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E-MRS Spring Meeting 2004  
May 24-28, 2004

## SYMPOSIUM H

Atomic scale materials design; modelling and  
characterization

Symposium Organizers:

Alain Estève, CNRS – LAAS, Toulouse, France

Jim Greer, University College, Cork, Ireland

Mehdi Djafari Rouhani, University of Toulouse, France

Anatoli Korkin, NANO & GIGA SOLUTIONS, Gilbert AZ, USA

Papers will be published in Computational Materials Science

# E-MRS 2004 SPRING MEETING

## SYMPOSIUM H

Tuesday, May 25, 2004

Morning

Session I: Polymer materials

Session chair: A. Korkin

- H-I.01** 09:00 -Invited- VAN DER WAALS DENSITY FUNCTIONAL THEORY CALCULATIONS OF POLYMER INTERACTIONS  
**Jesper Kleis** and Elsebeth Schröder, Department of Applied Physics, Chalmers University of Technology and Göteborg University, 41296 Gothenburg, Sweden  
We study the mutual interactions of simple polymer segments within the framework of density functional theory (DFT). We primarily focus on two polymers, polyethylene (PE) and polyvinylchloride (PVC), but our scheme applies more generally to geometrically simple polymers. From first principles DFT calculations we extract the geometrical structure of the polymers and their short-range interaction energy. Conventional implementations of DFT do not treat the long-range interactions correctly, but by using a systematic correction scheme we find the long-range van der Waals (dispersion) energy contribution of the polymer-polymer interaction.
- H-I.02** 09:30 MODELING CURRENT TRANSPORT IN ORGANIC LIGHT-EMITTING DEVICES (OLEDs)  
H.L. Kwok, Centre for Advanced Materials and Related Technologies, University of Victoria, Victoria V8W 3P6, Canada  
There has been some substantial interest in studying current transport in organic light emitting devices (OLEDs) because of their potential as solid-state light sources. While some of the physics remain to be resolved, there is in place a fair amount of understanding on the device operation to develop a working model for properties such as the J-V characteristics. This paper is an extension of an earlier publication<sup>1</sup> to model mathematically the rate of exciton formation in OLEDs based on bimolecular recombination. The earlier work relies on knowing the spatial distribution of the carrier densities and this allows one to study position dependent properties such as selective doping in OLEDs. Our current work extends the previous model to include space charge effect at low bias and suggests a possible mechanism bridging the transition between space charge limited current at low bias and recombination current at large bias. To validate our model, we compared our simulation results to data reported in the literature in the case of a ITO/TPA-PPV/Al device<sup>2</sup>. In particular, effort was spent to explain the existence of a current peak at low bias in the J-V characteristics. Our overall result appears to suggest that the operation of the OLEDs may well be accounted for by a simple model involving the capture of space charge injected holes at some unknown sites (possibly "trap" centers). This is followed by "recombination", which appears to be strictly limited by the availability of the electrons within the active region. The transition from space charge limited current to recombination current could explain the existence of the current peak at low bias.
- H-I.03** 09:45 STABILITY IN POLYSILANES FOR LIGHT EMITTING DIODES  
Asha Sharma(a), U. Lourderaj(b), Deepak(a), N. Sathyamurthy(b) and Monica Katiyar(a), (a)Dept. of Materials & Metallurgical Engg. & Samtel Centre for Display Technology, Indian Institute of Technology, Kanpur, India, (b)Dept. of Chemistry, Indian Institute of Technology, Kanpur, India  
Polysilanes are Si-backbone polymers with organic substituents which exhibit photoluminescence in the UV or NUV region. They can be used as active sources for electroluminescence devices mainly suitable for blue emission. We have examined four polysilanes, namely polydi-n-butylsilane (PBBS), polydi-n-hexylsilane (PDHS), polymethylphenylsilane (PMPS) and poly[bis(p-butylphenyl)silane] (PBPS), which have been reported<sup>[1]</sup> as active materials in LEDs. Among these, PBPS LED shows the greatest durability of the device at room temperature and NUV-EL is observed continuously for over 12 hours. For PBBS, PDHS and PMPS either room temperature EL is not observable or the device life time is very short. Understanding the factors influencing the stability of PBPS would help design polymers that are better. Attempts have been made to investigate the cause of instability of PBBS, PDHS and PMPS in comparison to PBPS where four polysilanes differ only in the substituents attached to the main chain. Ab initio (CIS/6-31g\*) and semi-empirical (AM1/PECI=8) calculations have been done to ascertain the relative stabilities of different electronic states. Potential energy curves plotted as a function of the Si-Si bond distance reveal that the first singlet (S1) state is stable for these polysilanes. However the lowest triplet (T1) state is repulsive, leading to the dissociation of the molecule. The dissociation of triplet state (T1) seems to be preceded by an intersystem crossing between the S1 and higher triplet states, mediated by vibronic coupling. The relative stability of the four polysilanes is correlated to the energy difference between the different triplet states. References: [1] Suzuki et al., IEEE Journal of Selected Topics in Quantum Electronics, Vol.4, No.1, 1998, p.129

**H-I.04** 10:00 DENSITY FUNCTIONAL TIGHT BINDING SIMULATION OF ACETONITRILE UNDER HIGH PRESSURE  
Sylvain Beaucamp and Didier Mathieu, Commissariat à l'Énergie Atomique, Centre du Ripault, BP16, 37260 Monts, France and Viatcheslav Agafonov, Laboratoire de Chimie Physique, EA PIMIR 2098, Faculté de Pharmacie, 31 Avenue Monge, 37200 Tours, France  
Density Functional tight Binding (DFTB) method proved useful to simulate the evolution of chemical systems on application of high pressures. However as it not optimized to describe van der Waals forces. Problems may be expected at lower pressures, especially for system for high symmetry compounds or low density crystals. Because of high symmetry and nitrile moiety unfavorable for high density packings, acetonitrile might be a difficult case. Actually, present calculations show that relaxation of the observed X-ray crystal structure of acetonitrile using DFTB leads to a loss of symmetry. Therefore, symmetry constraints have been implemented in the program. At higher pressures, symmetry constraints are not necessary. The simulation of the acetonitrile crystal at very high pressures allow us to sample the potential energy surface of nitrile systems and might provide some insight into the loss of unsaturated moieties for nitrile polymers under pyrolysis in vacuum.

10:15 **BREAK**

## Session II: Oxide materials I

Session chair: A. Estève

**H-II.01** 10:45 -Invited- CHARACTERISATION OF OXIDE DISPERSION-STRENGTHENED STEEL BY EXTENDED X-RAY ABSORPTION SPECTROSCOPY  
**C. Degueldre**(a), S. Conradson(b) and W. Höffelner(a), (a)Laboratory for Material Behaviour, Paul Scherrer Institute, 5232 Villigen, Switzerland, (b)Los Alamos National Laboratory, Los Alamos NM 87545, USA  
The Oxide Dispersion-Strengthened (ODS) steel PM2000 has been tested by Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy as well as studied for its behaviour under irradiation using SRIM. The samples were investigated as received and consisted of yttria nano-particles (around 20 nm in size) dispersed in the ferritic alloy. TEM investigations show the yttria nano-particles still well crystallised even after the mechanical and thermal treatments for the ODS preparation. The yttria nano-particles dispersed in the ferritic matrix present a Y absorption edge that can be used to analyse the atomic environment of Y. In fact the EXAFS analysis shows that the yttria phase is not cubic as it may be expected. The paper discusses the atomic environment of Y assuming potential changes e.g. cubic – monoclinic during thermal treatments as it may be postulated. The SRIM results show that the yttria nano-particles appear more transparent than the steel matrix with regard to the H or He irradiations. These results demonstrate the value of EXAFS for the characterisation of a nano-structured material such as ODS. The structure of the dispersed yttria nano-particles is not accessible by classical XRD. The EXAFS analysis of these yttria nano-structured ODS will be studied as a function of thermal treatments and irradiation conditions.

**H-II.02** 11:15 -Invited- MULTIMILLION ATOM MOLECULAR DYNAMICS SIMULATIONS OF NANOSTRUCTURES ON PARALLEL COMPUTERS  
**P. Vashishta**, University of Southern California, USA

**H-II.03** 11:45 -Invited- MONTE CARLO SIMULATIONS OF SILICON NANOCRYSTALS IN AMORPHOUS SILICON DIOXIDE  
G. Hadjisavvas and **P.C. Kelires**, Physics Department, University of Crete, P.O. Box 2208, 710 03 Heraclion, Crete, Greece  
Si nanocrystals (nc) embedded in a-SiO<sub>2</sub> have been extensively studied in recent years because of their photoemission properties. Various models have been proposed to explain the source of light emission, such as quantum confinement and localized surface states. However, some important issues still remain unclear. For example, since confinement depends on the size and density of the nanocrystals, it is essential to know their stability in the amorphous matrix as they become smaller. Also, the atomic structure of the interface, i.e., kind and proportion of bonds, is a crucial parameter, yet it is not well known. We present here results of Monte Carlo simulations which shed light onto these issues. In our approach, the generation of the embedding a-SiO<sub>2</sub> structure is achieved via a modified Wooten-Winer-Weaire method. Starting from crystalline beta-cristobalite, the network is amorphized through bond-breaking and switching moves. The Si nc is positioned at the center of the cell. The energies are calculated using the Keating potential. We introduce bond-conversion moves of the type Si-Si to Si-O-Si, and vice versa. This allows us to study interdiffusion in the system. We find a significant proportion of Si-O-Si bridge bonds at the interface, not considered previously. A penetration of oxygen into the nc, limited to few Angstroms, is observed. From an oxidation-number analysis, it comes out that the width of the interface is about seven Angstroms. The energetics show that the nc's are slightly metastable (small positive formation energies). The interaction between the nc's exhibits well-defined minima. We found a critical diameter of 1.5 nm, below which the nc's are unstable (heavily deformed).

**H-II.04** 12:15

A DENSITY FUNCTIONAL THEORY STUDY OF THE OXIDATION OF THE Si-RICH SiC SURFACE  
E. Wachowicz(a,b), R. Ruralski(c,d), P. Ordejón(c) and P. Hyldgaard(a), (a)Department of Applied Physics, Chalmers University of Technology, 41296 Göteborg, Sweden, (b)Institute of Experimental Physics, University of Wrocław, Pl. Maxa Borny 9, 50294 Wrocław, Poland, (c)Institut de Ciència de Materials de Barcelona (ICMAB--CSIC), Campus de Bellaterra, 08193 Barcelona, Spain, (d)Laboratoire Collisions, Agrégats, Réactivité, UMR5589, Université Paul Sabatier, 118 route de Narbonne, 31062 Toulouse cedex, France

SiC-based microelectronics is a candidate for a future replacement of the current Si-based technology. One of the main advantages of SiC over other wide band-gap semiconductor materials is the existence of a native oxide (SiO<sub>2</sub>). We present our theoretical study of the very first stages of oxidation on Si-rich 3C-SiC(001) surface. Total-energy density functional theory (DFT) calculation of different on- and near-surface O adsorption sites were performed. All calculations were done with the `siesta` code using GGA and a large basis set. We performed exhaustive convergence tests for the O<sub>2</sub> molecule dissociation energy, for the clean surface (substrate), and for the single-oxygen adsorption energies. We determine both the most favorable and stable adsorption sites and correlate the adsorption energy with the lattice distortion. We find that the near-surface adsorption is strongly favored and can arise both as intra-bond and interstitial oxygen incorporation. Finally, we use extensive DFT calculations to study the double-oxygen adsorption and test for correlation effects in the SiC surface oxidation process.

**H-II.05** 12:30

LAYERED SURFACE-OXIDE STRUCTURES ON Mg(0001)

Elsebeth Schröder(a) and Adam Kiejna(b), (a)Department of Applied Physics, Chalmers University of Technology and Göteborg University, 41296 Gothenburg, Sweden, (b)Institute of Experimental Physics, University of Wrocław, Plac M. Borny 9, 50-204 Wrocław, Poland

First principles density functional theory (DFT) calculations reveal the formation of a two-dimensional layered structure on the Mg(0001) surface in the initial stages of oxidation. The mixed oxygen-magnesium layers sit on top of an almost unchanged Mg(0001) surface, at least up to 3 monolayers of oxygen coverage. The layer separation of 2.3-2.7 Å is such that in addition to the strong short-range interactions also the long-range interactions, like the van der Waals forces, contribute to the interlayer binding. Conventional implementations of DFT are unable to treat such long-range interactions, and we use a recently introduced functional [Phys. Rev. Lett. 91, 126402 (2003)] for layered systems to consistently include the van der Waals interactions between the oxide layers.

