microscopy (FIM), or more technological applications such as particle accelerators and vacuum interrupters, it is of great importance to understand the response of surface defects on the field. How strongly atoms on a metal surface or on a semiconductor surface are charged in response to strong

EP2 61

electric fields and what is the difference in the mechanisms of surface charge formation can help to understand the atomic behavior in the presence of strong electric fields. We perform electronic structure calculations to study rough features on the Si (100) surface under the influence of external electric field. Charge-transfer dynamics is followed by applying the SIESTA code. Further we use Mulliken and Bader charge analysis tools to estimate the charge excess and depletion on the defects and in their close vicinity. Furthermore, we compare the data obtained for Si surface structural defects with the same defect obtained for metallic electronic structures in the rough Cu surface simulations.

add to my program (close full abstract)

13:30 **Magneto-optic study of undoped and Mn-doped ZnO thin films**

Authors : F. Oliveira (1), M.F. Cerqueira (1), M.I. Vasilevskiy (1), T. Viseu (1), J. Ayres de Campos (1), A.G. Rolo (1), I. Bogdanović-Radović (2) and E. Alves (3)
Affiliations : (1) Centro de Física, Universidade do Minho, Campus de Gualtar 4710-057 Braga, Portugal; (2) Rudjer Boskovic Institute, Bijenicka cesta 54, 10000 Zagreb, Croatia; (3) Associação Euratom/IST, Instituto de Plasmas e Fusão Nuclear, Instituto Superior T?cnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001, Lisboa, Portugal

Resume : Diluted magnetic semiconductors (DMS) are a promising candidate to produce the next generation of electronic spin devices. DMS are obtained by doping the lattice of the host semiconductor material with magnetic atoms. This doping usually does not destroy the crystal lattice of the semiconductor (as confirmed by Raman spectroscopy) and, in principle, free carriers can interact with magnetic atoms to produce a spontaneous magnetization according to the RKKY mechanism. Since DMS films are transparent, Faraday effect measurement is a suitable experimental method to detect the weak magnetic signal of the thin films. Results of our magneto-optical study, performed by using the Faraday effect measurements on undoped and Mn-doped ZnO thin films (thickness around 500 nm) grown by RF magnetron sputtering, with the Mn contents ranging from 0.4 to 5.3 at.%, will be presented. The films are nanocrystalline, with wurtzite structure, a typical crystalline grains size of 20 nm and a preferential orientation of the c-axis perpendicular to the surface. Our results show a linear behaviour of the Faraday angle with the Mn dose. The Verdet constant of ZnO:Mn as a function of the Mn content has been determined, indicating a paramagnetic behaviour at room temperature.

EP2 62

add to my program (close full abstract)

13:30 **Influence of the impure fluorine ions on the electronic structure and optical properties of cadmium molybdate compounds**

Authors : V. Chornii, S. Nedilko, Yu. Hizhnyi, T. Nikolaenko, M. Slobodyanik, O. Gomenyuk(1), V. Sheludko (1)
Affiliations : Taras Shevchenko National University of Kyiv, 64, Volodymyrs'ka str., 01601 Kyiv, Ukraine (1) Oleksandr Dovzhenko Hlukhiv National Pedagogical University, 24 Kyjevo-Moskovs'ka st., 41400, Glukhiv, Ukraine

Resume : The cadmium molybdate CdMoO4 are well-known scintillation and phosphor materials currently used in various technological applications. Doping of CdMoO4 with F impurities can be done in wide range of dopant concentrations, from several thousands of ppm to synthesis of anion-substituted material CdMoO3F2. Such doping leads to definite changes in optical, in particular, luminescence properties of cadmium molybdate hosts. In this work, the sequence of cadmium molybdate compounds with various F content is considered in theoretical calculations of the electronic structure. The electronic structures are calculated by the Full-potential Linear Augmented Plane Wave (FLAPW) method realized in Wien2k program package [1]. Perfect CdMoO4, fluorine-doped CdMoO4:F in which the oxygen-to-fluorine ratio ranges from 16:1 to 4:1 as well as perfect CdMoO3F2 crystals are treated in geometry-optimized calculations. Structures of the one-electron bands, spatial distributions of the electron densities, optical absorption and reflection spectra are calculated and analyzed. Obtained results are compared with available experimental data of luminescence and optical spectroscopy of pure and fluorine -doped cadmium molybdate crystals. [1] P. Blaha, et. al., 2001, ISBN 3-9501031-1-2.

EP2 63

add to my program (close full abstract)

13:30 **Surface plasmon resonance enhancement of visible range photoluminescence in Au-ZnO nanocomposite films synthetized by reactive magnetron sputtering**

Authors : W. Chamorro 1 2, P. Miska1 2, F. Soldera3, F. Mucklich3, P. Pigeat1 2, D. Horwat1 2
Affiliations : 1 Université de Lorraine, Institut Jean Lamour, UMR7198, Nancy, F-54011, France 2 CNRS, Institut Jean Lamour, UMR7198, Nancy, F-54011, France 3 Departame of Materials Science and Engineering, Saarland University, D-66123 Saarbrücken, Germany

EP2 64

Resume : Surface plasmon resonance (SPR) allows to metal nanoparticles as gold to absorb optical radiation in the visible range with a high efficiency. Subsequent effects such as enhanced electrical near field can be applicable for the surface-enhanced Raman spectroscopy for sensors and other optical devices. One of the advantages of the use of ZnO as a matrix is that it change the dielectrical interface, can stabilize the metallic nanoparticles and can handle the SPR wavelength1, 2. The presence of defects in ZnO not only interacts with the Au plasmon but can modify the emission behavior of this matrix. In this work we present Au-ZnO nanocomposite films that exhibit the SPR effect. Syntheses of Au-ZnO films were performed by reactive DC-magnetron co-sputtering of Zn and Au targets and we varied experimental conditions such as Au composition and annealing temperature. The introduction of gold in ZnO leads to changes in the photoluminescence response. The exciton signal of ZnO vanishes due to non-radiative processes that include the gold Fermi level. However, there is an enhancement of the emission on the visible range which strongly increases upon annealing of the films and development of SPR. XRD confirms the presence of Au nanoparticles with a 5 nm diameter with SPR absorption centered at a wavelength of 590 nm measured by UV-Vis spectrophotometry. The Au SPR is not responsible for the visible range emission but enhances the emission of particular defects presents in the ZnO matrix.

add to my program (close full abstract)

13:30 **Effect of grain refinement by severe plastic deformation on the evolution of the microstructure of a 316L austenitic stainless steel during ion irradiation**

Authors : Prasath Babu REVATHY RAJAN, Auriane ETIENNE, Isabelle MONNET, Bertrand RADIGUET, Xavier SAUVAGE, Nariman A. ENIKEEV, Rualan Z. VALIEV
Affiliations : Groupe de Physique des Matériaux, UMR-CNRS 6634, Université de Rouen, 76801 Saint Etienne du Rouvray cedex, France; CIMAP, CEA/CNRS/ENSICAEN/Universite de Caen-Basse Normandie, F-14070 Caen Cedex 5, France; Institute of Physics of Advanced Materials, Ufa State Aviation Technical University, Ufa 450000, Russia

Resume : In pressurized water reactors (PWR) internal structures, bolts that connect the baffle plates are commonly made up of 316L austenitic stainless steel. Some observations report the failure of several bolts due to Irradiated Assisted Stress Corrosion Cracking (IASCC). In order to limit radiation damage, that is a cause of IASCC, a 316 stainless steel with refined grains was elaborated by high pressure torsion (HPT) technique (430°C, 6GPa load) of a 316L steels in Ufa State Aviation Lab, Russia. This material has a grain size several orders of magnitude lesser than the coarse grained material. This nanograined material was annealed at 450°C and irradiated in Jannus facility (CEA Saclay) with Fe5+ ions of 10MeV at 450°C to achieve a uniform damage level of 5dpa. The microstructure of the as-deformed material as well as its evolution during annealing and irradiation were characterized by Atom Probe Tomography (APT) and Transmission Electron Microscopy (TEM) at the Groupe de Physique des Matériaux (University of Rouen). The difference in microstructure and defect structure evolution will be discussed in great detail.

EP2 65

add to my program (close full abstract)

13:30 **Molecular dynamics simulation study of grain boundary effect on stress and mass transport in metallic thin films**

Authors : Tomasz Zientarski-1, Dariusz Chocyk-2
Affiliations : 1Department for the Modelling of Physico-Chemical Processes, Maria Curie-Sklodowska University, ul. Gliniana 33, 20-614 Lublin, Poland, email: martom@dyzio.umcs.lublin.pl 2Department of Applied Physics, Lublin University of Technology, ul. Nadbystrzycka 38, 20-618 Lublin, Poland, email: d.chocyk@pollub.pl

Resume : Many important properties of polycrystalline materials are strongly influenced by grain boundaries. High purity metals are polycrystalline materials and they are usually used for fundamental research and for commercially pure materials in modern applications. It is widely known that the structure of grain boundary in these materials influence their mechanical and physical properties. Therefore, the knowledge about the grain boundary effect is very important to understand properties of this systems. To investigate the grain boundary size effect on thin film mechanical properties, we modeled a system with grain boundaries. For simplified polycrystalline geometries, we propose model mimics films intersected by the grain boundaries. To simplify calculation, in our model, we use the grain of rectangular shape. The interactions between metal atoms are described by embedded atom method. The simulation was performed for three-dimensional systems with x-y periodic boundary conditions at a several size of grain boundaries. The grain boundary size was also changed. Simulations show that depending on the size of grain boundaries and a mismatch of the lattice constant in grain and in boundaries leads to various evolution of stress.

EP2 66

We applied the kinematical scattering theory for the structural characterization of crystal structures and atomic stress method to analyze simulation data. Relation between stress and diffusion for different size of grain boundaries will be discussed in detail.

add to my program (close full abstract)

13:30 **Irradiation as a tool for interface defect modification in a-Si:H/c-Si heterojunction solar cells**

Authors : A. Defresne, O. Plantevin, I. P. Sobkowicz, Pere Roca i Cabarrocas
Affiliations : CSNSM, Univ Paris-Sud, CNRS/IN2P3, Orsay, France; CSNSM, Univ Paris-Sud, CNRS/IN2P3, Orsay, France; LPICM-CNRS, Ecole Polytechnique, 91128 Palaiseau, France; LPICM-CNRS, Ecole Polytechnique, 91128 Palaiseau, France

Resume : a-Si:H/c-Si heterojunction solar cells have reached record efficiencies of 24.7%. They consist of a n-type crystalline silicon wafer on which a thin (~10 nm) p-type hydrogenated amorphous silicon (a-Si:H) layer is deposited by plasma enhanced CVD at low temperature (~200 °C). The electrical contact is usually achieved by sputtering a thin transparent conducting oxide (80 nm thick) on the cell. Both sputtering and plasma deposition processes may introduce defects at the c-Si/a-Si:H interface which in turn will determine the conversion efficiency of the cell. The goal of this study is to understand the fundamental aspects of this interface via defect formation using a controlled introduction of point defects. Ion implantation of Argon at low energy (1 to 20 KeV) allows the modification of the a-Si:H thin layer. We can control the depth and concentration of irradiation defects by varying the ion energy and fluence. The defect concentration maximum is adjusted at a depth between 4 nm and 20 nm, while defect concentration is changed over 4 orders of magnitude between 1010 cm-2 and 1013 cm-2. The changes in the effective lifetime of minority carriers upon defect creation or annealing are characterized via photoconductance and photoluminescence measurements. The role of hydrogen diffusion within the amorphous silicon layer under low energy ion irradiation and thermal annealing is tentatively proposed as the origin of the heterojunction interface modification and correlated to the solar cell characteristics.

EP2 67

add to my program (close full abstract)

13:30 **INTENSE GREEN PHOTOLUMINESCENCE IN GdAlO3-d POWDERS (d= 0.0, 0.1 AND 0.2)**

Authors : Kh. Dhahri (a), M. Bejar (a), E. Dhahri (a), F. Amaral (b,c), M.A. Sousa (c), M.J. Soares (c), M.F.P. Graça (c)
Affiliations : (a) Laboratoire de Physique Appliquée, Faculté des Sciences, B.P. 1171, 3000 Sfax, Université de Sfax, Tunisie; (b) Polytechnic Institute of Coimbra, 3045-601 Coimbra, Portugal; (c) I3N and Physics Department, University of Aveiro, 3810-193 Aveiro, Portugal;

Resume : Nanocrystalline GdAlO3-d□ powders were prepared by means of solid state-reaction process. The parent compound GdAlO3 (d= 0.0) has a broad electronic band gap of 5.0 eV and do not present photoluminescence (PL) emission. This work aims to study the effect of oxygen deficiency in the GdAlO3-d□ compounds on the establishing of PL signal. X-ray diffraction patterns show that these compounds powders present a single perovskite phase and crystallize in the orthorhombic structure with the absence of a structural transition when increasing the oxygen deficiency. The optical study has exposed a very intense green photoluminescence (PL) emission, observed at room temperature and centered at 530 nm using a 350 nm excitation line. The experimental results revealed that the oxygen deficiencies VO z, where VO z = VOx, VO•, and VO••, created in the orthorhombic structure of GdAlO3-d□ compounds, is able to induce the green emission. These results can be explained by the formation of intermediary energy levels into the band gap due to the oxygen deficiencies.
Keywords: Perovskite, oxygen deficiency, photoluminescence

EP2 68

add to my program (close full abstract)

13:30 **Nanodefects in oxides doped LiF cdrystals**

Authors : L. Lisitsyna, V. Lisitsyn
Affiliations : Tomsk State University of Architecture and Building, sq. Soljianajia 2, Tomsk, 634003 Russia; National Research Tomsk Polytechnic University, av.Lenina 30, Tomsk, 634050 Russia

Resume : The results obtained in the study of LiF crystals doped with oxides of different polyvalent metals (Li, W, Fe or Ti) allow us to conclude that the growth of crystals is accompanied by the self-organization of defects with the formation of nano-sized regions which, in addition to polyvalent metal ion(s), contain oxygen in different states (O2–, OH–, O2) and intrinsic lattice defects. The length of such nano defect reaches at least five interionic distances. Hence the cross section of the capture of electronic excitations by nano defects can be 100

EP2 69

–1000 times greater than that by point defects. This means that the nano defects are sinks of electronic excitations, while in undopped crystals electronic excitations are uniformly distributed in the crystal volume. It is found that nano defects having their own spatial and energy structure determine both type and the parameters of radiation-induced processes. So it is established that in doped LiF crystals: (i) dose dependences of F2 color centers accumulation has character different from that in undoped crystals; (ii) in the absorbed doses less than 104 Gy electron pulse repetition rate does not affect the efficiency of F2 centers creating, whereas in the non-activated crystals such a dependence is observed. Assumed that in bulk of the nano defects main mechanism of creating of F2 color centers is correlation mechanism based on the decay of an exciton into a Frenkel pair in the region of the generated F color center.

add to my program (close full abstract)

13:30 **Stress changes in thin films bonded on polycrystalline substrate: molecular dynamics simulation**

Authors : Dariusz Chocyk 1, Tomasz Zientarski 2,
Affiliations : 1Department of Applied Physics, Lublin University of Technology, ul. Nadbystrzycka 38, 20-618 Lublin, Poland; email: d.chocyk@pollub.pl 2Department for the Modelling of Physico-Chemical Processes, Maria Curie-Sklodowska University, ul. Gliniana 33, 20-614 Lublin, Poland; email: martom@dyzio.umcs.lublin.pl,

Resume : Mechanical and physical properties of materials in nanoscale are frequently dependent on grain boundaries. Grain boundaries play also an important role in stress generation during growth. In many proposed growth models sources of stress in late stages are connected with mass transport along the boundaries. Therefore, a detailed knowledge about mechanism of diffusion through the grain boundaries is very important to understand properties of this systems. Numerical simulations method are commonly used to study the diffusion length, grain boundary thickness, and the average grain size. In this work we focused on stress changes of deposited films onto the surface consisting of several strips and rows. We consider a surface intersected by the grain boundaries to study influence of the grain boundary size and lattice mismatch on stress in film. We used a three-dimensional molecular dynamics simulations. To simplify calculation, in our model, we use the grain of rectangular shape and the Lennard-Jones (LJ) potential. The LJ potential is not adequate for specific materials. We have chosen this potential to capture the generic feature of such systems. Additionally, the application of simple LJ potential is also motivated by simplification of numerical calculations. Influence of lattice mismatch and grain boundary size on stress will be discussed in detail.

EP2 70

add to my program (close full abstract)

13:30 **An object kinetic Monte Carlo study of the influence of high grain boundary density on He retention in tungsten**

Authors : G. Valles(1), I. Martín-Bragado(2), O. Peña-Rodríguez(1), R. González-Arrabal (1), J. M. Perlado(1), A. Rivera(1)
Affiliations : (1)Instituto de Fusión Nuclear, ETSI de Industriales, Universidad Politécnica de Madrid, C/ José Gutierrez Abascal, 2, E-28006 Madrid, Spain;(2)IMDEA Materials Institute, C/ Eric Kandel 2, 28906 Getafe, Madrid, Spain

Resume : Owing to its good properties, tungsten is proposed as a suitable material for both divertor in magnetic fusion reactors and first-wall armor in inertial fusion reactors. Nevertheless, the extreme irradiation conditions will lead to swelling, pore formation, cracking and exfoliation. These processes are thought to be related to helium retention in irradiation-induced defects. Nanostructured tungsten is nowadays under research because it could be less prone to detrimental effects than conventional polycrystalline tungsten mainly due to the resulting lower density of highly pressurized clusters. In this work, we present object kinetic Monte Carlo (OKMC) simulations of He pulse irradiation (1013 cm-2 per pulse at 625 keV) in both polycrystal and nanocrystal tungsten. We considered the grain boundaries as a drain for defects. At high doses (>5•1015 cm-2) the grain-boundary density plays a clear role: the higher the density the lower the He retention. In addition, the resulting He-vacancy cluster configurations depend on the grain boundary density that act as a drain for defects. Our results show that at reactor temperatures nanocrystalline W exhibits a clear reduction in the number of undesired pressurized vacancy clusters as compared to polycrystalline W. Finally, new experimental results supporting the validity of the simulations will be discussed.