12:45

**LUNCH**

Tuesday, May 25, 2004

Afternoon

Session III: Metals and inter-metallic materials

Session chair: P. Vashishta

- H-III.01** 14:00 -Invited- USING ATOMISTIC MODELING FOR MATERIALS DESIGN  
**M.I. Baskes**, Los Alamos National Laboratory, USA
- H-III.02** 14:30 POLARIZATION BEHAVIOUR IN SYSTEMS WITH COMPETING FERROELECTRIC/ANTIFERROELECTRIC INTERACTIONS  
**J. Milhazes, A. Cadilhe** and **S. Lanceros-Méndez**, Centro de Física da Universidade do Minho, 4710-057 Braga, Portugal  
In the mixed ferro- (FE) and antiferroelectric (AFE) system, there is competition between the FE and the AFE orderings. Random distribution of composition is the main source to produce frustration, which can increase local structural competition such that the long-range electric order disappears. Instead of a typical sharp FE or AFE phase transition, these systems are characterized by extremely rich x-T phase diagram, where phase coexistence [such as PE/FE, PE/AFE etc.] becomes a characteristic. In order to obtain locally a phase state, which is different from the disordered host, the minimal size of the short range ordered clusters must be big enough to show typical features of the long-range ordered phases. In this communication, a model for polarization and hysteresis loops based on the coexistence of FE and AFE regions will be presented. Based on our model, we simulated single and double hysteresis loops corroborated by experimental results. The fit to experimental results is sensitive to the relative values of the interaction constants, grain size, and temperature. The results of the model will be used to discuss the phase diagram of the mixed crystal system Betaine Arsenate / Betaine Phosphate, which shows with a rich variety of coexistence regions.
- H-III.03** 14:45 THE RESEARCH OF THE MECHANISM OF NON-VACATIONAL DISORDERING IN A TWO-DIMENSIONAL ALLOY OF Ni<sub>3</sub>Al INTERMETALLIDE  
**M.D. Starostenkov, M.B. Kondratenko, N.B. Cholodova, G.M. Poletaev**, Altai State Technical University, Department of General Physics, Barnaul, Lenin st. 46, Barnaul 656038, Russia  
The disordering processes, taking place at high temperatures in Ni<sub>3</sub>Al two-dimensional crystal were studied by the method of molecular dynamics. The crystal had the packing of atoms corresponding to the plane [111] of L12 superstructure. The interactions between atoms in the alloy were given by semiempirical potential Morse functions. The calculated block of the crystal was presented by the packing, containing to 105 atoms. The structure was repeated by periodical boundary conditions outside the block. The velocities of the atomic displacements in the calculated block of the crystal in the dependence on temperature were given in correspondence with Boltzman distribution. The computer experiment showed, that the disordering process took place at the temperature 1590 K at the absence of vacancies and other defects. The velocities of the movement of atoms in the crystal were given accidentally, that is why the temperature of the beginning of the disordering process and the sizes of the disordering areas changed at every experiment. They were obeyed to the definite statistics regularities. In this connection, the value of the diffusion coefficient appeared to be proportional to the sizes of the disordering areas. The disordering processes are characterized by the definite mechanisms of collective displacements of atoms, which can be presented by triangles, tetragons, pentagons, hexagons and more complicated figures. The estimation of the activation energy of collective displacements of atoms, forming the disordering areas in the alloy was made.
- H-III.04** 15:00 COMPUTER SIMULATION STUDY OF DISLOCATION DYNAMICS IN MOLYBDENUM  
**Y.L. Liu** and **C.H. Woo**, Department of Mechanical Engineering, The Hong Kong Polytechnic University, Hong Kong SAR, China  
In this study, subsonic, transonic and supersonic motions of an edge dislocation, under and applied stress, in BCC molybdenum were investigated using the molecular dynamics simulation. We considered the glide of an edge  $a/2\langle 111 \rangle (110)$  dislocation under the action of a pure shear stress, and focus on the damping mechanism against the dislocation motion in different regimes. We found that the kinetic energy radiation along the Z-direction is about 100 times larger than those along the other two directions. That means that the continuum model of plane elastodynamics (X-Y) can only account for a small portion of the kinetic energy radiation during the dislocation motion. We also found that the phonon drag force is too small to be the dominant energy dissipation mechanism for high-speed dislocations.
- H-III.05** 15:15 MULTI-SCALE MODELING OF MIGRATION AND STABILITY OF ELEMENTARY DEFECTS IN ALPHA-IRON  
**J. Dalla Torre, C.C. Fu, F. Willaime, J.-L. Bocquet, A. Barbu**, Service de Recherches de Métallurgie Physique, CEA/Saclay, France  
We have performed a multi-scale modeling of the evolution under isochronal annealing of the defects produced by electron irradiation in alpha-Fe. The stability and mobility of the relevant point defects and defect clusters (vacancies, self-interstitials, and small clusters of vacancies or interstitials) are determined by the SIESTA ab initio method. These results are then used as input data for an event-based kinetic Monte Carlo model (JERK) to simulate the defect-population evolution: defects may migrate, aggregate, dissociate or annihilate. We followed closely the conditions of existing experiments, where evolutions in the defect population are evidenced by abrupt changes in the resistivity of the sample (so-called recovery stages). We successfully reproduce all the recovery stages and we clearly attribute them to the migration or dissociation of specific defects. Dose effects, i.e. shifts of the recovery stages when the irradiation dose is increased, are also properly reproduced.

H-III.06 15:30

FP-LAPW INVESTIGATIONS OF ELECTRONIC STRUCTURE OF TaN AND TaC COMPOUNDS

M. Sahnoun(a), C. Daul(a), C. Demangeat(b), J.C. Parlebas(b) and M. Driz(c), (a)Département de Chimie, Université de Fribourg, Pérolles, 1700 Fribourg, Switzerland, (b)IPCMS-GEMM, UMR 7504 CNRS, 23, rue du Loess, 67034 Strasbourg Cedex 2, France, (c)Laboratoire de Sciences des Matériaux, Université Djillali Liabes - Sidi Bel Abbes, Algeria

The transition-metal carbides and nitrides possess many scientifically interesting and technologically important properties. On the microscopic level they display three different types of bonding characteristics: metallic, ionic, and covalent. This unusual combination of bonding mechanisms manifests itself in their macroscopical properties. They exhibit ultrahardness, for example, many binary types of carbide have microhardness values between 2000 and 3000 kg/mm<sup>2</sup> values which lie between those of Al<sub>2</sub>O<sub>3</sub> and diamond. This property has resulted in an extensive use of carbides as cutting tools and for wear-resistant surfaces. However, the nitrides are hard, but are not as hard as the carbides. A second striking property of these materials is their very high melting points as well as metallic conductivity. Perhaps the important property of this type of compounds is their defect structure, they often crystallize in the sodium chloride (rocksalt) structure, and they are fairly simple to treat theoretically. It has been demonstrated recently that the stoichiometry of rocksalt tantalum nitride (TaN) can be tuned by N<sub>2</sub> pressure and temperature, yielding material that ranges from highly conductive to insulating. Tantalum nitride was also found to be promising material for other applications, such as diffusion barriers in copper interconnects on Si chips, and to make compact thin-film resistors. The Ta-N system is relatively unexplored and, unlike e.g. the Ti-N system, it exhibits a remarkable richness in the array of equilibrium and metastable phases that can form; indeed more than eleven have been reported, where very little is known about their relative stability. In this work, and using density functional theory we investigate the atomic and electronic structure of cubic TaN structure. Based on the calculated energetic and electronic structures, our results point on geometries optimizations, densities of states and bands structures. Also for comparison, we treated tantalum carbide TaC, and see the effect of changing the nitrogen by carbon on different parameters. Elastic properties are also treated and will be presented here. The density functional theory (DFT) calculations performed for this materials use the first-principles full-potential linearized plane wave (FLAPW) method with both exchange-correlation functionals LDA and GGA.

15:45

**BREAK**

Session IV: Deposition techniques and growth

Session chair: M.I. Baskes

H-IV.01 16:15 -Invited-

VAPOR DEPOSITION OF THIN METALLIC FILMS: ATOMISTIC MONTE CARLO SIMULATIONS  
**J. Dalla Torre**, Service de Recherches de Métallurgie Physique, CEA/Saclay, France

H-IV.02 16:45 -Invited-

SEEDING GROWTH OF SURFACE-ALIGNED NANOSTRUCTURES BY SURFACE ASSEMBLY OF ATOM-SCALE METALLIC WIRES

**Per Hyldgaard** and Bengt I. Lundqvist, Department of Applied Physics, Chalmers University of Technology, 41296 Gothenburg, Sweden

The (00-1) surface of kappa-phase Al<sub>2</sub>O<sub>3</sub> provides conditions for an automatic surface assembly of parallel atom-scale metallic wires mutually separated by 8.4 Å and insulated by the surrounding oxide [PRL 90, 236803 (2003)]. We summarize the flexible-ionic oxide behavior responsible for this predicted metallic-wire surface assembly and discuss the low- and high-temperature limits on the formation of the one-dimensional electron gas, i.e., on the atom-scale metallic-wire behavior. We furthermore document that the metallic wires serve to selectively bind graphite sheets with a prespecified orientation. We discuss how this reactivity can seed controlled growth of graphitic nanostructures aligned on surfaces and between predefined surface locations (for example, between contacts and near electrostatic gates).

H-IV.03 17:15

SELF-ORGANIZATION IN A MODEL OF STRAINED EPITAXY

Vasyl Tokar(a,b) and Hugues Dreyssé(a), (a)Institut de Physique et Chimie des Matériaux de Strasbourg, 23 rue du Loess, 67037 Strasbourg, France, (b)Institut of Magnetism, National Academy of Sciences 36-b Vernadsky str, 03142 Kiev-142, Ukraine

In heteroepitaxy, a lattice size mismatch between the substrate and the adlayer is common and is a major factor influencing both the layer growth mode and its morphology. In this contribution, we propose an atomistic model for the growth of submonolayer by considering pair interactions. By assuming a coherent deposition, the systems is projected on a lattice gas model in a way similar to cluster expansion in the theory of alloy /1/. The 1D case has been solved exactly /2/. It is possible to show, that if the nearest-neighbors interaction is attractive and if the lattice size mismatch is large enough, at low temperature the atoms self assemble into size calibrated clusters. Moreover if the next-nearest-neighbors interaction is also attractive, the clusters display self-organisation. For certain range of lattice size mismatch, it is even possible to have self-assembly at finite temperature which vanishes at T =0K. For thicker layers the kinetics of self-organization will be addressed. /1/ V. Tokar et H. Dreyssé, Phys. Rev. B 68 (2003) 011601 V. Tokar et H. Dreyssé, J. Phys. : Cond. Matter (2004) /2/ V. Tokar et H. Dreyssé, Phys. Rev. E 68 (2003) 195419

- H-IV.04** 17:30 **MODELLING OF LAYER EPITAXIAL GROWTH: SURFACE MORPHOLOGY AND GROWTH MODE TRANSITIONS**  
Vladimir I. Trofimov, Ilya V. Trofimov, Institute of Radioengineering & Electronics of RAS, 11/7 Mokhovaya Street, 125009 Moscow, Russia and Jong-Il Kim, School of Information Technology and Engineering Korea University of Technology and Education, Chung Nam-Do, 330-708 Seoul, Korea  
 Recently, we have proposed a simple kinetic model for layer epitaxial growth [1], which combines a rate equation approach and a feeding zone that allows accounting for an interlayer adatoms exchange, and consists of an infinite set of rate equations for adatom and 2D island density and coverage in successive layers. With this model it has clearly been shown on how with decreasing adatom surface diffusivity and/or increasing the Ehrlich-Schwoebel (ES) barrier height the growth mode crosses over from a smooth layer-by-layer to a rough 3D growth, and a corresponding phase diagram of the growth mode in the parameter space has been constructed. This paper reports on a systematic study the effect of the critical nucleus size, the island collision behaviour (impingement/coalescence) and the existence (in the case of heteroepitaxy) of two different adatom mobilities: heterodiffusion in the first layer and self-diffusion in all the next layers on the epitaxial growth. Special emphasis is placed on the identification of the elementary growth processes that affect the critical island size for the next layer nucleation and thus govern the growth mode transitions. It is shown that the increase of a critical nucleus size favours a smooth growth, whereas the island collision behaviour weakly influences on the growth mode transitions but affects on the scaling properties of the nucleation kinetics. The effect of two adatom mobilities depends on the relation between hetero- and self-diffusivity: a slower heterodiffusion leads to a smoother initial growth and retards the transition to a rough 3D growth, whereas a faster heterodiffusion promotes that transition.  
 [1] V.I. Trofimov, V.G. Mokerov, *Comput. Mater. Sci.* 17 (2000) 510.
- H-IV.05** 17:45 **MORPHOLOGICAL INSTABILITIES AND CRITICAL THICKNESS FOR DISLOCATION GENERATION IN EPITAXIAL THIN FILMS**  
Biao Wang and C.H. Woo, Department of Mechanical Engineering, The Hong Kong Polytechnic University, Hong Kong SAR, China  
 Thin films, particularly those deposited by epitaxy, have become increasingly important in many practical applications, most obviously in relation to the production of electronic, opto-electronic and magnetic devices. During epitaxial growth, lattice mismatch results in the generation of dislocations, when the film thickness increases beyond a critical value. The presence of such dislocations causes degradation of the performance of the thin film. Due to its obvious technological importance and scientific interest, study on this critical phenomenon has been actively pursued. In this investigation, we determine the critical thickness for dislocation nucleation. The perturbation theory will be used to first derive the solution for a slightly undulating surface. The morphological evolution and instabilities of the film will then be investigated. Assuming dislocation nucleates from the surface cusps, a criterion can be derived to determine the critical thickness for a piezoelectric thin film. Based on the criterion, detailed calculations are carried out, and the results compared with the experimental and MD simulation results.
- H-IV.06** 18:00 **GROWTH OF THE THREE-DIMENSIONAL SiC CLUSTERS ON Si MODELLED BY KMC**  
J. Pezoldt, FG Nanotechnologie, Zentrum für Mikro- und Nanotechnologien, TU Ilmenau, Postfach 100565, 98684 Ilmenau, Germany, A.A. Schmidt, V.S. Kharlamov, K.L. Safonov and Yu.V. Trushin A.F. Ioffe Physico-Technical Institute, Polytekhnicheskaya 26, 194021 St. Petersburg, Russia, E.E. Zhurkin, St. Petersburg State Polytechnic University, Polytekhnicheskaya 29, 195251 St. Petersburg, Russia  
 The formation of silicon carbide nanocluster on silicon substrates by MBE deposition of carbon provides a variety of applications, such as anti dot structures, nanowire heterostructures, wave guides and arrays of tips for cold cathode emission. The SiC formation on Si is unusual for semiconductor systems with large lattice mismatch due to the formation of a Si<sub>1-x</sub>C<sub>x</sub> solid solution, a formation of two dimensional 3C-SiC in this solid solution, and a subsequent step transforming the two-dimensional (2D) clusters into three-dimensional (3D) clusters for overall stress minimization. At the same time there are strong experimental evidences that under some experimental conditions 2D clusters could exist even at relatively high coverages. To study the transition from the 2D to the 3D cluster during SiC nucleation and growth the kinetic Monte Carlo method was used. Silicon and carbon atoms are allowed to exchange between the fixed sites of the 3D lattice with the symmetry of the diamond lattice (to simulate the growth of the 3C-SiC polytype mainly observed in growth experiments). The fitting parameters were estimated by means of molecular dynamics simulation as well as by comparing the data obtained with the experimental AFM, RHEED and TEM results.

Wednesday, May 26, 2004

Afternoon

Session V: Nanostructure properties

Session chair: M. Djafari Rouhani

- H-V.01** 14:00 -Invited- ATOMIC-SCALE STM EXPERIMENTS ON SEMICONDUCTOR SURFACES/ TOWARDS MOLECULAR NANOMACHINES  
**Prof. Dujardin**, Laboratoire de Photophysique Moléculaire, Orsay, France
- H-V.02** 14:30 STRUCTURAL DEPENDENCE OF OPTICAL PROPERTY OF SINGLE-WALLED BORON NITRIDE NANOTUBES  
R.Q. Zhang and M.F. Ng, Department of Physics and Materials Science, City University of Hong Kong, Hong Kong SAR, China  
The optical properties of different single-walled boron nitride nanotubes (SWBNNTs) with respect to their chirality, tube length, and tube diameter are examined with a time-dependent localized-density-matrix approach based on a semiempirical Hamiltonian. Comparisons to single-walled carbon nanotubes (SWCNTs) are made where appropriate. It is found that the optical gap of SWBNNTs is independent of the chirality with a given tube diameter. The gap is 5.78 eV at a tube diameter of about 5.6 Å, in contrast to SWCNTs, in which the optical gap depends strongly on the chirality, especially when the tube diameter is small. It is also found that SWBNNTs mainly show one major absorption peak below 6 eV, which is very different from the multi-peak features of SWCNTs. Moreover, the optical properties of SWBNNTs are also found to be strongly anisotropy and significantly high in absorption intensity regardless of the chirality, suggesting a good potential in advanced applications such as ultraviolet light absorption.
- H-V.03** 14:45 SELF-ORGANIZING PROCESSES IN CRYSTAL LATTICES AND FORMATION OF STRUCTURES OF NANOMETER DIMENSIONS  
I.V. Tereshko, V.V. Glushchenko, A.M. Tereshko, R.V. Petrov and V.V. Abidzina, Belarusian - Russian University, Prospect Mira 43, 212005 Mogilev, Belarus  
The present paper is aimed at studying nonlinear effects in solids induced by interaction of low-energy ion with surface of crystal lattices. We showed by a computer simulation (used a molecular dynamics method) that nonlinear oscillations in the system of coupled atomic oscillators were excited. The dependence of each atom displacement on the time passed after stopping the external influence was investigated. The formation of atomic clusters with nanometrical dimensions, running autosolitons, long-lived undamped oscillations in local ranges were observed. Such modifications in materials could be understood within the conception of only active self-organizing processes in crystal lattices, where the energy transition from vibration mode to a progressive one takes place. We also showed experimentally by the electron microscopy method that in the samples of armco-iron irradiated by a low-energy ion a microcrystalline and nanocrystalline structure were formed. These investigations confirm the results of our computer simulation.
- H-V.04** 15:00 L10- ORDERING KINETICS IN FePt NANO-LAYERS: MONTE CARLO SIMULATION  
M. Kozłowski, R. Kozubski, Institute of Physics, Jagellonian University, Reymonta 4, 30-059 Krakow, Poland, V. Pierron-Bohnes, Institut de Physique et Chimie des Matériaux de Strasbourg, 23, rue du Loess, BP43, 67034 Strasbourg CEDEX 2, France  
Ordering kinetics in L10-ordered FePt nano-layers has been studied by Monte Carlo (MC) simulation implemented with Glauber dynamics and vacancy atomic-jump mechanism. Nano-layers were simulated by imposing two-dimensional periodic boundary conditions upon a sample of AB binary system with L10 superlattice. Various models of surfaces limiting the sample, as well as various vacancy histories (creation and annihilation) were considered. Atomic pair-interaction energies in two co-ordination shells were evaluated on the basis of Cluster-Expansion "ab-initio" calculations carried out for FePt. Strong effect of the layer thickness on L10 structure stability and ordering kinetics was observed. The results are discussed in terms of detailed atomic-jump statistics analysed as a function of the number of atomic layers composing the simulated FePt thin film.
- H-V.05** 15:15 NANOSCALE EFFECTS ON THE NANOMECHANICAL PROPERTIES OF MULTIFUNCTIONAL MATERIALS  
C. Charitidis, S. Logothetidis, Laboratory for Thin Films, Nanosystems and Nanometrology, Department of Physics, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece  
Nanoscale measurements of mechanical and tribological properties play an important role in many emerging fields, such as surface engineering, magnetic storage disks, biomedical coatings and microelectromechanical systems. The understanding of scale effects is especially important, since surface to volume ratio grows with miniaturization and surface phenomena dominate. Nanoindentation and nanoscratching test are now commonly used for the evaluation of the functionality of the film-substrate compound can be satisfactorily used for the multifunctional materials characterization and microsystems. In the present study nanoscale effects on the nanomechanical performance of two multifunctional materials with applications in an increasing number of technical fields and high added-value areas are considered. In specific, the following cases are presented and discussed: i) The dependence of hardness of multilayered a-C films and the role of the intrinsic material length, namely the total (100 nm) and bilayers thickness (10 - 45 nm), where it was found that the reduction of the bilayer thickness results in film's strengthening, ii) The dependence of the dominant friction mechanisms and surface damage mechanisms on the applied load for flexible polymeric components. Load dependent transitions in both the scratch and the friction responses are considered and discussed, in the load range 1-25 mN and resultant deformation in nanoscale. The friction mechanism in the low-load range was adhesion. In the intermediate and high load ranges, adhesion, elastic and plastic deformations and ploughing mechanisms contributed to the friction behavior.

- H-V.06** 15:30 **MODELING THE OPTICAL PROPERTIES OF SI-CAPPED GERMANIUM QUANTUM DOTS**  
N. Skoulidis, H. Polatoglou, Department of Physics, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece  
 Over the last years the quantum dots have gained great importance because of their special properties. A very interesting case is that of the Ge quantum dots Si capped as that structure emits / absorbs light in the near infrared and visible area. Experimentally has been found that the Ge quantum dots Si capped have different shapes, size distribution, strains etc. which are strongly depended on their preparation method, and influence the properties of the material. While one can study many different individual cases by building atomistic models, relaxing them with an atomistic potential and calculate the optical properties such as absorption, we choose a specific atomistic model to study systematically the effects of strain, size and aspect ratio so as to probe their relative importance on the electronic and optical properties. In particular we start with a given number of Ge atoms, forming dome dots in a Si matrix arranged in a plane and by keeping the number of Ge atoms constant we reduce the aspect ratio, which leads to an increase of the base area of each quantum dot, and therefore reduces their distance. At some aspect ratio the quantum dots will join together and form a slab of some atomic layers of Ge embedded in Si. The interesting physics in this model is that we can continuously change the character of the electronic states close to the energy gap from 0D to 2D. Regarding the strains we distribute them in different ways between Si and Ge. A quite varied behavior is observed, while some trends can be noticed. The reasons for these trends will be discussed.
- H-V.07** 15:45 **MODELLING OF A SELFORGANIZATION PROCESS LEADING TO PERIODIC ARRAYS OF NANOMETRIC AMORPHOUS PRECIPITATES BY ION IRRADIATION**  
 F. Zirkelbach, M. Häberlen, J.K.N. Lindner and B. Stritzker, Universität Augsburg, Universitätsstrasse 1, 86135 Augsburg, Germany  
 High-dose ion implantation at certain conditions has recently been shown to result in the formation of selforganized periodic arrays of nanometric inclusions. The inclusions may have either spherical or lamellar shape and arrange themselves periodically. The phenomenon seems to be of general nature, as such nanoarrays have been observed for quite different implantations, e.g. O+ or C+ into Si, Ar+ into Al<sub>2</sub>O<sub>3</sub> and Si+ into SiC. In the present work we focus on high-dose carbon implantation into silicon. The effect is thought to be the consequence of supersaturation with impurity atoms, followed by precipitation of an amorphous phase. Upon amorphization stress fields build up and facilitate locally further ion induced amorphization. This, together with impurity diffusion into the amorphous volumes and recrystallization of impurity depleted volumes leads to the selforganized evolution of these arrays. In order to investigate if the above model can explain the formation of periodic nanoarrays a simple Monte-Carlo code was developed considering nucleation, growth, diffusion, amorphization and recrystallization. First results will be presented and compared with data obtained by XTEM studies.
- 16:00 **BREAK**

## Session VI: Quantum investigation of complex systems

Session chair: J. Greer

- H-VI.01** 16:30 -Invited- **THE STEADY-STATE OF HETEROGENEOUS CATALYSIS STUDIED BY FIRST-PRINCIPLES STATISTICAL MECHANICS**  
**Prof. Reuter**, Fritz-Haber-Institut, Germany
- H-VI.02** 17:00 -Invited- **NANOCATALYSIS WITH ALUMINAS**  
**Prof. Pantelides**, S. Rashkeev, S. Wang, K. Sohlberg, M. Glasoff, A. Borisevitch, S. J. Pennycook Vanderbilt University, Nashville, TN, USA, and Oak Ridge National Laboratory, Oak Ridge, TN, USA  
 Aluminas are complex oxides that are used widely in catalysis. We will report results of first-principles calculations and atomically resolved Z-contrast imaging and electron-energy-loss spectroscopy that allow us to unravel the fascinating aspects of these materials and their catalytic behavior on the nanoscale. In addition, the mechanism of stabilizing catalytic behavior at high temperatures by the addition of La has been elucidated
- H-VI.03** 17:30 -Invited- **AB INITIO CALCULATIONS OF ELECTRONIC EXCITATIONS/ CHALLENGES AND RECENT PROGRESS**  
**Prof. Reining**, Laboratoire des Solides Irradiés, Polytechnique, France
- H-VI.041** 18:00 **QUANTUM MECHANICAL CALCULATION OF SOLID STATE EQUILIBRIUM RUTHENIUM AND RHODIUM RUTILE VS CORUNDUM PHASES**  
M.H. Grillo, Accelrys GMBH, Germany
- H-VI.05** 18:15 **THEORETICAL INVESTIGATION ON THE GRAFTING OF CHAIN ORGANO-SILANES ON SILICA SURFACES**  
A. Dkhissi, L. Jeloica, A. Estève and M. Djafari Rouhani, LAAS-CNRS, France

Thursday, May 27, 2004

Morning

Session VII: Surfaces

Session chair: J. Gavartin

- H-VII.01** 08:30 -Invited- AN AB INITIO STUDY OF TITANIUM-TETRA-ISO-PROPOXIDE (TTIP) ABSORPTION MECHANISM ON Si (100) SURFACE  
**A. Palma**, Istituto per lo Studio dei Materiali Nanostrutturati (CNR-ISMN), Via Salaria Km 29.3, 00016 Monterotondo Scalo (RM), Italy and **A. Alavi**, Chemistry Department, University of Cambridge, Lensfield Road, Cambridge, U.K.  
DFT based methods with plane wave expansion pseudopotentials are used to unravel the absorption mechanism of TTIP on Si(100) surface during the early stage of its deposition at room temperature. The Silicon surface was modelled by a 4\*4 slab made of 4 Si layers: the bottom layer was saturated with H atoms, while the two upper layers were completely free to relax. Ab-initio Car-Parrinello (CP) dynamics have been performed at 600K for about 10 picoseconds. Our preliminary results show that the TTIP is bound to the surface through one of its terminal methyl group in coincidence of a H atom transfer from the same methyl group to the surface.
- H-VII.02** 09:00 INVESTIGATION OF SPUTTERING AND OXYGEN DESORPTION PROCESSES BY BINARY COLLISION APPROXIMATION METHOD  
**A.A. Dzhurakhalov** and **S.E. Rahmatov**, Arifov Institute of Electronics, F.Khodjaev Str.33, 700125 Tashkent, Uzbekistan  
In present work the peculiarities of the formation of the primary knock-on recoil atoms and oxygen desorption processes under conditions of low-energy grazing ion bombardment of Ag(110) surface have been investigated by computer simulation. The present computer code for a calculation of the ion and recoil trajectories is based on the binary collision approximation (BCA). The possibilities of this code are following: 1) to carry out the calculations without inelastic energy losses or with their inclusions on one of three models: Kishinevsky, Firsov, Oen-Robinson (for light particles); 2) to vary the interaction potentials: Born-Mayer, Moliere, Biersack-Ziegler-Littmark; 3) to compute the time integral or to use the hard sphere model; 4) to calculate the parameters of the scattering ions and recoil atoms for different values of mass ratio of colliding particles; 5) to determine the contributions of the recoil atoms formed from the first three crystal layers to the sputtering yields; 6) to calculate different characteristic of desorption of adsorbed molecules. These calculations do not require the change of code structure and may be performed by choice input parameters. The energy and angular distributions of particles sputtered and desorbed from the surface, as well as their yields have been calculated and studied in detail. These distributions of sputtered particles from clean and oxygen coverage Ag(110) surface have been considered.
- H-VII.03** 09:15 THE PECULIARITIES OF THE INTERACTION OF DIVACANCIES WITH INTERSTITIAL BOUNDARIES IN TWO-DIMENSIONAL COMPOSITES OF Ni<sub>3</sub>Al-AL AND Ni<sub>3</sub>Al-NI SYSTEMS  
**M.D. Starostenkov**, E.A. Dudnik, General Physics Department, Altai State Technical University, 46 Lenin st, 656038 Barnaul, Russia and **I.A. Demina**, G.V. Popova, East-Kazakhstan State University, 19 Serikbaeva st, 492010 Ust-Kamenogorsk, Kazakhstan  
The mechanisms of the movement of divacancies relatively to interphase boundaries in two-dimensional nanocrystal metallic composites were studied in the present paper. The areas of free volume appear at the formation of nanocrystal composites. Free volume can consist of the pairs of closely situated vacancies. The interaction of bivacancy with interphase boundaries of Ni<sub>3</sub>Al-Ni and Ni<sub>3</sub>Al-Al type was investigated by the methods of molecular dynamics. The packing of atoms in the studied structures was corresponded to the packing of planes [111] of FCC lattice and L12 superstructure of the metal. It was found, that the pair of vacancies transformed into more energetically profitable configuration at the temperature 100 K. The configuration consisted of three vacancies and self-centering interstitial atom. Such complex was more movable in comparison with a single vacancy. The interaction of the divacancy with interphase boundaries of different types had typical peculiarities. The divacancy moved inside the boundary or along it in the case of interphase boundary. It depended on the width of the boundary. The movement of the vacancy took place near the interphase boundary at the presence of interphase boundary, consisting of the atomic rows of Ni. The divacancy complex was movable enough with the growth of temperature to 400 K.
- H-VII.04** 09:30 -Invited- STABILITY, ELECTRONIC AND STRUCTURAL PROPERTIES OF DEFECTED ZnSe/GaAs(001) HETEROSTRUCTURES  
**A. Stroppa**, M. Peressi Università degli Studi di Trieste, 34100 Trieste, Italy and INFN-DEMOCRITOS Simulation Center, Trieste, Italy  
ZnSe/GaAs(001) heterostructures with controlled native stacking fault density can be successfully grown, characterized by a Zn-rich interface composition and rather low band alignments [A. Colli et al., Appl. Phys. Lett. 83, 81 (2003)]. Recent experimental characterizations suggested the presence of a thick intermixed region of a defect (Zn,Ga)Se alloy with a substantial concentration of Ga vacancies. In order to exploit the possibility of defect compound and/or alloy formation at the interface, which should be lattice mismatched with respect to the binaries constituting the heterojunction, we compare the relative stability of some selected interface morphologies, chosen taking into account charge neutrality arguments, performing accurate density functional ab-initio pseudopotential calculations. Our results remarkably show that some interfaces with Ga vacancies are indeed favoured in a wide range of conditions over many other configurations, including the simplest neutral ones with anion and/or cation mixing, despite the accumulation of additional local strain in comparison. We investigated also the electronic properties of the defect interfaces, allowing to suggest some particular interface morphologies which are compatible with the observed compositions and measured band alignments.