EP2 71

add to my program (close full abstract)

13:30 **Understanding the origin of the dead-layer at the La0.7Ca0.3MnO3/SrTiO3 Interface**

Authors : Juan Rubio-Zuazo 12, Alicia de Andrés2, and Germán R. Castro 12

EP2 72

Affiliations : 1 SpLine Spanish CRG BM25 Beamline at the ESRF BP 220-38043 Grenoble Cedex, France 2 Instituto de Ciencia de Materiales de Madrid-ICMM/CSIC; Cantoblanco, E -28049 Madrid, Spain

Resume : La1-XCaxMnO3–type perovskite-manganese oxides exhibit a wide variety of interesting physical properties which originate from mutual coupling among spin, charge and lattice degrees of freedom. They present, in the Ca doping range between 0.15 and 0.5, a ferromagnetic –paramagnetic (F–M) phase transition accompanied by a metal – insulator (M–I) transition that results in a colossal magneto-resistance behaviour. In bulk La0.7Ca0.3MnO3 (LCMO), the transition temperatures TC and TMI raise for 33% Ca doping level reaching values close to room temperature. It is well-known the premature disappearance of such intrinsic properties for thin films. Typically the TC and TMI transition temperatures decreases as the film thickness is reduced being even absent for ultra-thin films. Such behaviour hampers the potential application of perovskite-manganese oxides in industrial devices. We have studied a series of epitaxial LCMO films with thickness between 2.4 and 27 nm grown on SrTiO3(001) (STO) by dc-sputtering. The magneto-electric measurements show a severe decrease of TC and TMI as the film thickness is reduced. The transition temperatures are absent for films with thicknesses below 2.4 nm. We have performed an extensive study, by X-ray Diffraction and low and high energy X-ray photoelectron spectroscopy, concerning the atomic structure, strain relaxation, oxygen vacancies and compositional and electronic (manganese valence) depth profile as a function of layer thickness.

add to my program (close full abstract)

13:30 **Ab initio simulation of the initial steps of the ODS particle formation process in bcc iron matrix.**

Authors : Yu. A. Mastrikov1, P. V. Vladimirov2, V.A. Borodin3, A. Gopejenko1, Yu.F. Zhukovskii1, E. A. Kotomin1, A. Möslang2

Affiliations : 1Institute for Solid State Physics, University of Latvia, Kengaraga str. 8, Riga, Latvia 2Institut für Angewandte Chemie, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Karlsruhe, Germany 3 National Research Centre Kurchatov Institute, 1, Akademika Kurchatova pl., Moscow, 123182, Russia

Resume : Reduced activation ferritic-martensitic steels (RAFM) strengthened by yttria precipitates are promising structure materials for future fusion and advanced fission reactors. Oxide dispersion strengthened (ODS) particles hinder dislocation motion effectively resulting in higher strength and better high-temperature creep resistance of ODS steels in comparison to basic materials. Implementation of ODS materials widen the operating temperature, as compared to conventional RAFM steels, as well as they are more radiation resistant. The size, shape and spatial distribution of ODS nanoparticles significantly affect both mechanical properties and radiation resistance. A deep understanding of the mechanism of the ODS particle formation at the atomistic level is essential for ODS steels production [1]. The very initial steps of the ODS particle formation process were modelled by first principles DFT/plane-wave method, as implemented in the computer code VASP 5.3. Stabilization of Y solute atoms in the alpha-Fe lattice was analysed in details. Interaction energies for various combinations of Y solute atoms and vacancies were obtained for use in the future kinetic Monte Carlo calculations. The most probable Y stabilization and precipitation reaction mechanisms were suggested. Y solute atoms create stable complexes with multiple vacancies. Stabilized by vacancies, Y solute atoms exhibit stronger attraction. [1] A. Gopejenko et.al. J. Nucl. Mater., 416, p. 40-44, 2011

EP2 73

add to my program (close full abstract)

13:30 **S-monolayer-doping of InGaAs films and its contactless characterization by Raman scattering**

Authors : R. Cusco [1] , N.Domenech-Amador [1] , P. Y. Hung [2] , W.Y. Loh [2] , L. Artus [1]

Affiliations : [1] Institute Jaume Almera (CSIC), Barcelona, Spain ; [2] SEMATECH, 257 Fuller Road, Suite 2200, Albany, NY 12203

Resume : Recently, the use of monolayer doping (MLD) has emerged as a promising approach to a controllable, nanoscale doping method for achieving ultrashallow junctions. We use Raman scattering to assess the impact of anneal temperature on activation of S dopant introduced by MLD. In0.47Ga0.53As films 20 nm thick were grown by MBE on 100nm In0.48Al0.52As barrier with InP substrate. The samples underwent sulfur monolayer doping [1] then capped with 5nm SiN and annealed at different temperatures. The dopant profile was determined with SIMS measurements and the sheet resistance and electron

EP2 74

carrier density was obtained from Hall measurements. While the electrical properties of such doped layers are routinely assessed by Hall measurements, contactless optical methods such as Raman scattering by LO-phonon-plasmon-coupled- modes (LOPCMs) have been shown to yield reliable determinations of the electron density in uniformly doped, bulk-like samples and such methods are of great interest to study doping in semiconductor nanostructures. Raman scattering measurements were performed in z(xy)-z configuration using the 514.5 nm excitation. Raman peaks associated with LOPCM modes were observed. The Raman spectra are analyzed in terms of the dopant/electron distribution and the Raman results are correlated with the SIMS and Hall data. [1] W. Y. Loh et al , VLSI Technology, International Symposium on Systems and Applications (VLSI-TSA), April 2013, Hsinchu, Taiwan

add to my program (close full abstract)

13:30 **Tailoring soft magnetic properties in amorphous FeZr films by low energy ion implantation**

Authors : Anders Hallén, Atieh Zamani, Reda Moubah, Gabriella Andersson, Martina Ahlberg,Petra E. Jönsson

Affiliations : Anders Hallén; KTH Royal Institute of Technology, School of ICT, P.O. Box Electrum 229, SE-164 40 Kista-Stockholm, Sweden Atieh Zamani, Reda Moubah, Gabriella Andersson, Martina Ahlberg Petra E. Jönsson; Department of Physics and Astronomy, Uppsala University, Box 516, SE 751 20 Uppsala, Sweden

Resume : Amorphous iron-zirconium (a-FeZr) films have been studied extensively, much due to their interesting magnetic properties. They show soft magnetic features with low coercive field and large magnetic saturation, but typical Curie temperatures for as-prepared samples are around 250 K. However, by for instance, introducing hydrogen, or employing different preparation schemes for the films, it is possible to increase the Curie temperature to above room temperature. The reason for the changes in the magnetic properties is still under discussion, but the direct exchange interaction is very sensitive to the Fe-Fe distance, and the introduction of extra atoms in the structure is believed to increase the Fe-Fe distance thereby enhancing the ferromagnetic properties. In this contribution we will show that the magnetic properties can also be changed by implantation of keV low mass ions at high fluence. In fact, the implantation technique allows a controlled tuning of magnetic properties of the a-FeZr films, for instance, the Curie temperature within a range of 230 to above 400 K using proper choice of ion, energy and fluence [1,2]. In this study a-Fe0.93Zr0.07 thin films of a thickness of about 40 nm are prepared by magnetron sputtering on Si substrates, where the films are sandwiched between two 5 nm thick layers of Al0.7Zr0.3. Ion implantation is then performed at room temperature using a Danfysik implanter and beam currents low enough to prevent any significant sample heating during the implantation. The implantation technique also makes lateral patterning of the surface, using lithographic techniques, possible. In this way one- and two-dimensional structures of various sizes can be prepared which will help to better understand the magnetic behaviour of these films. The role of volume expansion due to the implanted ions and possible swelling effects due to displacement damage for increasing the Fe-Fe distance will be addressed. [1] A. Zamani et al., J. Magnetism and Magnetic Materials 346, 138 (2013) [2] R. Moubah et al., Appl. Phys. Express 6, 053001 (2013)

EP2 75

add to my program (close full abstract)