- H-VII.05** 09:45 MAINTAINING HALF METALLICITY AT NiMnSb/III-V SEMICONDUCTOR HETEROJUNCTIONS: THE ROLE OF SEMICONDUCTOR SUBSTRATE AND LOCAL INTERFACE TERMINATION **A.** Debernardi(a), **M. Peressi**(a,b) and **A. Baldereschi**(a,b,c), (a)Istituto Nazionale di Fisica della Materia (INFM), DEMOCRITOS Research Unit of Trieste, via Beirut 4/2, 34014 Trieste, Italy, (b)Department of Theoretical Physics, University of Trieste, Strada Costiera 11, 34014 Trieste, Italy, (c)Ecole Polytechnique Federal de Lausanne (EPFL), 1015 Lausanne, Switzerland  
Halfmetallic NiMnSb Heusler alloy has a lattice parameter compatible for a good matching with several conventional III-V semiconductor compounds. NiMnSb heterostructures have therefore recently attracted considerable interest to design devices making use of spin polarized electrons injected into conventional semiconductors. The interest in particular is to exploit those interfaces which maintain the peculiar half-metallic band structure. To this purpose we investigate different heterojunctions based on NiMnSb by pseudopotential density functional - local spin density method. The method is able to take accurately into account even tiny effects of the polarized band structure at the interface due to the strain and/or chemistry. We therefore address the combined effects of chemistry and of strain considering different III-V [001] oriented semiconductors substrates, giving raise to different strain conditions for the epitaxial magnetic layer. We consider also different interface terminations, investigating therefore the atomic-scale microscopic mechanisms governing the interface electronic structure. By comparative analysis, we suggest some possible interfaces which are compatible with maintaining the desired half-metallicity.
- H-VII.06** 10:00 TIGHT BINDING MODELLING OF BAND OFFSETS IN NANOSCALE HETEROSTRUCTURES **H. Hakan Gürel**, Özden Akonco and Hilmi Ünlü, Department of Physics & Informatics Institute, Istanbul Technical University, Maslak Istanbul 80626, Turkey  
We present a tight binding view of the modeling of band offsets of nanoscale heterostructures. The model considers the nonorthogonality of the  $s^3$  set of orbitals of adjacent atoms and spin-orbit coupling and uses the Hartre-Fock atomic energies and interacting matrix element, obtained by fitting existing band structures for bulk materials, to determine the valence band energies at 0 K (H. Ünlü, Physica Status Solidi, B-235, pp. 248-253 (2003)). The valence band offsets are then obtained by taking the difference between the valence band energies which are screened by the optical dielectric constants of bulk materials at any temperature, pressure, and alloy composition. It is found that the model predictions compare very well with experiment for the band offsets for many heterostructures. The model predicts a crossover between  $E_{g\Gamma}$  and  $E_{gX}$  at about  $P=40$  Kbar for GaAs, in agreement with measurements of Goni et al., Phys. Rev. B 36, 1581 (1987)). The calculated pressure effects on the valence band offsets are found in good agreement with measurements of Woldorf et al. (J. Vac. Sci. and Tech., **B 4**), 1043 (1986) for (Al,Ga)As/GaAs and Lambkin et al. (Phys. Rev. **B 39**), 5546 (1989)) for AlAs/GaAs quantum wells for pressures below 60 Kbar. Also, the calculated small increase in  $\Delta E_v$  is in qualitative agreement with the superlattice band calculations of Johnson et al. (Phys. Rev. Lett., **61**), 1093 (1988)).
- 10:15 **BREAK**
- 10:45-12:45 **POSTER SESSION**
- H/P.01** COEXISTENCE OF HIGH TEMPERATURE SUPERCONDUCTIVITY AND ANTIFERROMAGNETISM **Krzysztof Kucab**, Grzegorz Górski, Stanislaw Topolewicz and Jerzy Mizia Institute of Physics, University of Rzeszów, Poland  
We analyze the competition between high temperature superconductivity and antiferromagnetism. We use the extended Hubbard model containing following matrix elements in the Hamiltonian - single-site Coulomb repulsion  $U$  - single-site (subscript "in") exchange interaction,  $J_{in}$ , - two-site charge - charge, exchange, pair exchange and assisted hopping interactions  $V$ ,  $J$ ,  $J'$ ,  $\Delta$ . In our model we introduce the possibility of antiferromagnetic ordering by dividing the crystal lattice into two interpenetrating sublattices  $\alpha$ ,  $\beta$ . We use Hartree-Fock approximation for all interactions except the strong on-site Coulomb repulsion. The self-energies  $\Sigma_{\gamma}^{\sigma}(\epsilon)$  ( $\gamma=\alpha,\beta$ ) are calculated within the Alloy Analogy Approximation. To obtain the superconducting critical temperature  $T_C$  and the Néel's temperature  $T_N$  we solve the coupled equations of motion for the Green functions. The results show that the antiferromagnetism at half-filling dumps the superconductivity of the  $d$ -wave and  $s_0$ -wave symmetry.
- H/P.02** MODEL BASED OPTIMIZATION OF SOME GROWTH PROCESS PARAMETERS OF A Nd:YAG CYLINDRICAL BAR GROWN BY EDGE -DEFINED FIM-FED GROWTH (E.F.G.) METHOD **L. Braescu**, Department of Mathematics, Polytechnical University of Timisoara, P-ta Regina Maria No. 1, Timisoara 300004, Romania, A.M. Balint, Department of Physics, West University of Timisoara, Blv. V. Parvan No.4, Timisoara 300223, Romania, St. Balint, Department of Mathematics, West University of Timisoara, Blv. V. Parvan, No.4, Timisoara 300223, Romania  
The main purpose of this paper is to find those values of the pressure  $p$ , die radius  $r_0$ , pulling rate  $v$  and temperature  $T_0$  at the meniscus basis which assure the growth of a Nd:YAG monocrystal (blue laser) cylindrical bar with a prescribed diameter  $2r_f$  and for which the non-uniformities of the surface of the bar, due to small uncontrollable oscillations of the pulling rate  $v$  and melt temperature  $T_0$ , are minimum possible. For a set of the values of  $p$  and  $r_0$  we find those couples  $(v, T_0)$  for which the grown crystal radius is equal to a desired radius  $r_f$ . For a pressure  $p$  and a die radius  $r_0$  we find that couple  $(v, T_0)$  for which the amplitude  $A$  of the change of  $r_f$ , due to small oscillations of  $v$  and  $T_0$ , is minimum. Finally we identify the pressure  $p$ , the die radius  $r_0$  and the  $(v, T_0)$  couple for which the amplitude  $A$  is minimum possible. Numerical results are given for a Nd:YAG cylindrical bar of 5 (mm) diameter, grown in a furnace in which the vertical temperature gradient is  $k=33$  (K/mm) for the following three types of uncontrollable oscillations of  $v$  and  $T_0$ :  $v=0.001$  (mm/s),  $T=1$  (K);  $v=0.01$  (mm/s),  $T=10$  (K) and  $v=0.02$ (mm/s),  $T=20$  (K), respectively.

- H/P.03** MODEL BASED PREDICTION OF THE EFFECTS OF THE OSCILLATIONS OF THE PRESSURE IN THE FURNACE IN THE CASE OF AN EDGE-DEFINED FIM-FED GROWTH SYSTEM  
L. Braescu, Department of Mathematics, Polytechnical University of Timisoara, P-ta Regina Maria No. 1, Timisoara 300004, Romania, A.M. Balint, Department of Physics, West University of Timisoara, Blv. V. Parvan No.4, Timisoara 300223, Romania, St. Balint, Department of Mathematics, West University of Timisoara, Blv. V. Parvan No.4, Timisoara 300223, Romania  
 In this paper the usual mathematical model, which permits to compute the evolution in time of the radius  $r=r(t)$  and the meniscus height  $h=h(t)$  in the case of cylindrical bars, grown from the melt by edge-defined film-fed growth (E.F.G.) method, is considered. What is specific is that the growth process takes place not in a vacuum and the pressure  $p$  in a furnace can oscillate. The effect of these oscillations is investigated and it is shown that if the pressure  $p$  increases, then the wetting width  $w$  decreases but the contact angle  $\theta$ , the meniscus height  $h^*$  and the crystal radius  $r^*$  increase. In other words, if the pressure oscillates then  $w$ ,  $\theta$ ,  $h^*$ ,  $r^*$  oscillate too. Numerical results for a 5 [mm] diameter of Nd:YAG cylindrical bar are given and the computed effect of the pressure oscillation is simulated.
- H/P.04** A MODEL BASED CONTROL PROCEDURE FOR OF THE SHAPE OF A Nd:YAG CYLINDRICAL BAR GROWN BY EDGE-DEFINED FILM-FED GROWTH (E.F.G.) METHOD WHEN THE PRESSURE IN THE FURNACE OSCILLATES  
L. Braescu, Department of Mathematics, Polytechnical University of Timisoara, P-ta Regina Maria No. 1, Timisoara 300004, Romania, A.M. Balint, Department of Physics, West University of Timisoara, Blv. V. Parvan No.4, Timisoara 300223, Romania, St. Balint, Department of Mathematics, West University of Timisoara, Blv. V. Parvan No.4, Timisoara 300223, Romania  
 The main purpose of this paper is to give a model based proof of the fact that the effect of the variations of the pressure  $p$  can be compensated by an adequate variation of the pulling rate  $v$  in order to assure a constant diameter of the Nd:YAG cylindrical bar, grown from the melt by E.F.G. method. For that, using a nonlinear model, we find the pulling rate and the pressure couples for which the system of differential equations, which governs the evolution of the crystal radius  $r=r(t)$  and the meniscus height  $h=h(t)$  in the case of cylindrical bar, has asymptotically stable steady-state solution  $(r^*, h^*)$ . By interpolation we find the dependences  $r^*=r^*(p, v)$ ,  $h^*=h^*(p, v)$  and the set  $S$  of those couples  $(p, v)$  for which  $r^*(p, v)=r_f$ , where  $r_f$  is a desired radius. Using the curves  $S$  we show that, if during the growth the pulling rate  $v$  and/or the pressure  $p$  are changed, then the crystal radius is changed too. For a given variation of the pressure, during the growth, we give a control procedure i.e. a procedure to change adequately the pulling rate in order to obtain a single crystal with the prescribed radius  $r_f$ .
- H/P.05** EFFECTS OF METALLIC CONTACTS ON SILICON NANOSTRUCTURES STUDIED QUANTUM MECHANICALLY  
C. Summonte and A.M. Mazzone, C.N.R.-Istituto IMM, Sezione di Bologna, Via Gobetti 101, 40129 Bologna, Italy  
 The purpose of this study is to get insight into the effects of metallic contacts on nanocrystalline silicon material. Therefore the Hartree-Fock formulation at semiempirical level and DFT have been applied to silicon grains coated with aluminum atoms. The semiempirical method is used for routine calculations whereas DFT serves as benchmark of the accuracy of the semiempirical calculations. The calculations describe the effects induced by the presence of the metallic atoms on the grain structure and electronic charge. In fact, the structural and electronic properties of the grains appear perceptibly altered by the metallic overlayer and the strength of bonding is generally lowered in the structures with the contacts. Furthermore the built-in potential across the entire device exhibits a functional dependence on the geometry of the grain and of the contacts which could be usefully applied for the fabrication of unconventional Schottky barriers devices.
- H/P.06** MOLECULAR DYNAMICS SIMULATIONS OF ATOMIC-SCALE SLIDING FRICTION OF a-, nc-SiC AND c-C SURFACES  
V.I. Ivashchenko, P.E.A. Turchi(b), V.I. Shevchenko(a), L.A. Ivashchenko(a) and O.K. Porada(a), (a)Institute of Problems of Material Science, NAS of Ukraine, Krzhynzhovskyy Str. 3, 03680 Kyiv-142, Ukraine, (b)Lawrence Livermore National Laboratory (L-353), P.O. Box 808, Livermore CA 94551, USA  
 We use molecular dynamics calculations to simulate a slide of a-SiC/ c-C and nc-SiC/c-C systems interacting via the Tersoff empirical potential. The bulk a-SiC sample was generated by means of cooling the melt to 300 K. Nano-structured SiC was generated by using the same approach, provided that the part of atoms were fixed to embed a 3C-SiC islet into the amorphous matrix. a-SiC, nc-SiC and c-C slabs were generated by equilibrating the corresponding bulk samples with imposing two-dimensional periodic boundary conditions. The sliding slabs have outside reservoirs, where external normal and tangential forces are applied to each atom. The reservoirs are thermostated to maintain a constant low temperature. The friction coefficient ( $k$ ) and atomic structure of sliding interfaces are studied as a function of sliding velocity ( $V$ ), temperature ( $T$ ) and applied load ( $FN$ ). It was found that, at velocities lower  $0.1 c$ , where  $c$  is the longitudinal sound speed in a-SiC,  $k$  is a decreasing function of  $V$ ,  $T$  and  $FN$ . No mixing was observed at the sliding interface, although a weak diffusion of atoms from the diamond slab takes place at highest  $V$ . The friction has an initial transient before reaching an apparent steady state. This transient is characterized by the dynamic formation of microstructure of the sliding surfaces. In the case of the nc-SiC/c-C sliding system, during the transient, the crystallite transforms into an amorphous fragment.
- H/P.07** MOLECULAR DYNAMICS SIMULATIONS OF THE ATOM-BY-ATOM DEPOSITION OF a-SiC FILMS  
V.I. Ivashchenko(a), P.E.A. Turchi(b), V.I. Shevchenko(a), L.A. Ivashchenko(a), O.K. Porada(a), and G.V. Rusakov(a), (a)Institute of Problems of Material Science, NAS of Ukraine, Krzhynzhovskyy Str. 3, 03680 Kyiv-142, Ukraine, (b)Lawrence Livermore National Laboratory (L-353), P.O. Box 808, Livermore, CA 94551, USA  
 Empirical molecular dynamics simulations and the recursion procedure are applied to study the atomic and electronic structures of a-SiC thin films. The films are generated by means of the condensation of a diluted Si-C vapor on a crystalline silicon substrate similarly to the atom-by-atom deposition. The as-deposited films are annealed at different temperatures. Growth kinetics, bonding configuration, chemical ordering, cohesion, relaxation effects, surface roughness, atomic level stress and electronic properties of the films are investigated as a function of the deposition parameters: vapor temperature, applied particle force, substrate and annealing temperatures. For comparison, the bulk and film samples of a-SiC were also generated from the melt. The main theoretical findings on a-SiC films are in rather good agreement with experimental evidences.

- H/P.08** CURRENT TRANSPORT IN A SILICON NANOWIRE ENDED BY ALUMINUM ATOMS  
A.M. Mazzone and V. Morandi, C.N.R.-Istituto IMM, Sezione di Bologna, Via Gobetti 101, 40129 Bologna, Italy  
 The current state of the art in the evaluation of the structural and electronic properties of bulk samples, surfaces and clusters has greatly advanced and many simulation methods at a  $\$$  level are available. A major problem remains in the evaluation of the transport properties and the studies dealing with this characterization are few. This study attempts an advancement in this area and the Boltzmann transport formalism has been coupled with Density Functional for the evaluation of the conductivity and other basic transport properties. As a benchmark, the method has been applied to the evaluation of the current in a linear silicon nanowire ended with aluminum atoms. The calculations describe the effect of the geometrical parameters of the wire on its transport properties.
- H/P.09** THE LOCAL INELASTIC ELECTRON -POLAR OPTICAL PHONON INTERACTION IN MERCURY TELLURIDE  
O.P. Malyk, Lviv Polytechnic National University, Semiconductor Electronics Department, Bandera Street 12, 79013 Lviv-13, Ukraine  
 In [1] the mechanism of electron - polar optical phonon scattering was considered in view of inelastic character of scattering within the framework of a precise solution of the stationary Boltzmann equation. There was exhibited that the usage of standard model of electron - polar optical phonon scattering reduces to a disagreement between the theory and experiment in temperature range  $> 100$ ; According to our opinion this model has following shortages: 1) the use of macroscopic parameter - permittivity- is not reasonable in microscopic processes; 2) the interaction potential of an electron with optical oscillations of a crystal lattice is long-range that contradicts the special relativity. The purpose of the present work is the build-up of such a model of scattering which at first would well match with experiment and secondly would not have the above mentioned shortages. The short-range interaction potential of an electron with polar optical phonons is found by the way of solution of a Poisson equation in the limits of one unit cell. Thus the unit cell is substituted by an orb of effective radius  $R = \frac{a}{2}$ ;  $a$  (  $a$  - lattice constant) the magnitude which lays within the limits from half of smaller diagonal up to half of greater diagonal of a unit cell. Magnitude  $\approx 0.628$  is picked so to adjust the theory with experiment. The calculation shows that the theoretical electron mobility is well coincides with experiment that testifies that the model, offered us, adequately describes the process of electron - polar optical phonon scattering. It was established that the intraband scattering is the basic scattering mechanism in the interval  $> 100$  T. [1]. O.P. Malyk . Accepted to publication in Journal of Alloys and Compounds.
- H/P.10** THE EXACT SOLUTION OF A STATIONARY BOLTZMANN EQUATION FOR THE SEMICONDUCTOR WITH ISOTROPIC DISPERSION LAW  
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 The description of transport phenomena in semiconductors usually carried out on the basis of Boltzmann equation with usage of a relaxation time approximation or variational method. However, these methods are approximate and therefore do not allow to answer a question: as far the selected quantum mechanical models of charge carrier scattering is correctly described a physical reality? The aim of the present work is the precise solution of the stationary Boltzmann equation that will allow directly to determine the adequacy of the charge carrier scattering model to physical reality. The solution of Boltzmann equation is considered here in the case when the magnetic field directed along Z-axis  $B = \{0, 0, B\}$  and electric field has components  $E = \{E_x, E_y, 0\}$ . The solution is found in the form of series expansion of nonequilibrium distribution function with respect to carrier energy. After the substitution of the solution into Boltzmann equation and double integration over the quasimomentum one can obtain the system of the algebraic equations relatively to the values  $f_n$ . This system of the nonlinear algebraic equations can have different types of solutions. Therefore there is a necessity of a selection of physical solutions among a totality of mathematical solutions of the system. The following criteria of selection of solutions is offered:  $J_z = J_{zn} + J_{zp} = 0$ ,  $J_{zn}$ ;  $J_{zp}$  - electron and hole components of Z-component of a current density vector. For selection of physical solutions among the totality of obtained solutions it is necessary to determine at a given value  $n = 0, 1, 2 \dots$  the components of a conductivity tensor and compare them with experiment.
- H/P.11** THE ADSORPTION OF ETHYLENE ON THE Si(001)(2x1) SURFACE BY COAXIAL IMPACT COLLISION ION SCATTERING SPECTROSCOPY  
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 The adsorption of ethylene (C<sub>2</sub>H<sub>4</sub>) on Si(001)(2x1) surface has been focused on a simple model system - small and unsaturated hydrocarbon molecules on Si(001)(2x1). Despite a variety of experimental and theoretical studies, the adsorption sites (so called the di- $\sqrt{3}$  structure and tetra- $\sqrt{3}$  structure) are still debated. Moreover, there is other argument whether the Si dimers are intact or cleaved after ethylene adsorption on Si(001)(2x1). In order to elucidate this controversial issues clearly, ethylene has been non-dissociatively chemisorbed on the Si(001)(2x1) at room temperature in the exposure range of 100-200L, and ethylene on Si(001)(2x1) surface was investigated by coaxial impact collision ion scattering spectroscopy (CAICISS). To confident out results definitely, the computer simulations with a two-dimension trajectory count method were performed and compared with experimental results.
- H/P.12** DIFFUSION-LIMITED REGIMES IN PERCOLATIVE TO COMPACT SUBSTRATES  
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 We simulated a two-species annihilation model in a two dimensional substrate from a fractal percolative structure to a compact square lattice limit. The kinetics of the system is modified, as we vary the percolation probability  $p$  from values above  $p_c$  to one. The time evolution of concentration of one particle species shows various decaying regimes. In diffusion-limited reaction regime, we find a non-mean-field kinetics behavior due to the spatial inhomogeneities of particle concentration. An explanation of this behavior is given in terms of particle domain kinetics. Major interest in this type of model resides in its applications on irregular-surfaces reactions.

**H/P.13****MONTE CARLO GROWTH AND IN SITU CHARACTERISATION FOR Al<sub>x</sub>Ga<sub>1-x</sub>As HETEROEPITAXY**

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The use of photoemission current oscillations and reflection high-energy diffraction (RHEED) intensity oscillations has proven to be a powerful tool to understand growth mechanisms of GaAs, AlAs and Al<sub>x</sub>Ga<sub>1-x</sub>As in molecular beam epitaxy (MBE) [1,2]. One important feature immediately recognized by all, is the close relationship between the RHEED intensity and photoemission current oscillations and the growth rate of deposited films. We presented here a kinetic Monte Carlo model describing the growth of Al<sub>x</sub>Ga<sub>1-x</sub>As heterostructure including a local photoemission model with RHEED intensity for comparison. The model assumes growth under As rich conditions typical for MBE, so a As<sub>2</sub> molecules in physisorbed aspect, will bond immediately above a group III atoms once their configuration is favourable. Growth is controlled by the migration of group III atoms to reach a position to increase the number of their nearest neighbours. With this model, we have examined the Al<sub>x</sub>Ga<sub>1-x</sub>As morphology with 0 < x < 1. We show a roughness Al<sub>x</sub>Ga<sub>1-x</sub>As front profile for high Al concentrations. In fact, versus x, an increase in photoemission current with a decrease in oscillations amplitude are noted and an increase in the time required to achieve bilayer growth of Al<sub>x</sub>Ga<sub>1-x</sub>As is shown. The same observations are shown for RHEED oscillations. These features are explained by the lower diffusivity of Al compared with Ga adatoms which is confirmed experimentally essentially when x exceeds 0.4 [3] References [1] J.J. Zinck and D.H. Chow, Appl. Phys. Lett. 66(1995)3524. [2] J. Zhang, J.H. Neave, B.A. Joyce, P.J. Dobson, P.N. Fawcett, Surf. Sci. 231(1990)379. [3] H. Morkoc, T. Drummond, W.Kopp, R. Fisher, J. Electrochem.Soc, Vol 129(1982)824

**H/P.14****NANO-SCALE DECOMPOSITION IN DISCONTINUOUSLY TRANSFORMED Fe-Ni-Cr-N ALLOYS UPON AGING**

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Interface diffusion plays a central and rate-determining role in phase transformations. In supersaturated solid solutions, the precipitation processes often occurs through grain boundary diffusion leading to the generation of fine lamellae, growing in a cooperative fashion with the matrix, in a number of engineering materials. In the alloy 33, based on Fe, Cr, Ni, with high content of N, we have developed isothermal aging treatments at 700°C, during time intervals ranging from 1 to 1002 hour, aiming at determining the kinetics of discontinuous precipitation observed in this system. A key factor governing the compositional redistribution is the difference of solute partitioning mechanisms of Cr (substitutional) and N (interstitial) atoms. In one hand, the precipitate lamellae are nitrides and the depleted lamellae are austenite solid solution. It is of fundamental importance to determine the stoichiometry of the nitride and, on the other hand, measure the diffusional fields left in the depleted lamellae. This effort requires high spacial resolution analytical electron microscopy given the nano-scale width of the precipitate and also the submicron spacing between them. This study, currently in progress, has also revealed under diffraction contrast in the transmission electron microscopy a secondary decomposition in both the original and depleted matrix, consisting of coherent homogeneous precipitates of few nanometers.

**H/P.15****Cu-ALKALI ION EXCHANGE IN GLASS: A MODEL FOR THE COPPER DIFFUSION BASED ON XAFS EXPERIMENTS**

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Cu-alkali ion exchange is a suitable way to dope superficial layers of silicate glasses well beyond the Cu solubility limits, with the possibility of controlling nanocluster nucleation and growth by subsequent proper treatments. The ion exchange process gives rise to a peculiar copper distribution, with the possible presence of different oxidation states, namely, Cu<sup>+</sup> and Cu<sup>2+</sup>. The modelization of the copper diffusion process is necessary for defining an effective preparation protocol for the copper-doped composites. In this framework, suitable techniques capable to investigate the local atomic environment of Cu atoms are crucial. With this aim, X-ray absorption fine structure (XAFS) spectroscopy in reflection mode was performed using a synchrotron source on different ion-exchanged samples. Based on the experimental results, a developed phenomenological model is used to describe the diffusion process.

**H/P.16****ERBIUM AND SILVER LOCAL ENVIRONMENT IN CO-DOPED GLASSES FOR OPTICAL AMPLIFICATION**

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Rare-earth doped silicate glasses have gained much attention due to their potential application in several fields, especially for optical amplification. The increase of Er<sup>3+</sup> efficiency has been investigated by introducing broadband sensitizer species, such organic complex, silicon nanocrystals, or metals such as silver. The knowledge of local environment of both erbium and sensitizer species is crucial for the understanding of the physical mechanism giving rise to efficiency gain and for the development of an effective preparation protocol for these materials. With this aim, an extended x-ray absorption fine structure (EXAFS) spectroscopy experiment was performed on samples co-doped with Er and Ag via a combined sol-gel and ion exchange route. Silver atoms resulted either dispersed in the matrix or aggregated in Ag multimers or nanoclusters. EXAFS spectroscopy has demonstrated to be a particularly suitable technique for studying the local order around dopant atoms, due to its sensitivity to diluted samples and the possibility to characterize both oxide phase and multimers formation.

- H/P.17** EXTENDED MOLECULAR DYNAMICS SIMULATIONS OF INTERFACES AND DEFECTS: ELASTIC FLEXIBLE BOUNDARY CONDITIONS  
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Molecular dynamics simulations are performed to investigate the atomic processes of the relaxation of defects created during adhesion of semiconductor interfaces. Suitably fitted empirical potentials of the Tersoff or the bond order type are applied to consider sufficiently large model sizes and relaxation times relevant for macroscopic structures. The systems are coupled elastically to the bulk continuum surroundings instead of using periodic boundary conditions. The coupling is performed by means of the elastic multipole expansions for the displacement fields in the continuum region, with the expansion coefficients being treated as dynamic variables along with the positions of atoms in the atomistic region. The corresponding equations of motion for the new variables are derived from an extended Lagrangian. The method of using elastic flexible boundary conditions is tested investigating energy and configurations of typical dislocations structures. The simulations enable to predict the bonding processes and forces of perfect or disturbed surfaces in dependence on steps, facets, reconstructions, adsorbates, mistilt, twist rotation, etc. The comparison of the relaxed interface structures with experiments is possible using simulated electron micrographs on the basis of the molecular dynamics structure models. The main attention is focused to the square networks of screw dislocations resulting from a twist misorientation of wafers upon bonding as well as to arrays of 60° dislocations due to surface steps.
- H/P.18** GENETIC ALGORITHM APPROACH FOR NANOSCALE CONDUCTING WIRES  
Hiroshi Mizuseki, Nobuaki Igarashi, Rodion V. Belosludov, Amir A. Farajian, and Yoshiyuki Kawazoe, Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan  
Over the next ten years, the forty-year miniaturization revolution in silicon-based microelectronics will approach its ultimate, nanometer-scale limits. Thirty years ago Aviram and Ratner (1) have first demonstrated how an organic molecule could function as a molecular rectifying diode to realize electronic devices in nanometer-scale electronic systems. However, it is currently very difficult to predict which molecules would be suitable for fabricating such devices, because the number of organic molecules that are available is enormous. In this study, we propose that a Genetic Algorithm (GA) could be used to survey molecules to determine those which would be appropriate for practical molecular devices(2). The molecules that were identified in this study have a long rigid shape and delocalized frontier orbitals. The properties of the molecule that we identified were satisfactory, with a specific length and a small HOMO-LUMO gap, which are necessary attributes to connect with other functional molecules. This study was performed through Special Coordination Funds for Promoting Science and Technology from the Ministry of Education, Culture, Sports, Science and Technology of the Japanese Government and a Grant for Basic Science Research Projects from the Sumitomo Foundation. (1) A. Aviram and M. A. Ratner, Chem. Phys. Lett. Vol. 29 (1974) 277. (2) H. Mizuseki, N. Igarashi, R. V. Belosludov, A. A. Farajian, and Y. Kawazoe, Mater. Sci. Eng., C, Vol. 23 (2003) 807.
- H/P.19** MONTE-CARLO SIMULATION OF GIANT MAGNETORESISTANCE AND PHASE SEPARATION IN A RANDOM-FIELD MAGNETIC POLARON MODEL  
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The magnetoresistive effect due to phase separation was investigated in a random-field small-magnetic-polaron model. The phase-separated state was showed in an inhomogeneous lattice that was induced by a random-field. The co-occurrence of ferromagnetic/paramagnetic phase separation and metal/insulator transition was observed and the conductance was simulated using tunneling-electron mechanism. The insulating behavior in high temperature and the metallic one in low temperature were studied by fitting the zero-field resistivity as a function of temperature. When a magnetic field is applied on the system, an evident magnetoresistance effect appears. We compared the calculated magnetoresistance with that in real manganites and found a qualitative agreement between them.
- H/P.20** MONTE-CARLO SIMULATION ON THE DIPOLE ALIGNMENT IN FERROELECTRIC SQUARE LATTICE  
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The dipole alignment configuration in a multi-domained ferroelectric lattice of cubic symmetry is simulated using the Monte-Carlo method based on the Ginzburg-Landau model. It is revealed that the gradient energy associated with the spatial discontinuity of the dipole alignment near the domain walls results not only in a 90°-domain configuration, but also distorted dipole alignment on the walls. The simulation shows that such a distorted alignment pattern is thermodynamically preferred at low temperature. The effect of the alignment distortion on the ferroelectric phase transition is discussed and it is found that the ferroelectric transition temperature shifts to a slightly lower temperature when there is a larger number of allowed orientation states for the dipoles.
- H/P.21** BUCKY SHUTTLE MEMORY SYSTEM BASED ON BORON-NITRIDE NANOTUBE  
Won Young Choi, Jeong Won Kang and Ho Jung Hwang, Chung-Ang University, Seoul, Korea  
We investigated the internal dynamics of a bucky shuttle memory system, consisting of three C60+s encapsulated in (10, 10) boron-nitride nanotubes and filled Cu electrode. Energetics and operating response of the shuttle-memory-element proposed were examined by using classical molecular dynamics simulations of the C60+ shuttle in the boron-nitride nanotube capsule under the external force fields. For the stable operations of the shuttle memory device, the periods and the magnitudes of the operating force fields were investigated.