15:45 Break

16:00 PLENARY SESSION

Back

PROGRAM VIEW : 2014 Spring
MY PROGRAM : 2014 Spring

Symposium : E

Defect-induced effects in nanomaterials

26 May 2014 | 27 May 2014 | 28 May 2014 | **29 May 2014** | 30 May 2014

hide a

start at	Subject	Num.
	Nanostructures in silica : William Weber	
09:00	**Enhanced optical functionalities in silica by doping with Au-based nanostructures.** **Authors :** T. Cesca, B. Kalinic, C. Maurizio, C. Scian, P. Mazzoldi, G. Mattei **Affiliations :** University of Padova, Dept. of Physics and Astronomy and CNISM, Padova, Italy **Resume :** Au-based nanostructures have been the object of strong interest from the scientific community in these years for their linear and nonlinear optical properties. Recently our group demonstrated that enhanced optical functionalities in nanophotonics can be obtained when sub-nanometric Au nanoclusters (made by less than 20 atoms) are formed by ion implantation in silica. Due to quantum confinement effects such molecule-like Au aggregates are characterized by discrete energy levels allowing for efficient radiative relaxation at room temperature. Moreover, the formation of a near-infrared luminescence band correlated to electronic surface states at the Au nanostructures was revealed to be the mechanism that triggers the energy-transfer to photoemitting systems as Er ions and makes sub-nanometric Au nanoclusters very efficient nanoantennas for the Er emission. This has important technological entailments in optoelectronics where many research efforts are being done in these years to increase the small cross-section for Er excitation. In this work we will present the results of some very recent experiments aimed at elucidating the photophysical nature of the interaction between molecule-like Au-based nanoaggregates and Er ions. The results demonstrate that the energy-transfer process is indeed a non-radiative coupling mechanism occurring at very -short range with characteristic length comparable to interatomic distances.	EO101
	add to my program (close full abstract)	
09:30	**Influence of doping on the optical properties of silicon nanocrystals embedded in SiO2** **Authors :** M. Frégnaux, R. Khelifi, Y. Le Gall, D. Muller and D. Mathiot **Affiliations :** Université de Strasbourg, CNRS, Laboratoire ICube (UMR 7357), 23 rue du Loess, BP 20, F - 67037 Strasbourg cedex 2 **Resume :** Co-implantation, with overlapping implantation projected ranges, of Si and doping species (P, As, B) followed by a thermal annealing step is a viable route to form doped Si nanocrystals (NC) embedded in SiO2. This presentation deals with optical characterizations of both doped and undoped Si NC prepared by this method. The NC effective presence in the oxide layer and their crystallinity is verified by Raman spectrometry. Photoluminescence (PL) and PL excitation measurements reveal quantum confinement effects and a gradual PL quenching with increasing dopant concentrations. In undoped NC, the measured Stokes shift remains constant and its value ~0.2 eV is almost twice the Si–O vibration energy. This suggests that a possible radiative recombination path is a fundamental transition assisted by a local phonon. PL lifetime investigations show that PL time-decays follow a stretched exponential. Using a statistical model for luminescence quenching, a typical radius of ~1.1 nm is obtained for As- and P-doped NC, consistent with our previous atomic probe tomography (APT) analyses. APT also demonstrated that n-type dopant (P, As) are efficiently introduced in the NC core, whereas p-type dopant (B) are located at the NC/SiO2 interface. This observation could explain the failure of the luminescence quenching model to determine B-doped NC size. All together these experimental	EO102

observations question on possible different carrier recombination paths in P or As doped NC compared to B one's.

add to my program (close full abstract)

09:45 **Structural and electrical properties of heavily arsenic doped silicon nanocrystals embedded in silicon oxynitride films**

Authors : F Ehrhardt1, C Ulhaq-Bouillet2, G Ferblantier1, D Muller1 and A Slaoui1
Affiliations : 1- Laboratoire ICube, Universit? de Strasbourg, CNRS UMR 7357, 23 rue du Loess, B.P. 20, F-67037 Strasbourg , France 2-Laboratoire IPCMS, UMR CNRS-UdS 7504, 23 rue du Loess, BP43, 67034 STRASBOURG, France

Resume : Silicon nanocrystals have been extremely studied these recent decades as they can be very useful in many applications such as electronic and photovoltaics devices. These Si nanocrystals are most often embedded in an insulating dielectric matrix such as SiO2, SiNx or SiCx. On the other hand, doping the Si nanocrystals can enhance their applicability. However, due to the self-purification effect in the nanocrystal, the doping is thermodynamically unfavorable. Nevertheless, investigations are still progressing in this field. Furthermore, effects of the doping on the size and crystallinity of the Si nanoparticles as well as on the charges transport is still not unclear. This paper investigates the structural and electrical properties of arsenic doped SiON layers containing silicon nanoparticles (Si:SiON). The arsenic atoms were introduced by ion implantation followed by a high temperature annealing. We show that the incorporation of arsenic at a high doping level lead to a increase of the Si nanoparticles size by more than a factor 3, namely from ~4-5 nm to more than 15-25 nm. Moreover most of the arsenic atoms are preferentially located inside the silicon nanoparticle, and the lattice parameter is comparable to that of bulk silicon even with a doping level of about 25 at%. Additionally, the crystalline fraction of the nanoparticles is higher than for the undoped structures crystalline. The results are discussed on the basis of a modeling of the Si crystal growth. Finally, we show that the electrical conduction in the heavily arsenic doped Si-SiON structure is limited by the tunnel oxide thickness between the large Si nanoparticles.

EO103

add to my program (close full abstract)

10:00 **Break**

Effect of defects on properties of nanomaterials : Christina Trautmann

10:30 **Defect-Engineering in Silicon Nanostructures for Enhanced Thermopower**

Authors : N. Bennett (1,2), D. Byrne (1), A. Cowley (1).
Affiliations : (1) Nanomaterials Processing Lab., School of Electronic Engineering, Dublin City University, Dublin 9, Ireland; (2) Institute of Mechanical, Process and Energy Engineering, School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh, EH14 4AS, United Kingdom.

Resume : In the past five years, research in thermoelectric (TE) materials has intensified thanks to the exciting potential of thermoelectric nano-materials. Traditionally the best performing TE materials have been often scarce, expensive and toxic, making it a challenge to adopt thermoelectrics for wide-scale energy harvesting. More recent research has shown that nano-structuring materials can greatly reduce their thermal conductivity (k). With reduced k, nano-structured silicon – which is plentiful, low-cost and non-toxic – becomes a competitive TE material. However, further optimisation is required to make silicon a truly state-of-the-art TE material. Using defect-engineering, we show that by manipulating the internal crystal nano-structure of silicon, an additional enhancement in thermoelectric performance is possible. This is revealed by extracting thermal conductivity, electrical resistivity and Seebeck coefficient, alongside imaging by scanning and transmission electron microscopy. In addition to silicon's thermal conductivity being reduced, a second important parameter – the thermopower – can be significantly increased. This important finding has the potential to propel nanostructured silicon closer to becoming a state-of-the art TE material.

EO111

add to my program (close full abstract)

10:45 **Europium doping of β-Ga2O3 bulk crystals and nanowires**

Authors : M. Peres [a], M. Felizardo [a], N. Franco [a,b], L.C. Alves [a], E. Alves [a,b], K. Lorenz [a,b], E. Nogales [c], I. López [c], B. Méndez [c], J. Piqueras [c], J. Rodrigues [d], T. Monteiro [d], E. G. Víllora [e], K. Shimamura [e]
Affiliations : [a] Instituto Superior Técnico (IST), Campus Tecnológico e Nuclear,

EO112

Estrada Nacional 10, P-2695-066 Bobadela LRS, Portugal; [b] IPFN, IST, Portugal; [c] Dpto. Física de Materiales, Universidad Complutense de Madrid, 28040 Madrid, Spain; [d] Departamento de Física e i3N, Universidade de Aveiro, 3810-193 Portugal; [e] National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan
Resume : β-Ga2O3 is well known for its properties as a transparent conductive oxide for the visible and UV range. The recent success in the production of high quality, single crystalline wafers is now opening the way to develop β-Ga2O3 based electronic and optoelectronic devices. Furthermore, the synthesis of nano- and microstructures as well the optical functionalization with rare earth ions promise new applications in nanotechnology, photonics and sensing. β-Ga2O3 bulk single crystals as well as β-Ga2O3 nanowires (NWs) were implanted with Eu ions with different fluences and at different temperatures. The structural properties were investigated by Rutherford Backscattering Spectrometry/ channeling and X-ray diffraction and the typical 5D0→7Fj intraionic transitions of Eu3+ have been studied by cathodoluminescence, photoluminescence and ionoluminescence. Implantation at room temperature leads to amorphisation for fluences above ~1E15 at/cm2. This lattice damage can be efficiently removed by rapid thermal annealing at ~1100 °C. However, in the case of bulk crystals, Eu could not be incorporated on substitutional sites and a decreased Eu3+ emission is observed by photoluminescence when compared to NWs. Implantation at elevated temperature (~600 ºC) yields a significant reduction of implantation damage, incorporation of Eu on substitutional Ga-sites and an improved optical activation. This result suggests that ion implantation at elevated temperature could be a better process than post-implant thermal treatment.

11:00 **Role of defects in optical properties of germanium quantum dots**
Authors : S. Saeed, K. Dohnalova, T. Gregorkiewicz
Affiliations : Van der Waals-Zeeman Institute, University of Amsterdam, The Netherlands
Resume : In order to include the infrared part of the solar spectrum in photovoltaic conversion, new materials with small band-gap energy are required. Among such materials Ge- and SixGe1-x quantum dots (QDs) can be excellent choices. Moreover, one might expect that efficient carrier multiplication should take place in these QDs due to the parallel bands of the indirect band structure, which would enable highly efficient conversion of the high energy wing of the solar spectrum. For such applications, optical properties of these materials should be studied at room temperature. However, the physical mechanisms behind the photoluminescence (PL) from Ge-based nanostructures are still not very well understood. Defect- and exciton-related PL bands from Ge -QDs have been reported, with the excitonic PL being usually supressed by the defect emission. In this contribution we report on the comprehensive study of room temperature optical properties of differently grown GeQDs embedded in various matrices. Time-resolved PL and induced absorption spectroscopy shows some interesting results among them one is possibly the first ever report on multiple exciton generation in GeQDs.