- H/P.22** QUANTITATIVE CHARACTERIZATION OF THE MESOSCOPIC SURFACE ROUGHNESS IN A GROWING ISLAND FILM  
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Surface roughness strongly affects on physical properties of thin films and plays a key role in the so-called surface enhanced phenomena, e.g., such as the giant Raman scattering, so a quantitative characterization of the surface morphology is of great importance for materials science. In this paper, a quantitative description of statistically rough surface generated in thin film growth process via 3D island mechanism is presented. Analysis is based on the statistical model of a random nucleation and growth of hemispherical islands taking into account the growing island collisions at late stages [1]. Analytical expressions for a number of surface relief parameters: the rms surface roughness, the roughness coefficient, the surface profile height (depth) distribution and the package density factor providing a rather complete quantitative description of the evolving surface morphology during growth process in different condensation regimes are derived. It is shown that the surface profile height distribution is a non-Gaussian with a negative skewness and that the rms roughness and the roughness coefficient kinetics can be represented as a universal (independent of a condensation regime) unimodal function of either coverage or film thickness with a maximum just prior the completed film formation. The scaling behaviour of the surface roughness is analysed. The nonmonotonic surface roughness dynamics in a film growth process predicted by the model is well consistent with experimentally observed physical properties behaviour in growing film. [1] V. I. Trofimov, V. A. Osadchenko, Growth and Morphology of Thin Films (in Russian) Moscow, Energoatompubl. 1993, 272 pp.
- H/P.23** ELECTROMAGNETIC CHARACTERISTICS OF YBCO CERAMICS SUPERCONDUCTOR  
Sang Heon Lee, Department of Electronics Information and Communication Engineering, Sun Moon University, Asan, Chung Nam, South Korea  
An electromagnetic memory effect in YBaCuO system is studied. A voltage drop across a superconducting sample is observed on the external magnetic field. The voltage drop continues to appear after the removal of the magnetic field. This phenomenon is considered as a nonvolatile memory effect. The appearance of the voltage drop is resulted from the trapping of magnetic flux. The voltage drop in the sample increases or decreases depending on the direction of applied magnetic flux less than  $2 \times 10^{-3}$  T. The fact that the material used is porous and contains many grain boundaries suggests us a junglegym-like path in a current flow model for our studied system. The mechanism of the memory effect can be explained by applying this model. Our studied model is considered to be composed of a super conduction part and a finite resistance part, respectively. In general, the super conduction parts are considered to be located in parallel and connected to both sides of the sample. The super conduction parts cause to exhibit zero voltage. Since the shape of the super conduction part is very complicated like the junglegym, it should be assumed that there are both wide and narrow paths. The narrow path will be destroyed by the effect of an appropriate value of magnetic flux which causes the voltage drop across the sample. The destroyed regions will be increased with the increase of the magnetic flux. This causes an increase in the voltage drop. In conclusion, our studied model implicates that there are some defect regions for trapping the external magnetic flux in order to generate the trapped magnetic flux which causes the memory effect.
- H/P.24** ELECTROMAGNETIC PROPERTIES OF BPSCCO CERAMICS  
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The electromagnetic characteristics in BiPbSrCaCuO superconductor was studied. In the measurement of differential conductance, it was cleared that the mechanism of magnetic effect could not be explained by using conventional flux flow model. As a result of measuring the inductance of coils inserted by BiPbSrCaCuO ceramics, the inductance of coils increased with increasing external magnetic field and current. By changing the density of external magnetic flux, changes in inductance of a coil in which a superconducting bar inserted were also measured. The results showed that the filament model was valid to explain the mechanism of the occurrence of a voltage in superconducting sample. It was concluded that the electromagnetic characteristics arose from the interaction between the trapped magnetic flux and weak link of the filament formed in the superconducting bulk
- H/P.25** MEASUREMENT OF ATTRACTION FORCE BETWEEN AFM TIP AND SURFACE OF DIELECTRIC THIN FILMS WITH DC-BIAS  
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SiO<sub>2</sub> and ZrO<sub>2</sub> thin films were deposited on n-Si (100) wafers by sputtering method. The thickness of films was measured by ellipsometry to be between 2 – 70 nm. The attractive force between the atomic force microscope (AFM) tip and the surface of dielectric thin films (SiO<sub>2</sub> and ZrO<sub>2</sub>) was measured with a Solver P47H SPM by applying DC-bias between the AFM tip and the n-Si substrate. The measurement is carried out in dry nitrogen atmosphere. As the surface of dielectric thin film moves towards the AFM tip, the attraction force increases gradually and finally jumps to a maximum value. There is a Van Der Waals interaction between the AFM tip and the surface of dielectric films under 0 electric field. When a DC voltage is applied, the attractive force, which should be mainly columbic, increases noticeably. This force decreases with increasing film thickness, and is higher for ZrO<sub>2</sub> than for SiO<sub>2</sub> films, indicating that the columbic interaction may be related to the dielectric property of the films. It is hopeful that the intrinsic properties of the ultra thin dielectric films may be revealed by further theoretical modelling using these force-distance curve data as measured by AFM with DC-bias.

- H/P.26** AB INITIO SIMULATIONS ON AgCl(111) SURFACE AND AgCl(111)/a-Al<sub>2</sub>O<sub>3</sub>(0001) INTERFACE.  
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The conductivity and other properties of solid-solid interfaces are of great fundamental and applied interest [1]. In this study, large-scale first-principles calculations have been performed for AgCl(111) surface and AgCl(111)/a-Al<sub>2</sub>O<sub>3</sub>(0001) interface using both Hartree-Fock method combined with the electron correlation corrections (HF-CC), as implemented into computer code CRYSTAL98, and Density Functional Theory (DFT), realized in plane-wave VASP code. A number of properties have been calculated and analyzed for the AgCl(111) slabs with varied thickness as well as for the AgCl(111)/a-Al<sub>2</sub>O<sub>3</sub>(0001) interface. In order to find the atomic structure of both silver chloride surface and its interface with corundum, we performed and discuss detailed structure optimization. For resolving the problem of mismatch of the lattice constants for both contacting crystalline structures, the interfacial bilayer of AgCl adsorbate has been simulated with steps. The most favourable adsorption sites for Ag<sup>+</sup> and Cl<sup>-</sup> ions on the interface have been found to be over substrate upmost O<sub>2</sub><sup>-</sup> ions and Al<sub>3</sub><sup>+</sup> axes, respectively. Theoretical results are also discussed in the light of conductivity measurements. [1] J. Maier, Progr. Sol. State Chem. 23 (1995) 171.
- H/P.27** KINETIC MODEL FOR PRODUCTION AND GROWTH OF DUST PARTICLES IN THE PLASMAS OF ELECTRONEGATIVE GASES  
B.F. Gordiets\*, A. Pinyol and E. Bertran, Departament de Física Aplicada i Òptica, Universitat de Barcelona. Avinguda Diagonal 647, 08028 Barcelona, \*On leave from Lebedev Physical Institute of the Russian Academy of Sciences, Moscow, Russia  
A kinetic model for production and growth of clusters and dust particles in the low-pressure low temperature plasmas of electronegative gases is developed and presented. Comparison of this model with experimental results has been carried out with silicon-related films with embedded nanoparticles obtained by plasma enhanced chemical vapour deposition processes. The model takes into account the different processes: ionisation, dissociation and dissociative attachment of the main molecules; the electron attachment and detachment for respectively neutral and negative charged clusters and grains; the secondary electron emission from grains; the joining (association) of monomers to the clusters and grains; the ion recombination involving electrons and ions as well as particle coagulation and diffusion losses. The model describes the particle generation and growth from monomer radical up to grains of submicronic dimensions. The formulas and equations are presented to calculate (in the framework of our model and with some approximations) the particle density, their average dimension  $\langle n \rangle$ , the charge distribution function of grains and their average charge  $Z_p$ . Other important parameters such as neutral and negatively charged cluster function distribution are also calculated according to number "n" of monomers in clusters; critical dimension  $n^*$  and fluxes of particles across the point  $n^*$ . The value of  $n^*$  determines the rate for production of such dust particles, which dimension  $\langle n \rangle$  and concentration can increase in time. The calculation is also given for average dimension of particles, those which are found in deposited films.
- H/P.28** INTRA-MOLECULAR PROPERTIES OF DMeOPPV STUDIED BY QUANTUM MOLECULAR DYNAMICS  
Helena M.G. Correia, Marta M.D. Ramos, Departamento de Física, Universidade do Minho, Largo do Paço, 4700-320 Braga, Portugal  
When we introduce methoxy electron donor groups into a poly(para-phenylene vinylene) (PPV) chain, substitution will lead to the appearance of unique electronic properties at molecular scale which should affect the overall properties of light-emitting diodes based on these polymers. Self-consistent quantum molecular dynamics calculations have been used to provide information on intra-molecular properties of poly(2,5-dimethoxy-para-phenylene vinylene) (DMePPV), which are relevant for the modelling and characterization of polymer light-emitting diodes at nanometric length scale. We focus our attention in those properties that have been somewhat neglect in previous literature: the effect of chain length on the ionization potential and electron affinity, the charge distribution associated with positive and negative charge carriers and their intra-molecular mobility when an electric field is applied.
- H/P.29** QUANTUM MODELLING OF POLY(VINYLLIDENE FLUORIDE)  
Helena M.G. Correia, Marta M.D. Ramos, Departamento de Física, Universidade do Minho, Largo do Paço, 4700-320 Braga, Portugal  
The addition of inverted monomer units during the conventional polymerization of poly(vinylidene fluoride) (PVDF) is an unavoidable phenomenon. Although extensive studies have been conducted on PVDF because its ferroelectric, pyroelectric and piezoelectric properties, the effects of monomer inversion on the properties of this polymer at molecular scale are not fully understood. Therefore, we have used a method combining molecular dynamics with a self-consistent semi-empirical quantum mechanical method to study the effects of both chain length and monomer inversion on the electronic properties of individual PVDF chains, such as the dipole moment and the polarizability. The effects of monomer inversion on the electronic and vibrational spectra are also discussed.
- H/P.30** ATOMISTIC MODELLING OF PROCESSES INVOLVED IN POLING OF PVDF  
Marta M.D. Ramos, Helena M.G. Correia, S. Lanceros-Méndez, Departamento de Física, Universidade do Minho, Largo do Paço, 4700-320 Braga, Portugal  
Poling processes play an important role in the design and preparation of many ferroelectric materials for practical uses in the field of sensors and actuators. Particularly, the processing of piezoelectric beta-poly(vinylidene fluoride) (beta-PVDF) involves the mechanical stretching in order to transform the extruded alpha-phase into the beta-phase and the poling of this later material in order to optimize the piezoelectric response. This poling process affects the orientation of the dipolar moments of the beta-chains and improves the alpha-beta transformation. Poling processes in general and in PVDF in particular are still quite empirical because a firm understanding of the physical processes involved in poling has not been fully established. In the present work we use a self-consistent quantum molecular dynamics method to study the effect of the electric field at a chain level both in alpha and beta chains of PVDF in order to discuss the experimental results obtained for poled and non-poled beta-PVDF. The orientation of the dipolar moments in each chain as a function of a chain size and electric field and the accompanying structural modifications due to these reorientations will be the main parameters discussed.

- H/P.31** NOVEL LANTHANIDE COMPLEXES FOR VISIBLE AND IR EMISSION  
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 Complexes formed by a light harvesting antenna (conjugated ligand) and a transition metal ion combine the advantages of a large absorption cross section with sharp emission, large Stokes shift, long emission lifetimes and the possibility of accessing the IR region of the spectrum through the use of Er and Nd ions. The population of the excited states of the ion takes place through an efficient resonant energy transfer process involving the ligand triplet states. We have synthesized and studied novel ligands based on an azamacrocyclic, which imparts a high stability to the complex, combined with the well known antenna hydroxyquinoline. We have obtained the Eu<sup>3+</sup> and Er<sup>3+</sup> complexes in which the antenna is directly coordinated to the metal. Excitation within the ligand absorption band produces the emission of the ion at 612 nm and 1540 nm for Eu<sup>3+</sup> and Er<sup>3+</sup> respectively, thus showing an efficient energy transfer process. Quantum chemical calculations of the ligand energy levels will be used to obtain indication on their overlapping with the ion levels.
- H/P.32** SECOND-MOMENT INTERATOMIC POTENTIAL FOR GOLD AND ITS APPLICATION TO MOLECULAR-DYNAMICS SIMULATIONS  
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 We have obtained a new interatomic potential for Au in the framework of the second-moment approximation to the tight-binding model by fitting to the volume dependence of the total energy of the metal, computed by first-principles calculations. The scheme was validated by calculating the bulk modulus, elastic constants, vacancy formation energy and relaxed surface energies of Au, that were found to be in good agreement with experiment. We also have performed molecular-dynamics simulations at various temperatures and we have determined the temperature dependence of the lattice constant, mean-square displacements, as well as the phonon density of states and the phonon dispersion curves of the metal. The agreement with the available experimental data is much better than previous works based on the same approximation, but resulting from fitting to several measured data.
- H/P.33** ELECTRONIC STATES ASSOCIATED WITH TILT BOUNDARY IN GaN  
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 Numerous theoretical studies have been performed on native defects and dislocations structures in order to explain the origin of the yellow luminescence observed in GaN thin film. However, the results are still under debate. Crystals of GaN grown by molecular-beam epitaxy on (0001) sapphire show [0001] low and high angles grain boundaries. The atomic structure of these boundaries may modify the electronic states of the valence and the conduction bands and consequently, may influence the opto-electrical properties of the semiconductor. Recently, atomistic studies of a variety of [0001] tilt boundaries with various misorientation angles have been reported [Béré and Serra, Chen et al.]. It was shown that the structural units associated with all the boundaries could be explained in terms of combinations of the three cores of the 1/3[1-210] edge dislocation. In the present work, the electronic structures of tilt boundaries were investigated by atomic computer simulation using Density-Functional-based Tight-Binding approach (DFTB). Electronic states specific to the boundaries geometries will be discussed in comparison with those in GaN bulk and dislocations. A. Béré and A. Serra, Phys. Rev. B 66, 085330 (2002) J. Chen, P. Ruterana and G. Nouet, Phys. Rev. B 67, 205210 (2003)
- H/P.34** NUMERICAL SIMULATION OF FILM THICKNESS DISTRIBUTION IN ELECTRON-BEAM CO-EVAPORATION  
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 This study deals with Monte Carlo simulation of the physical phenomena involved during materials transport using electron-beam evaporation. Simulation of thickness and composition distributions of deposited layers are compared with experimental measures, in the case of three metals (copper, aluminium, titanium) evaporated simultaneously from independent sources. First the deposition is performed under vacuum (10<sup>-1</sup> Pa) which allow to assume that : &#61623; there is no collision between ambient and evaporated particles, &#61623; the particles condense immediately when they are in contact with a wall. When a gas is introduced inside the vacuum vessel, the first assumption is not still valid and collisions between ambient and evaporated particles must be taken into account. At the temperature of interest the electronic excitation of the vapor is significant and energy transfer between the electronic and translational modes of energy affects the flow. Moreover, as the vaporisation rate is large, in the immediate vicinity of the evaporation sources, translational equilibrium is not achieved between the atoms that leave the surface, their velocity in the direction normal to the surface must be positive. The problem is treated in terms of the formation of a Knudsen layer. After this hydrodynamical discontinuity, the evaporated particles diffuse into the atmosphere of the chamber until their mean free path is large enough to consider a molecular description which is then treated by a Monte Carlo model.
- H/P.35** LOCAL VIBRATIONAL MODES OF Zn-H-As DEFECTS IN GaAs, ZnSe AND ZnTe  
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 The hydrogenation of the zinc acceptor in GaAs (Zn<sub>Ga</sub>), and As acceptor in ZnSe (As<sub>Se</sub>) and in ZnTe (As<sub>Te</sub>), are studied by computer modeling using a pseudopotential density-functional method. For these complexes, we found that the lowest energy location for hydrogen is near the bond-center (closer to As) between Zn and As atoms. Also for GaAs:ZnH, ZnSe:AsH and ZnTe:AsH, antibonding As-H units were found to be metastable by 0.4, 0.5 and 0.7 eV above the ground state, respectively. The calculated local vibrational modes and deuterium induced shifts fall within 4% of the experimental data, and the observed decreasing trend of the absolute frequencies from GaAs:ZnH, ZnSe:AsH and ZnTe:AsH follows a local expansion of the Zn-H-As bond lengths.

- H/P.36** MODELIZATION OF THIN FILM GROWTH  
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 A 3-Dimension Monte-Carlo simulation of the growth of realistic thin films is presented. To characterize thin film properties, a sample of sufficient size is needed. Yet, to model a few tens or even hundreds of nanometers of thin film, the number of atoms needed is huge. This makes impractical to use molecular dynamics approaches, even semiclassical ones, because of the amount of calculus involved. We developed a Monte-Carlo semi-empirical approach to simulate the 3D structure of a thin film. The aim of this work is to simulate thin films that can be used to model its mechanical, electric and chemical behaviour at a mesoscopic level.
- H/P.37** ATOMIC SCALE ANALYSIS OF YBa<sub>2</sub>Cu<sub>3</sub>O<sub>y</sub> BY LOW-ENERGY ION SCATTERING  
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 Investigation of composition and crystal structure of multicomponent single crystal surfaces and dynamics of their change in the process of ordering and under ion bombardment has important meaning in processes of nano- and microelectronics, connected with epitaxial growth of crystals and layer-by-layer analysis of their surface. In the present work the trajectories, energy and angular distributions of 5-15 keV Ne, Ar, Kr, Xe ions scattered on chains of atoms - components of YBa<sub>2</sub>Cu<sub>3</sub>O<sub>y</sub> single crystal yttrium ceramics at grazing incidence has been investigated by computer simulation in binary collision approximation. This method was also used for determination of oxygen atom contents in the Cu-O basis plane. It has been shown that in the case of YBa<sub>2</sub>Cu<sub>3</sub>O<sub>y</sub> unlike of the one component targets, calculated energy and angular distributions are more complex. Comparison of energy-scattering angle dependencies for different atomic chains on the surface of YBa<sub>2</sub>Cu<sub>3</sub>O<sub>y</sub> single crystal become possible, firstly, to distinguish of scattering on simple and mixed chains, secondly, to determine the difference in distances between atoms in chain and thirdly, to establish the difference between composition of mixed chains. Comparison of the computer simulation results with experiment data allows permitting the reliable and express method for diagnostics of surface of the high-T<sub>c</sub> materials. This technique can be useful for atomic scale surface analysis of complex compounds and alloys.
- H/P.38** COMPARISON OF C60 ENCAPSULATIONS INTO CARBON AND BORON-NITRIDE NANOTUBES  
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 This presentation will show that the features of C60 encapsulation into boron-nitride nanotubes (BNNTs) are similar with that into carbon nanotubes (CNTs), whereas the encapsulating and the internal dynamics of the C60@BNNT are different from those of the C60@CNT. Since the C60 encapsulation into the BNNTs is energetically more stable than that into the CNTs and the suction force on the C60 molecule induced by the BNNTs is higher than that by the CNTs, the C60 encapsulation into the BNNT is achieved faster than that into the CNT. The internal dynamics of the C60 molecule inside the BNNT is also different from that inside the CNT, because the C60@CNT system includes only one long-range interaction of C-C whereas the C60@BNNT system includes both long-range interactions of C-B and C-N. Because of the difference of the binding energies and the equilibrium distances between C-B and C-N, the C60 molecule frequently collided against the BNNT wall in our MD simulations. At low temperature, the energy dissipation of the C60@CNT system was mainly achieved at the both end edges of the CNT, where the C60 molecule is under the restoring (or sucking-in) forces. The energy dissipation of the C60@BNNT was achieved from the collisions against the BNNT wall as well as at the both end edges of the BNNT.
- H/P.39** MODELING OF FLUX-FLOW FOR SUPERCONDUCTING FLUX FLOW TRANSISTOR WITH NANOBIDGE  
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 We performed numerical simulations and experiments on flux flow transistor controlled by the magnetic field generated by a control current I<sub>com</sub>, which regulates the critical current I<sub>cr</sub> through the weak link of the bias line I<sub>b</sub> and the control current. We have fabricated superconducting flux flow transistor with nanobridge from epitaxial YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7- $\delta$</sub>  thin films with thickness 350 &#13210; and bridge width 600 &#13210;, and length 5 &#13211;. The form of this device is patterned using by photolithography and electron-beam lithography. The YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7- $\delta$</sub>  films were wet etched by 0.67% HNO<sub>3</sub> and dry etched by inductively coupled plasma system. The most important steps of the patterning process are the baking procedure used to vulcanize the electron beam resist, the etching time for aqueous solution of nitric acid(HNO<sub>3</sub>), and the inductively coupled plasma etching process. We reviewed a model to describe the current-voltage characteristics measured on nanobridge operating in the flux creep regime. This model allows for computation of the penetration depth, the maximum velocity, the pinning energy, and the critical current as a function of control current I<sub>com</sub> circulating in the control line. Besides this model predicts the dependence of the critical current intensity on the spacial distribution of an applied magnetic field induced by the control current. Comparing the measured and the theoretical results shows that the device model agrees with those expected from the YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7- $\delta$</sub>  flux flow transistor with nano-scale channel.
- H/P.40** QUENCHING-DEPENDENT REVERSIBLE MODIFICATION OF ELECTRONIC STRUCTURE OF PROTON-IMPLANTED SILICON  
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 Fourier-transform infrared (FTIR) studies of proton-implanted silicon were performed in the temperature range 8 K to 300 K. Samples were annealed at 400-450oC and subsequently were heat-treated at a temperature in the range of 70-300oC with following quenching to room temperature in water. FTIR data taken at near-liquid He temperatures reveal that well-known higher-order IR bands related to <100> self-interstitials are quenching-dependent in proton-implanted silicon and their behaviour correlates with the behaviour of far IR absorption lines associated with hydrogen-related shallow donor nanoclusters. The origin of this quenching-dependent reversible modification of electronic structure of proton-implanted silicon is discussed.

- H/P.41** ELECTRONIC EXCITATIONS IN THE Er(8-HYDROXYQUINOLINE)<sub>3</sub> COMPLEX: A THEORETICAL STUDY USING THE SPARKLE MODEL  
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The lanthanide complexes have been applied as emitting materials and are expected to show long luminescent lifetimes and the line-like emission of the metal ions. Being their emission in the infrared region of great technological interest for telecommunication applications, it is important to study the factors that could be able to increase the electro- or photoluminescence quantum efficiency. We report here the results of a theoretical study on the triplet and singlet states involved in the energy transfer mechanism, using as model system the Er(8-hydroxyquinoline)<sub>3</sub> complex. The energy level ordering of the ligands is calculated using the INDO/S-CI model and compared with those of the metal ion. The geometry of the lanthanide complex has been obtained by using a sparkle methodology (i.e. by replacing the lanthanide ion with a suitable effective ion centre) in the framework of the semiempirical AM1 Hamiltonian.
- H/P.42** MD SIMULATION OF LOW-ENERGY SMALL CLUSTER BOMBARDMENT OF CRYSTAL SURFACES AT GRAZING INCIDENCE  
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In the case of grazing incidence the trajectories of projectiles as well as the interaction processes are very complexity, application of analytic approaches are impossible and that is why it is necessary applying the computer simulation. In this work the molecular dynamics (MD) simulation has been used for investigation of small particle-surface interaction processes at grazing incidence. The interaction potential between projectile and target atoms is the universal Biersack-Ziegler-Littmark potential, the interactions between substrate atoms or atoms of molecules have been described by Lennard-Jones or Morse potentials. Both cluster scattering processes and sputtering of target atoms have been studied for the target models as the isolated atomic chains, surface semichannels, two and three dimensional targets. The trajectories of projectiles and recoil atoms as well as some parameters of scattering particles have been calculated. By comparison of these results with analogous results of BCA (binary collision approximation) calculation it was shown that the interaction and accompanying processes in the case of cluster bombardment are drastically changed than those in atomar bombardment. The advantages of application of grazing incidence for mentioned processes are discussed.
- H/P.43** FORMATION OF ALUMINIDE PHASES ON Ti SUBSTRATE DURING ANNEALING AND ION IRRADIATION  
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The aluminum layer on the titanium substrate has been formed by thermal deposition. The structural formation of aluminide phases on the Ti substrate has been studied. The sequence of structural transformations at the Ti/Al interface is limited by the reaction temperature and time. The sequence of aluminide phase formation is occurred in compliance with Ti-Al equilibrium phase diagram. At the initial stages at the Ti/Al interface the Al<sub>3</sub>Ti alloy starts forming as a result of interdiffusion, and gradually the whole aluminum film is spent on the formation of this layer. The Al<sub>3</sub>Ti layer decomposes with the increase of temperature (>600C). At 800C the two-phase (Ti<sub>3</sub>Al + TiAl) layer is formed on the titanium surface. The TiAl compound is unstable and later on with the increase of the exposure time at 800C gradually transforms into the Ti<sub>3</sub>Al. The chain of these successive transformations leads to the formation of the continuous homogeneous layer consisting of the Ti<sub>3</sub>Al compound on the titanium surface. At temperatures exceeding the allotropic transformation temperature (>900C) the Ti<sub>3</sub>Al compound starts decomposing. Ion irradiation influences on kinetics of phase transformation. The irradiation-induced defects produced by prior ion irradiation of Ti substrate accelerated formation of aluminide phases.
- H/P.44** KINETIC MODEL OF THIN FILM GROWTH  
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The production of thin films that contain two chemical components, A and B, has been studied theoretically. It is assumed that the film production is due to "flaky" (layer-on-layer) deposition and that every layer can have components A and B. In general, the chemical bonds A-A, A-B and B-B are formed between A and B components arrived from gas phase and deposited on the surface. As a result, the old layer is covered by a new one, and chemical bonds A-A, A-B, B-B are created between A and B components from neighbouring layers, and between the neighbouring components from the same layer. A general kinetic model of such binary deposition is presented. The model includes the probabilities and rate coefficients for the elementary processes of gas (plasma)-surface interactions, and can be used for calculations of the macro characteristics of thin film production by PECVD. The master equations for densities of A and B components in the surface layers are formed, and their analytical and numerical solutions are obtained. The deposition and erosion rates, surface and volume densities of A and B components, as well as the relative volume of micro cavities within the films, are calculated as a function of probabilities for the elementary processes. The agreement of theory with experiment is obtained from a-Si:H and CN thin films resulting properties, which were prepared by SiH<sub>4</sub> PECVD and rf-magnetron sputtering assisted by ion beam, respectively.
- H/P.45** RF SPUTTERING DEPOSITION AND MAGNETIC CHARACTERISATION OF ND-FE-B THIN FILMS FOR MICROWAVE APPLICATIONS  
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Nonreciprocal ferrite devices, like circulators, are actually used under bulk form in the telecommunication field. To work properly, they need to be biased by a magnetic field which can be provided by a bulk magnet. The current challenge is to integrate these circulators with a multi-layer form on a unique substrate (MMIC technologies). This study deals with the realisation by rf magnetron sputtering and the characterisation of NdFeB thin magnetic films; they are likely to polarize a soft ferrite layer. To do this, the easy axis of the magnetic layers must be perpendicular to the film plane. The effect of deposition parameters on structure, magnetic properties and composition of the films has been studied in a multilayer Si/Ti (200 nm)/NdFeB(1000 nm)/Ti (200 nm). The Ti underlayer prevents Fe-Ti reactions and the Ti overlayer avoids Nd oxydation. The hard polycrystalline magnetic phase Nd<sub>2</sub>Fe<sub>14</sub>B has been identified. Its coercive field is about 0.6 Tesla.