EO11 3

11:15 **Silicon LEDs fabricated using Plasma Ion Implantation**
Authors : M.P. Bradley, S. Purdy, J.R. McLeod
Affiliations : Dept. of Physics & Engineering Physics University of Saskatchewan
Resume : The Bradley Lab at the University of Saskatchewan (U of S) fabricates silicon LEDs using a process of plasma ion implantation (PII) followed by annealing to make a nanocrystalline buried layer. This buried layer has some features in common with porous silicon but is much more robust because it is self-capped and therefore mechanically robust as well as stable against contamination by environmental gases. The peak emission wavelength of these silicon LEDs is tunable by varying the implant process parameters (ion species implanted, ion fluence, depth of implant, and the annealing temperature/time profile). The quantum efficiency of these LEDs is strongly dependent on the annealing parameters. This talk will review different LED fabrication recipes developed at the U of S and will discuss possible paths to improve device quantum efficiency.

EO11 4

11:30 **Hindering Influence of Surface Point-Defects for Photoactivity on TiO2(110)**
Authors : I. Lyubinetsky, Z.-T. Wang, N. A. Deskins, M. A. Henderson
Affiliations : Pacific Northwest National Laboratory, Richland, WA, USA
Resume : Surface point-defects are expected to act as charge trapping and/or recombination centers in various photoinduced processes. However, the direct

EO11 5

impact of surface defects on photoreactivity is not well explored. We present the first observation of a suppressing effect of oxygen vacancy (VO) defects on photoreactivity of TiO2(110). Direct scanning tunneling microscopy imaging reveal a pronounced site-selectivity in the hole-mediated photooxidation of trimethyl acetate (TMA) on TiO2(110) upon ultra-violet light irradiation, wherein the reaction readily occurs at regular Ti sites but is completely inhibited at VO defects. Utilizing electron energy loss spectroscopy and density functional theory, we show that the lack of reactivity of TMA groups adsorbed at VO's cannot be attributed to either a less active adsorption conformation or electron transfer from the VO defect. Instead, we propose that the excess unpaired electrons associated with the VO promptly recombine with photoexcited holes approaching the surface, effectively 'screening' TMA species at VO site. We also show that this screening effect is spatially short-ranged, being predominately localized at the VO, and only mildly affecting TMA's at adjacent Ti sites. The direct impact of O vacancies on TMA photoreactivity over TiO2(110) is expected to have similar implications for other hole-mediated (e.g., photooxidation) reactions in which adsorption at or near electronic point-defects is possible. Furthermore, the localized i

add to my program (close full abstract)

11:45 **Swift heavy ion beam modification of rutile TiO2 for photo-catalysis applications**

Authors : R. Sanz1, L. Romano1-2, V. Scuderi1, M. Zimbone1, G. Impellizeri1, J. Jensen3, V. Privitera1
Affiliations : 1.IMM-CNR MATIS, via S. Sofia 64, 95123 Catania, Italy 2.Dipartimento di Fisica e Astronomia, Università di Catania, via S. Sofia 64, 95123 Catania, Italy 3.Thin Film Physics Division, Department of Physics, Chemistry and Biology – IFM, Linköping University, SE-581 83 Linköping, Sweden

Resume : TiO2 is a well know material for photo-catalysis applications. The anatase TiO2 phase has been widely studied for this purpose due to its higher photo-catalytic yield compared to rutile TiO2, in spite of its higher band-gap energy and less stability than rutile phase. However, recent experiments demonstrate the degradation of anatase due to an ageing effect, which could limit the application of this phase for its extensive use in photo-catalysis. Therefore, although rutile phase present a lower photo-activity it could represent a better choice for long-term use in photo-catalysis reactions as it is more robust under aggressive pH and temperature conditions. Previous works on ion beam induced modification of rutile single crystals have showed an increased chemical reactivity towards biomolecules. In this contribution we present results on the structural, compositional and UV photo-activity characterization of rutile TiO2 substrates after having been exposed either Ti (100 keV) or Br (25 MeV) ion beams. The results show: i) the disappearance of photo-catalytic properties of keV ion modified substrates, ii) a noticeable increase of the photo-activity yield of the swift heavy ions (SHI) modified substrates, without detectable degradation of their properties under acid environments. These results will be discussed in terms of ion induced damage and subsequent structural and surface modification, pointing at the unique effects of SHI for modifying TiO2 properties.

EO116

add to my program (close full abstract)

12:00 **Lunch**

Reshaping of nanomaterials by swift heavy ions : Mark Ridgway

14:00 **Novel nanowire and nanotube structures produced by ion-track technology**

Authors : C. Trautmann1,2, I.Alber1, L. Movsesyan1, 2, A. Spende1,2, M.E. Toimil-Molares1
Affiliations : 1 GSI Helmholtz Centre for Heavy Ion Research, Planckstr. 1, Darmstadt, Germany; 2 Technische Universit?t Darmstadt, Alarich-Weiss-Str. 4, Darmstadt, Germany

Resume : The ion-track technology based on MeV-GeV ion beams greatly benefits from the fact that each ion projectile creates a cylindrical track with a few nanometers in diameter. The small track size in combination with the large ion range (several tens of ?m) allows the fabrication of high-aspect ratio nanostructures. The track etching process provides great flexibility in adjusting their size and geometry under well controllable conditions [1,2]. Ion-track nanostructures are thus considered as excellent model systems to investigate the influence of size-effects on optical, electrical, magnetic, or thermal

EO121

properties. The development of suitable techniques to precisely tailor the dimensions, orientation, and surface properties of nanowires is illustrated by several novel examples including: ? Metallic and semiconducting self-supporting 3D nanowire networks of adjustable interconnectivity and high mechanical stability [3]. ? Nanowires synthesized by means of pulsed electrodeposition of Au-Ag-Au segments. Dissolving one of the component creates capacitively and conductively coupled dimers of adaptable gap size and with interesting surface plasmon properties [4]. ? Nanotubes (Al2O3, TiO2, SiO2) of adjustable wall thickness produced by atomic layer deposition in ion track membranes. [1] C. Trautmann, Micro- and Nanoengineering with Ion Tracks, in: Ion beams in Nanoscience and Technology R. Hellborg, H. Whitlow, Y. Zhang (Eds.), Topics Appl. Physics 110, 215?264 (2009) Springer-Verlag. [2] M. E. Toimil-Molares, Beilstein J. Nanotechnol. 3 (2012) 860 ? 883. [3] M. Rauber, I. Alber, S. M?ller, R. Neumann, O. Picht, C. Roth, A. Sch?kel, M. E. Toimil-Molares, W. Ensinger, Nano Lett. 11 (2011) 2304-2310. [4] I. Alber, W. Sigle, F. Demming-Janssen, R. Neumann, C. Trautmann, P.A. van Aken, M.E. Toimil-Molares, ACS Nano 6 (2012) 9711-9717.

add to my program (close full abstract)

14:30 **Stopping Power Dependence on Shape Elongation of Zn Nanoparticles under Swift Heavy Ion Irradiations**

Authors : H. Amekura, N. Ishikawa, N. Okubo, S. Mohapatra, D.K. Avasthi
Affiliations : National Institute for Materials Science (NIMS), Tsukuba, Japan; Japan Atomic Energy Agency (JAEA), Tokai, Japan; Guru Gobind Singh Indraprastha University, New Delhi, India; Inter-University Accelerator Centre (IUAC), New Delhi, India

Resume : The mechanism of the shape elongation of metal NPs in amorphous silica is still an issue under debate. Up to recent, one of the most referred mechanisms was the synergy effect between the in-plane stress generation due to the ion hammering and transient melting of NPs due to the thermal spikes. Contrarily, recent molecular dynamics (MD) simulations reproduced the elongation of Au NPs without assuming the hammering. However, the simulation induced not only the shape elongation but also the amorphization of Au NPs, which has never been experimentally confirmed. In this paper, the elongation efficiency of Zn NPs in silica was evaluated under irradiations with seven different combinations of ion-species and energies, ranging from 200 MeV Au^13+ ions to 1.7 MeV Si^+ ions. The elongation efficiency was determined by the optical dichroism spectroscopy. The Se values of Si ions of 8, 50, and 140 MeV in silica (in Zn) were 3.22, 3.20, and 2.20 keV/nm (4.93, 6.58, and 4.72 keV/nm). While the "Se in silica" monotonically decreases with the energy, the "Se in Zn" shows a peak in the middle. Since the experimentally observed elongation efficiency monotonically decreased with the energy, the "Se in silica" describes better the elongation efficiency than the "Se in Zn". The origin will be discussed.

EO12 2

add to my program (close full abstract)

14:45 **In-situ study of shape variations in metallic nanoparticles irradiated with swift heavy ions**

Authors : O. Peña-Rodríguez, J. Olivares, A. Rivera, L. Rodríguez-Fernández, A. Crespo-Sosa, J.C. Cheang-Wong, and A. Oliver
Affiliations : 1Instituto de Fusión Nuclear, UPM, José Gutiérrez Abascal 2, E-28006 Madrid, Spain 2Centro de Micro-Análisis de Materiales, UAM, Cantoblanco, E-28049 Madrid, Spain 3Instituto de Óptica, CSIC, C/Serrano 121, E-28006 Madrid, Spain 4Instituto de Física, UNAM, A.P. 20-364, México D.F. 01000, México

Resume : The shape deformation (elongation) of metallic nanoparticles (NPs) embedded in a dielectric matrix produced by irradiation with swift heavy ions is a phenomenon that has been known for some years. The prolate spheroids obtained in this way have their larger axis aligned with the incident ion beam direction, which can be advantageous for many applications. However, although this effect has been extensively studied and some theoretical models have been proposed, the origin of the deformation is not yet fully understood. One of the reasons that complicate this task is the lack of information concerning the intermediate stages of the deformation mechanism. In this work we have exploited the strong dependence of the surface plasmon resonance on the particle's shape and size to study in-situ the elongation of the NPs by means of optical absorption. The samples used in this study were composed nearly-spherical silver (gold) nanoparticles embedded in silica (TiO2). Then, by means of an irradiation with swift heavy ions, the "spheres" were transformed into spheroids. Optical absorption spectra were measured in-situ and the detailed deformation kinetics was calculated from a fit of these spectra. It was found that almost no deformation occurred until a certain fluence (ion- and sample-

EO12 3

dependant). After this point the elongation increases rapidly up to an aspect ratio value of ~3-4. Higher fluences only produce small increases of the deformation.

add to my program (close full abstract)

15:00 **Ion-Beam Shaping and Plasmon Mapping of Hollow Gold Nanoparticles**

Authors : P.-E. Coulon, J. Amici, M.-C. Clochard, I. Monnet, V. Khomenkov, C. Dufour, M. Kociak, L. Largeau, G. Rizza
Affiliations : LSI, Ecole Polytechnique, 91128 Palaiseau Cedex, France ; PMC, Ecole Polytechnique, 91128 Palaiseau Cedex, France ; CIMAP, 14070 Caen Cedex 5, France ; LPS, Bâtiment 510, Université Paris Sud XI, 91405 Orsay, France ; LPN, Site Alcatel de Marcoussis, Route de Nozay, 91460 Marcoussis, France

Resume : The importance of the ion-beam shaping technique relays in its unique capability to modify the morphology of nanoparticles (NPs) embedded within an amorphous host matrix. Consequently, ion-shaping technique is a route for downscaling the engineering of embedded NPs with a precision that is barely reachable with standard techniques. In this sense, the use of ion-shaped plasmonic crystals opens the way for advanced applications in the fields of bio-sensing or surface field enhanced spectroscopies (SERS). Although nowadays a vast literature exists on the ion-shaping technique, the deformation of hollow nanoparticles (HNPs) has not been reported yet. As spherical HNPs have a localized surface plasmon resonance between 700 and 800 nm, thus their elongation allows to explore deeper regions of the near-infrared region of the optical spectrum. Here, we show that swift heavy ion irradiation can be used to obtain vertical hollow NPs, with an aspect ratio increasing over 2. The deformation mechanisms have been studied by changing both the dimension of the HNPs and the thickness of the metallic shell. Experimental results are interpreted using the 3D-TS code. Finally, plasmon mapping is nanometer-scale spatial resolution is obtained by Electron Energy Loss Spectroscopy (EELS). This work represents a step forward for the development of an alternative route for the controllable fabrication of a whole family of nanostructures in vertical geometry with topologically tunable properties.

EO124

add to my program (close full abstract)

15:15 **STRESS FIELD/DISTRIBUTION AROUND SWIFT HEAVY ION TRACKS IN Al2O3**

Authors : J.H. O'Connell(a), V.A. Skuratov(b), N.Kirilkin(b), J. Neethling(a)
Affiliations : (a)CHRTEM, Nelson Mandela Metropolitan University, Port Elizabeth; (b) FLNR, Joint Institute for Nuclear Research, Dubna, Russia

Resume : Mechanical stresses in swift heavy ion irradiated radiation-resistant insulators are a subject of considerable practical interest in view of the simulation of fission product impact. To date, the build-up and accumulation of stress with swift heavy ion fluence and energy has been studied for a very limited number of ceramics and oxides using mainly X-ray diffraction techniques. Since the radiation damage and correlated stresses induced by swift heavy ions are concentrated within a small volume, surrounding the ion trajectory, it is also interesting to evaluate the stress state of irradiated crystals before and after overlapping of isolated ion track regions. The aim of this study is to collect data of lattice strain as a function of radial distance from the ion track centre using computational methods on TEM micrographs of the ion tracks. This data is of high importance to verify current computational models of track formation based on the temperature spike model. Single crystal Al2O3 crystals were irradiated with 710 MeV Bi and 167 MeV Xe ions and analysed using a JEOL ARM200F TEM

EO125

add to my program (close full abstract)

15:30 **Break**

Swift heavy ion irradiation and carbon-based materials : Marcel Toulemonde

16:00 **Confining ion tracks in 2D organic materials: the case of ultrathin polymer layers**

Authors : R. M. Papaléo 1, R. S. Thomaz 1, L. I. Gutierres 1, V. M. de Menezes 1, P. L. Grande 2, E. M. Bringa 3, C. T. Trautmann 4
Affiliations : 1 Faculty of Physics, Catholic University of Rio Grande do Sul, Porto Alegre, Brazil; 2 Institute of Physics, Federal University of Rio Grande do Sul, Porto Alegre, Brazil; 3 Instituto de Ciências Basicas, Universidad Nacional de Cuyo, Mendoza, Argentina; 4 Gesellschaft für Schwerionenforschung, Darmstadt, Germany

EO131

Resume : In the past 30 years, basic damage mechanisms and the physico-chemical changes observed in polymers irradiated by energetic ions have been thoroughly investigated for a multitude of polymeric systems and irradiation conditions. However, very little has been reported so far on nanoscale polymer systems and, in particular, on studies aiming a direct comparison of the "magnitude" of radiation effects under bulk and confinement conditions. In this contribution, we report on cratering associated to heavy ion tracks in 2D polymer nanostructures. We have used poly(methyl methacrylate) thin films as a model system to investigate confinement effects of ion tracks in one dimension by following the changes in radiation effects (for ions in an energy range from 20 MeV up to 2 GeV) as the thickness is systematically reduced down to ~2nm. We show experimental evidence, supported by molecular dynamics simulations, that surface effects produced by swift heavy ions associated to mass transport and particle ejection are weakened when the length of the ion track is spatially confined. The deviation from bulk-like behavior starts at a critical thickness hc as large as 40nm, initially because long range effects associated to cooperative action of excited material along the ion track are reduced. hc however depends on the type of effect being considered, being much smaller (~8-10nm) for effects more related to the localized heating at the track core (as the crater hole size).

16:30 **Atomistic simulations of ion irradiation-induced nanotracks**

Authors : Alejandro Prada 1, José Olivares 2, Ovidio Peña-Rodríguez 1, Mathieu Bailly-Grandvaux 1, María José Caturla 3, Eduardo Bringa 4, José Manuel Perlado 1,Antonio Rivera 1

Affiliations : 1. Instituto de Fusión Nuclear, Univerisdad Politécnica de Madrid, C/José Gutiérrez Abascal 2, E-28006 Madrid, Spain; 2. Centro de Micro-Análisis de Materiales, Universidad Autónoma de Madrid (CMAM-UAM), Cantoblanco, E-28049 Madrid, Spain; 3. Instituto de Óptica, Consejo Superior de Investigaciones Científicas (IO-CSIC), C/Serrano 121, E-28006 Madrid, Spain; 4. Independent Researcher CONICET, Instituto de Ciencias Básicas, Universidad Nacional de Cuyo, Mendoza, Argentina

Resume : The irradiation of silica with swift heavy ions produces a very high electronic excitation that eventually leads to the formation of nanometer sized tracks around the ion trajectory as well as surface effects such as high yield electronic sputtering. A full description of the underlying physical processes is very complex. It requires a detailed kinetic model for the electron system coupled to a molecular dynamics code to follow the atomic evolution. In this work, we ignore the details of the electron system evolution and apply a Molecular Dynamics (MD) model to describe the lattice evolution. For this purpose, we set the initial kinetic energy of the atoms in a cylinder of certain radius (3-5 nm) to be equal to the energy deposited by the incoming ion into the electron system. This approach is justified by the astonishingly broad range of phenomena that describes. In fact, for the first time, we show an atomistic model able to explain the nano-track radius, the velocity effect, the refractive index change, the defect generation rate, the defect saturation density or the electronic sputtering yield and distribution. As a conclusion, we will discuss the mechanisms for permanent modification of silica based on a sudden temperature raise that induces a huge thermal gradient followed by a shock wave and an ultrafast cooling process that determines the final atom rearrangement. Finally, the application of the model to embedded metallic nano-particles in silica will be discussed.

EO13 2

16:45 **Fluorescent nanodiamonds by low energy irradiation**

Authors : Paolo Coppo, Andrea Mazzocut, Alan Reynolds, Lorna Anguilano

Affiliations : Paolo Coppo; Andrea Mazzocut: Wolfson Centre Brunel University, Kingston Lane, Uxbridge, UB8 3PH United Kingdom Alan Reynolds; Lorna Anguilano: ETC Brunel University, Kingston Lane, Uxbridge, UB8 3PH United Kingdom

Resume : The use of nanodiamonds as luminescent biological probes is particularly intriguing, in view of their lack of reactivity and toxicity in vitro and in vivo.1 Nitrogen-Vacancy colour centres in diamond are commonly produced by irradiation of nitrogen rich diamond (type Ib) with high energy protons, electron or ion beams, followed by annealing at 600-800°C.2–4 Hereafter we investigated the use of a low energy (200KeV) TEM electron beam to generate the displacement of carbon atoms in commercially available nanodiamonds. The morphology, structure and optical properties of the samples were studied using a Scanning Transmission Electron Microscope coupled with a Gatan cathodoluminescence detector. XRD powder diffraction and a thorough investigation by steady state optical spectroscopy reveal new insights in this

EO13 3

promising material. In addition we explore the possibility to induce fluorescence in nanodiamonds (FNDs) by irradiation with a 60Co source, in all similar to those used in hospital environment for the treatment of cancer, in order to provide a more practical protocol to produce optically active nanodiamonds. 1. Wu, T.-J. et al. Nat. Nanotechnol. 8, 682–9 (2013). 2. Mochalin, V. N. et al. Y. Nat. Nanotechnol. 7, 11–23 (2012). 3. Boudou, J.-P. et al. Diam. Relat. Mater. 37, 80–86 (2013). 4. Chang, Y.-R. et al. Nat. Nanotechnol. 3, 284–8 (2008).

add to my program (close full abstract)

17:00 **Turning an organic semiconductor into a stable low-resistance material by ion implantation**

Authors : B.Fraboni1, A.Scidà1, P.Cosseddu2, Y.Q. Wang3, M. Nastasi4, S.Milita5 and A.Bonfiglio2

Affiliations : 1Dipartimento di Fisica e Astronomia, Università di Bologna, viale Berti Pichat 6/2, 40127 Bologna, Italy 2Dipartimento di Ingegneria Elettrica ed Elettronica, Università di Cagliari, piazza d'Armi, 09123 Cagliari, Italy and CNR-INFM S3 via Campi 213/a 41100 Modena 3Los Alamos National Laboratory MS-K771 Los Alamos NM 87545 USA 4 Center for Energy Sciences Research, University of Nebraska –Lincoln, Lincoln, NE U.S.A 5 IMM-CNR Bologna

Resume : The performance of organic electronic devices is steadily improving thanks to the advancement in understanding and controlling the organic material molecular structure and electron transport properties. Yet, a few major issues still need to be addressed, such as the achievement of an efficient charge carrier injection. The implementation of low contact resistance devices usually relies on interface physics (matching the metal electrode work function to the molecular energy levels of the semiconductors), or on dedicated device architectures. The electrical doping of organic films can be a very attractive way to further improve the efficiency of organic devices and ion implantation, the process often used to this aim in the fabrication of inorganic semiconductor devices, has not been yet applied to small molecule organic semiconductors on to organic materials. We report on the effects of low energy (30keV) ion implantation on thin films of Pentacene, carried out to investigate the efficacy of this process in the fabrication of organic electronic devices. Two different ions, Ne and N, have been implanted and compared, to assess the effects of a different reactivity within the hydrocarbon matrix. A strong modification of the electrical conductivity, stable in time, is observed following ion implantation. This effects is significantly larger for N implants (up to 8 orders of magnitude), that are here shown to introduce stable charged species within the hydrocarbon matrix, not only damage as is the case for Ne implants. Fully operational Pentacene thin film transistors have also been implanted and we show how a controlled N ion implantation process can induce stable modifications in the threshold voltage, without affecting the device performance. We have monitored the effectiveness of low-energy ion implantation in controlling and stabilizing the organic thin film resistivity over a long time (over 2000 hours), proving how ion implantation can be safely carried out on fully operational OTFTs. The electrical properties of the Pentacene layer and of the OTFT have been investigated by means of current-voltage and photocurrent spectroscopy analyses, while the structural modification induced by ion implantation have been characterized by depth resolved X-ray Photoemission Spectroscopy analyses.

EO13 4

add to my program (close full abstract)

17:15 **Modification of metal containing carbon films by swift heavy ion irradiation**

Authors : P.A.Karaseov1, A.I.Titov1, S.Kumar2, A.Tripathi2, D.K.Avasthi2, S.Mohapatra3

Affiliations : 1 State Polytechnic University, St.Petersburg, Russia 2 Inter University Accelerator Center, New Delhi, India 3. Guru Gobind Singh Indraprastha University, New Delhi, India

Resume : Ion beams are increasingly being used as a tool for synthesis and modification of nanostructures. It is demonstrated that ion beams can be used for synthesis of graphitic clusters to engineer the sp3/sp2 –bonding ratio and stress in insulating carbon thin films. Such transformation of insulating, diamond -like (sp3-bonded) carbon into conducting, graphite-like (sp2-bonded) carbon within the ion tracks has been demonstrated. Recently, it has been shown that swift heavy ion irradiation of carbon films results in the formation of conducting graphitic nanowires of about 8 nm in diameter embedded within the insulating carbon matrix. Use of swift heavy ion irradiation as a tool to synthesize conducting nanowires has been explored by a few groups. The field emission properties of carbon films are mainly dependent on the chemical bonding structure and the doping with metals (Au, Ag, Ni) into the carbon matrix. Modification of such doped material along ion track by swift heavy ion irradiation

EO13 5

is of great interest since it gives not only the way to engineer the sp3/sp2 – bonding ratio and stress in the film, but can give nanowires with significantly increased conductivity. In this contribution the route of swift heavy ion irradiation of carbon films combined with its doping for achieving highly conducting ion tracks in insulating carbon films will be presented. This work is supported by Russian RFBR (grants № 12-08-01197 and 13-02-92709) and DST of India.

add to my program **(close full abstract)**

Back

European Materials Research Society
23 Rue du Loess - BP 20 - 67037 Strasbourg Cedex 02 - France - Phone:+33-(0)3 88 10 63 72 - Fax:+33-(0)3 88 10 62 93 - emrs@emrs-strasbourg.com

PROGRAM VIEW : 2014 Spring
MY PROGRAM : 2014 Spring

Symposium : E

Defect-induced effects in nanomaterials

26 May 2014 | 27 May 2014 | 28 May 2014 | 29 May 2014 | **30 May 2014**

hide a

start at	Subject	Num.
	Nuclear materials I : Anatoly Dvurechenskii	
09:00	**Radiation damage evolution in nanocomposites** **Authors :** Blas Pedro Uberuaga **Affiliations :** Los Alamos National Laboratory, Los Alamos, New Mexico, USA 87545 **Resume :** Radiation damage evolution in nanocomposites As nuclear energy systems are taken to higher levels of radiation damage, there is greater need to develop materials that can withstand that damage. Nanocomposites, nanomaterials comprised of both a high density of internal interfaces and second phases, are one promising avenue for such materials. Most work on nanomaterials has focused on the role of the interfaces as sinks of point defects. Here, motivated by a series of experimental studies on oxide composites, we examine the other component of nanocomposites, the dual phase nature of the material. Using atomistic calculations, we examine defect behavior within these nanocomposites and use that insight to develop a mesoscale model of defect evolution of nanocomposites under irradiation. This model depends primarily on defect properties within each phase. We identify three regimes of steady-state defect behavior that depend on the relative thermodynamics and kinetics of the defects in the phases comprising the composite. Importantly, in one regime, defect populations are enhanced on one side of the interface and depleted on the other. Further, transient defect populations can exceed steady-state concentrations. The model captures the salient features observed in the experiments. We conclude that the evolution of irradiation-induced defects in one phase of the composite is strongly controlled by the defect properties of the other phase, offering a route to controlling defect evolution in these materials. add to my program (close full abstract)	EO14 1
09:30	**The effect of electron-ion interactions on the primary radiation damage in alpha -Fe** **Authors :** S. L. Daraszewicz, D. M. Duffy **Affiliations :** London Centre for Nanotechnology, Department of Physics and Astronomy, University College London (UCL), Gower Street, WC1E 6BT, London, UK **Resume :** The impact of electronic effects, such as the electronic stopping (e-s) and the electron-phonon (e-p) coupling, on the primary damage yield remains one of the most important unsolved challenges in the field of high-energy radiation damage modelling, which inhibits accurate predictions of long-term radiation damage in materials. Using classical molecular dynamics (MD), damped MD and two-temperature MD (2T-MD) we analyse the effects of electronic excitations in 50 keV and 100 keV primary knock-on atom (pka) cascades in alpha-Fe. We obtain detailed defect statistics for over two hundred simulations and demonstrate that the cascade dynamics and the resulting primary damage yield are highly sensitive to the choice of the treatment of electronic effects, with a variation of a factor of three in the number of residual defects predicted by the different models. We analyse the temporal defect evolution in detail and untangle the contribution of e-s and e-p coupling (and their parameter sensitivity) to the creation and annihilation of defects. It is the first systematic study of this type and it will therefore serve as an important reference for future modelling of high-energy radiation damage events, which will facilitate informed choices about the MD model to employ and enable valid comparisons between different studies. add to my program (close full abstract)	EO14 2

09:45 **Development of object kinetic Monte Carlo models for nanostructural evolution in iron alloys**

Authors : Monica Chiapetto, Lorenzo Malerba, Charlotte Becquart
Affiliations : SCK-CEN (Mol, Belgium), Université des Sciences et Technologies de Lille

Resume : We developed physically-based sets of parameters for object kinetic Monte Carlo (OKMC) simulations of the nanostructural evolution under irradiation of Fe alloys: our models proved to be able to describe the buildup of irradiation defect populations, in terms of density and size distribution, in both FeMnNi and FeCr alloys, model alloys for, respectively, bainitic and ferritic/martensitic steels for nuclear applications. The effects of the substitutional solutes of interest were introduced with different levels of approximation. Specifically, a “grey alloy” approach was applied, where the effect of the solute atoms is introduced by modifying the parameters that govern the mobility of both self-interstitial atoms (SIA) and vacancy clusters; namely, both are assumed to be slowed down by the presence of solutes. In particular, the slowing down of SIA clusters by Mn and Cr can be justified in terms of the interaction between these atoms and crowdions in Fe. This fact is exploited to introduce an explicit dependence of the parameters on solute concentration. With these models, irradiation processes up to < 1 dpa in different ranges of dose-rate and temperature were simulated, including post-irradiation annealing simulations, finding excellent agreement with experiments. Our simulations suggest that solute clusters are likely to form by heterogeneous nucleation on point-defect clusters.

EO143

10:00 **Break**

Nuclear materials II : Blas Uberuaga

10:30 **Mechanism of He impurity buildup-induced nanopore and fuzz formation in W**

Authors : A. Lasa, K.O.E. Henriksson, and K. Nordlund
Affiliations : Association Euratom-Tekes - Department of Physics, University of Helsinki, Finland

Resume : Recent experiments [1] have shown that W exposed to a He plasma becomes in a certain temperature range first nanoporous and eventually forms a low-density "fuzz"-like morphology. This unexpected effect can become a potentially serious problem in fusion reactors which are planned to have W in the inner plasma-facing wall. Using molecular dynamics and kinetic Monte Carlo simulations, we show that the effect can be understood to be due to initially mobile implanted He atoms becoming trapped in defects in the material. The immobile trapped He can absorb additional He, leading to growing nanobubbles. These bubbles can cause surface roughening via dislocation loop punching, and when sufficiently large, rupture at the surface leaving behing voids. The void formation explains the fuzz morpohology formation, and the balance of roughening and bubble rupture the experimentally observed scaling of fuzz layer thickness with the square root of fluence. [1] M. J. Baldwin and R. P. Doerner, Nucl. Fusion 48 (2005) 035001. [2] A. Lasa, S. K. Tähtinen, and K. Nordlund, EPL (2013), accepted for publication.

EO151

11:00 **He Blister Suppression by Swift Heavy Ions in Nanocrystalline ZrN**

Authors : A. Janse van Vuuren(a), V. A. Skuratov(b) J.H. Neethling(a), V.V. Uglov(c) and S. Petrovich(d)
Affiliations : (a)CHRTEM, NMMU, Port Elizabeth, South Africa, (b)FLNR, JINR, Dubna, Russia, (c)BSU, Minsk, Belarus, (d)VINCA Institute of Nuclear Sciences, BU, Belgrade, Serbia

Resume : Recent studies have shown that swift heavy ion irradiation may significantly modulate hydrogen and helium behavior in certain materials. This phenomenon is of considerable practical interest for various ceramics and semiconductors, specifically for candidate materials for use as inert matrix fuel hosts (IMs). IMs accumulate He via (n,□) reactions and will also be subjected to high energy fission fragments (FFs) in the nuclear reactor environment. The inherent properties of ZrN has led to its identification as a candidate IM. Certain studies have indicated that nanocrystalline (nc) materials have improved radiation tolerance compared to their micro- and single-crystalline counterparts. This suggests that nc-ZrN may have a superior radiation tolerance. In this study low energy He ions were used to simulate □-particles and high energy Xe and Bi

EO152

ions were used to simulate FFs. The combined effects of low and high energy radiation were also studied. TEM and SEM were used to study nc-ZrN irradiated with 30-40 keV He, 167 MeV Xe and 695 MeV Bi ions to fluences of 5×1016 cm-2, 2.65×1014 cm-2 and 1.5×1013 cm-2 respectively. The irradiated samples were annealed at temperatures between 600 and 1000 °C. He irradiation did not lead to amorphization of unannealed nc-ZrN. Post irradiation heat treatment resulted in blistering at depths corresponds to the end-of-range of the He ions. He/Xe irradiated samples revealed that the electronic excitation effects (EEEs) resulting from high energy Xe ions suppress He blister formation. nc-ZrN is prone to the formation of He blisters, which may lead to material failure and is therefore of concern for materials with nuclear applications. These effects may however be suppressed by the EEEs from high energy heavy ions.

add to my program (close full abstract)

11:15 **Nano-oxide nucleation and interaction with hydrogen in nano-composite steels**

Authors : M.G. Ganchenkova (1), V.A. Borodin (2)
Affiliations : (1) NRNU MEPhI, Kashirskoe Sh. 31, 115409, Moscow, Russia ; (2) NRC Kurchatov Institute, Moscow, 123182, Russia

Resume : Oxide-dispersion-strengthened (ODS) steels give an example of knowledge-based modification of a material at the nanolevel with the aim of predictably improve material's properties. Many experimental facts indicate that the oxide particle ensemble in the ferritic steel matrix develop via the co-precipitation of alloying atoms (Y, Ti, Al) with oxygen, which is strongly guided by the matrix lattice, as evidenced by orientational relations between oxide precipitates and the matrix. The kinetics of nucleation is very complicated and only several attempts to model the kinetics of oxide nucleation have been suggested. In this report we discuss an advanced model of oxide particle nucleation in ODS steels, which takes into account the recent data concerning the static and dynamic properties of the relevant impurity atoms in steel and the influence of the matrix lattice on impurity agglomeration. Based on this data, the model suggests a possible sequence of events involved in the oxide nucleation at the atomistic level. Important part played in nucleation by self-point defects, which is completely neglected in the modern theoretical models, is emphasized. Following the theoretical considerations, several atomistic configurations of small oxide clusters in bcc iron lattice were created and their stability was investigated using both first principles and classical molecular dynamics. The interaction of the simulated oxide nanoparticles with hydrogen dissolved in the lattice is discusse

EO15 3

add to my program (close full abstract)

11:30 **Raman microscopy as a defect microprobe for hydrogen bonding characterization in materials used for thermonuclear fusion applications**

Authors : C. Pardanaud1, Y. Addab1, C. Martin1, N. Mellet1, G. Giacometti1, P. Roubin1, B. Pegourie2, M. Oberkofler3, M Koppen3, T. Dittmar3, Ch. Linsmeier3, C. Hopf4, T. Schwarz-Selinger4, W. Jacob4
Affiliations : 1 Aix-Marseille Universit?-CNRS, PIIM, 13397 Marseille cedex 20, France; 2CEA, IRFM, 13108 Saint-Paul-lez-Durance, France; 3 Forschungszentrum J?lich GmbH, Institut f?r Energie- und Klimaforschung - Plasmaphysik, 52425 J?lich, Germany 4Max-Planck-Institute f?r Plasmaphysik, EURATOM Association, Boltzmannstr. 2, 85748 Garching, Germany.

Resume : One promising way to produce energy from nuclear fusion reaction is to magnetically confine a hot (D, T) plasma in thermonuclear fusion devices (called tokamaks) and to heat it to ignition. One of the inner walls? role is to transfer the heat loads produced by the fusion reaction to a cooling loop and then to a turbine for producing electricity. In the tokamaks, interactions between plasma and walls lead to impurity transport in the edge machine together with material migration/mixing. Depending on the location in the machine, the impinging particle flux and energy, the initial structure of the material? wall?s temperature is changed, affecting the efficiency of the fundamental mechanisms occurring. Then, it is a challenging question to predict what will be the walls? hydrogen content. This point has been achieved for carbon walls as many studies have yet been done. Especially, a campaign involving the Tore Supra tokamak has been dedicated to measure both the H and C behavior at the scale of the machine and on many years. However, due to the good affinity existing between C and H isotopes leading to a severe safety issue (namely, tritium retention), carbon is not envisaged for the next step machine: the ITER project. Be and W, in which H isotopes can also be retained, have been chosen as the wall materials. For these elements, many studies have to be done before we can be predictive. In this study, we will present the advantage of using Raman spectroscopy at the micron scale (H bonding,

EO15 4

structure/defect sensitive, non destructive,?) for fusion applications. As examples, we will use Tore Supra carbon tiles, beryllium implanted with deuterium ions resulting in the creation of D containing nanometric height domes, and tungsten oxides implanted with hydrogen ions.

add to my program **(close full abstract)**

11:45 **Final discussions**

12:15 **Lunch**

Back

European Materials Research Society
23 Rue du Loess - BP 20 - 67037 Strasbourg Cedex 02 - France - Phone:+33-(0)3 88 10 63 72 - Fax:+33-(0)3 88 10 62 93 - emrs@emrs-strasbourg.com