- H/P.46** FIRST PRINCIPLES CALCULATION STUDY OF MULTI-SILICON DOPED FULLERENES  
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 Introducing dopant atoms into a fullerene molecule gives us the possibility to modify and control its structural and electronic properties. Mass spectroscopy and photofragmentation experiments have given clear evidence on the existence of stable Si-doped heterofullerenes that can contain more than one heteroatom (or even twelve) in the carbon cage. The determination of largest number of Si atoms which can replace C atoms in the network without causing its breakdown still remains an open problem. Previously, first-principle calculations were used to elaborate an atomic-scale picture of stability and bonding in Si-doped fullerenes. Here we extend these calculations to a large number of Si atoms by optimizing the structures of heterofullerenes  $C_{54}Si_6$ ,  $C_{48}Si_{12}$  and  $C_{40}Si_{20}$ . We found that these cage networks are remarkably stable, yielding deformed and yet fairly regular fullerene geometries. Our results show that, at least for the case of zero temperature stability, highly heterogeneous fullerenes are conceivable nanomaterials which might be detected via suitable techniques of synthesis.
- H/P.47** STOCHASTIC SIMULATIONS OF THE SYNTHESIS OF NANOCRYSTALS IN REVERSE MICELLES  
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 In the past decade, semiconductor nanoparticles have attracted much attention arising from the fundamental scientific interest in understanding the transition of material properties from the bulk to molecular-like clusters and their potential applications. The main issue in the preparation of semiconductor nanocrystals is a careful control of particle size and, even more important, their size distribution. Among the several preparations proposed a popular method makes use of reverse micelles or water in oil microemulsions, undergoing to fast development in the last few years [1]. Nanoparticles can be obtained by using self-assembly molecules as a template, exploiting confined growth inside the surfactant film of microemulsion system. Stochastic simulation methods can be effectively exploited to account for the observed template effect of the microemulsion aggregate size on the nanocluster growth. In this contribution a computer program that simulate the time evolution of this process will be presented and the obtained outcomes discussed. The program is based on the Gillespie algorithm [2], a Monte Carlo procedure that exactly simulate the master equation associated with any chemically reacting system. This approach allows to describes into details all the reactions that take place in the systems, i.e. solute exchange among droplets, nucleation and growth of nanocrystals, solute sedimentation. Moreover, the size dispersion of the reverse micelles can be taken into account. The aim of this work is to get insight in all the microscopic reactions linked to macroscopic properties of the reacting system than can be opportunely regulate to obtain nanocrystals with the desired sharp size distribution.
- H/P.48** FIRST-PRINCIPLES STUDY OF CUBIC  $Al_xGa_{1-x}N$  ALLOYS  
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 Nitride semiconductors (GaN, AlN and InN) are grown on various substrates exhibiting large misfits, moreover, even between themselves, the large mismatches may act strongly and lead to miscibility gaps and composition fluctuations at the atomic scale. Following the need to accurately understand the In composition fluctuations and their role on the optical First-principles calculations, based on the full-potential augmented plane wave method within the local density approximation, are used to study the influence of alloying on the structural and electronic properties of cubic  $Al_xGa_{1-x}N$  ordered alloys in the chalcopyrite and luzonite structures. We have investigated the lattice parameters and band gap energies. The lattice constants exhibits a small downward bowing. From, the calculated band gap variation, we reported a very small bowing. We established the dependence of the band gap bowing parameter on the lattice constant and on the structural model used in the calculations. We observe a direct to indirect band gap crossover at  $x(Al)=0.51$ . The large dispersion of the value of the band gap bowing is discussed.
- H/P.49** LOW-ENERGY P+ION CHANNELING AND IMPLANTATION INTO Si(110), SiC(110), GaP(110) AND ASGa(110)  
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 Recently the computer simulation based on binary collision approximation was applied for the description of various processes accompanying the interaction of ion beams with a surface including for the description of medium and low energy ion channeling in homogeneous thin single crystals with lattices such as fcc and as diamond. In the present work a comparative investigation of 1-5 keV P+ ions channeling in thin and thick Si(110), SiC(110), GaP(110) and AsGa(110) crystals is carried out by computer simulation in binary collision approximation. The comparative investigation of trajectories, ranges, energy losses, angular and energy distributions, as well as depth profile distribution of low-energy P+ ions channeling in Si(110), SiC(110), GaP(110) and AsGa(110) have been carried out by computer simulation. It was shown that for paraxial part of a beam the main contribution to total energy losses comes from inelastic energy losses. It has been observed in details the dynamics of the change of the character of trajectories, the range and energy losses of channeled ions as well as the angular and energy distributions of ions transmitted through thin crystal versus the composition of single crystal, the impact parameters from the center of the channel and the initial energy. It has been established that for a paraxial part of a channeled beam the contribution of inelastic energy losses to the total energy losses is a main.
- H/P.50** CHARACTERISATION AND DEPTH PROFILES MEASUREMENTS OF SILICON NITRIDE THIN FILMS ON SILICON AND MOLYBDENUM SUBSTRATES BY AUGER ELECTRON SPECTROSCOPY  
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 $Si_3N_4$  thin films were deposited on Si or Mo substrates using a new technique of plasma enhanced chemical vapor deposition (PECVD). Depth profiles measurements were carried out on these  $Si_3N_4$  layers, as well as on the  $Si_3N_4$  /Mo and  $Si_3N_4$  / Si interlayer by Auger electron spectroscopy, associated to Argon ion sputtering. For the  $Si_3N_4$  films deposited on Mo substrates a sequence of three distinguishable zones was observed: the  $Si_3N_4$  layer; an interlayer containing Si-N, Mo-N, and presumably Mo-Si bonds; a diffusion zone of nitrogen into the Mo substrate. On the Si substrate a more usual depth profile was evidenced involving the sequence of the  $Si_3N_4$  layer, an interlayer zone with the presence of Si-N and Si-Si bonds, and finally the Si substrate.

- H/P.51** CHARACTERIZATION OF THE JAMMING STATE OF PRE-TREATED PATTERNED SURFACES BY EXTENSIVE MONTE CARLO SIMULATIONS  
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 We present an extensive Monte Carlo study of irreversible, sequential deposition of disks with short-range repulsive interactions, on a patterned surface. We perform, in this work, a detailed characterization of the jamming state, where no more disks can be adsorbed on the surface. In particular, we studied the effect of the substrate patterning on the coverage and on the particle distribution on the surface. To this end, we defined suitable parameters, namely, the radius of disks,  $r$ , the side of square regions,  $a$ , of where deposition can take place, and the distance,  $b$ , between such squares on the substrate. We observe regions in the  $a/r$  versus  $b/r$  diagram, with fundamentally different time dependences of the coverage, namely, exponential and power-law approaches to the jamming state. We show that the model, interpolates between the continuum to lattice random sequential adsorption, as we conveniently vary the above parameters. Moreover, we observe regions of the above diagram, where disks adsorb and form near crystalline order, while in order regions of the diagram, this ordering is absent. Our study is of interest to people working, for example, in the fields of self-assembled nanostructures, colloids, lithography, and nonequilibrium statistical physics as it provides key parameters and characterization of the jamming state.
- H/P.52** EFFET OF TUNGSTEN 0- 8wt.% ON THE OXIDATION OF Co-Cr ALLOYS  
A. Karaali(a), K. Mirouh(a), S. Hamamda(a) and P. Guiraldenq(b), (a)Département de Physique, Faculté des Sciences, Université Mentouri, Constantine, Algérie, (b)Département IFOS, Ecole Centrale de Lyon, 69131 Ecully cedex, France  
 The nature and the morphology of the present oxide layers on the surface of alloys have a great importance on the quality of the ceramic/metal bond. This study shows the effect of the tungsten addition on the formation and the growth of the oxide layers of the Co-Cr alloys at pre-oxidation temperatures 950 - 1050°C, thus including the temperature range of the ceramisation process which these alloys will undergo later. Their characterization, using the microprobe analysis, the scanning electron microscopy (SEM) and the x-rays diffraction, show the formation of two distinct layers; the first at surface is formed only of pure CoO while second is the mixture of CoCr<sub>2</sub>O<sub>4</sub> particles and of the tungsten oxide dispersed in a CoO matrix. The addition of the W element up to 8% modifies considerably the thicknesses of the formed layers while accumulating in the second layer thus blocking the diffusion of cobalt.
- H/P.53** A NANOSTRUCTURED BIOSENSOR BASED ON ENZYME IMMOBILIZATION IN LAYER-BY-LAYER FILMS  
V. Zucolotto, A.P.A. Pinto, A.P.U. Araújo, O.N. Oliveira Jr., Instituto de Física de São Carlos, USP, SP, CP 369, Brazil  
 A highly sensitive biosensor for halogenated organic compounds was achieved upon immobilization of the enzyme Cl-catechol 1,2 dioxygenase (CCD) in ultrathin nanostructured films. The films were obtained with the electrostatic layer-by-layer (LBL) technique, in which CCD was alternated with layers of poly(amidoamine) generation 4 (PAMAM G4) dendrimers. Thin films containing up to 40 PAMAM/CCD bilayers were assembled onto quartz substrates. The film growth step, which comprised the enzyme immobilization was confirmed via UV-VIS spectroscopy showing a linear increment in the absorption band at 280 nm as a function of deposited PAMAM/CCD bilayers. Atomic force microscopy (AFM) was employed in the morphological analyses as well as in the determination of the film thickness. The thickness per bilayer was found to be 14 nm with an average roughness of only 0.5 nm showing a very smooth adsorption of the components onto the substrate. Circular dichroism (CD) spectroscopy revealed that the conformation of the CCD macromolecules was the same either in solution or in the LBL film. The enzymes remained active for several days in the LBL nanostructure, which allowed the films to be used as biosensors for halogenated organic compounds, viz. catechol or Cl-catechol. More specifically, catechol detection was carried out by observing the formation of cis-cis muconic acid when the LBL film was immersed in a catechol solution. The acid is a product from the reaction between CCD and catechol, which displays absorption at 260 nm. Films with 10 PAMAM/CCD bilayers were employed to detect catechol in very dilute solutions, with concentrations as low as 10<sup>-11</sup> mol/L.
- H/P.54** ANALYSIS OF NANO-SIZED STRUCTURES IN HYDROGENATED AMORPHOUS SILICON-CARBON THIN FILMS  
D. Gracin, K. Juraic, P. Dubcek, A. Gajovic and I. Bogdanovic-Radovic, Rudjer Boskovic Institute, Zagreb, Croatia  
 The one micrometer thick hydrogenated amorphous thin films with high hydrogen concentration and variety of carbon to silicon ratio were deposited by magnetron sputtering and by PECVD (Plasma Enhanced Chemical Vapour Deposition). The local structural and chemical ordering of specimens were examined by vibrational spectroscopy (Raman and IR spectroscopy) while IBA (Ion Beam Analysis) e.g. RBS (Rutherford Back Scattering) and ERDA (Elastic Recoil Detection Analysis) were used in estimating the composition of films. The GISAXS (Grazing Incidence Small Angle X-ray Scattering) spectroscopy, performed on ELETTRA synchrotron radiation source (Trieste, Italy) was used for examination of samples homogeneity on nano-scale. For all of samples, the GISAXS results indicate presence of "particles", with characteristic linear dimensions between 1 and 6 nm, depending upon hydrogen and carbon concentration. In order to identify constitution of particles, their sizes and size distributions were correlated with the results of other methods. For most of specimens, the distribution of dielectric function, modelled by using effective medium approximation, suggests that the "particles" are agglomerates of small voids, whose size increases with carbon to silicon ratio and whose distribution broadens with hydrogen concentration.
- H/P.55** QUANTITATIVE ESTIMATION OF THE ORDER-DISORDER PHASE TRANSITION TEMPERATURE OF Ni<sub>3</sub>Al USING A FACE CENTERED CUBIC LATTICE MODEL WITH A RENORMALIZED POTENTIAL  
Ryoji Sahara(a), Hiroshi Mizuseki(a), Kaoru Ohno(b), and Yoshiyuki Kawazoe(a), (a)Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan, (b)Department of Physics, Graduate of School of Engineering, Yokohama National University, 240-8501, Yokohama, Japan  
 A Monte Carlo (MC) simulation is carried out to study thermodynamic properties of Ni<sub>3</sub>Al using a face centered cubic (FCC) lattice-gas model. To estimate the order-disorder phase transition temperatures of actual the system as quantitatively as possible, a Finnis-Sinclair-type potential, which has been widely used for molecular dynamics (MD) simulations, is applied in the model. In order to overcome some shortcomings of lattice-gas models such as neglecting internal entropy of the system, the potential is mapped onto FCC lattice using the renormalization technique (1)-(3). Using the renormalized potential as many-body interactions of MC simulation, we find the order-disorder phase transition temperatures of the system is greatly improved when compared with the case of using the original MD potential directly on the lattice. References: (1) K. Ohno, The Sci. Rep. Res. Inst. Tohoku Univ. A43, 17 (1997). (2) R. Sahara, H. Mizuseki, K. Ohno, S. Uda, T. Fukuda and Y. Kawazoe, J. Chem. Phys. 110, 9608 (1999). (3) R. Sahara, H. Ichikawa, H. Mizuseki, K. Ohno, H. Kubo, and Y. Kawazoe, accepted to J. Chem. Phys. (2004).

- H/P.56** **ATOMISTIC MODELLING OF METAL SULPHIDES**  
P.E. Ngoepe, S.P. Ntoahae, H.M. Sithole, Materials Modelling Centre, University of the North, Private Bag x1106, Sovenga 0727, South Africa, S.C. Parker, School of Chemistry, University of Bath, Claverton Down, Bath BA2 7AY, U.K., K.V. Wright, The Royal Institution of Great Britain, 21 Albermarle Street, London W1X 4BS, U.K.  
 In this study planewave pseudopotential method is mainly used to study structural and electronic properties of mineral metal sulphides/arsenides with a pyrite structure, such as FeS<sub>2</sub> and PtAs<sub>2</sub>, together with the platinum sulphides with a tetragonal structure. In particular the variation of these properties with pressure are studied. Empirical forcefields are derived for these compounds and validated by reproducing experimental structures, and they are used to investigate bulk and surface properties.
- H/P.57** **TRENDS IN ATOMIC DIFFUSION ON METALLIC SURFACES**  
Adele Carrado, Hervé Bulou, Christine Goyhenex, Institut de Physique et Chimie des Matériaux de Strasbourg, GSI, BP 43, 67034 Strasbourg cedex 02, France  
 The study of elementary processes of adatom migration is of primary importance for the understanding of growth of epitaxial layers or nanostructures. Many theoretical works have been devoted to atomic diffusion within various approaches but mainly in the aim to reproduce the experimental behavior of a single chosen system. Thus we attempt here to fill the lack of systematic studies in this field. We present molecular-dynamics calculations of adatom self diffusion on surfaces of transition or noble metals going from the 3d to 5d series. The second moment approximation (SMA) of the tight-binding formalism was used to calculate the atomic interactions. We found it to be a reliable method to characterize within a unique approach a sufficiently large amount of systems in order to deduce general tendencies on self diffusion on metals.
- H/P.58** **MOLECULAR MODELING OF DISLOCATION FORMATION AND PLASTIC DEFORMATION OF AN ORIENTED CRYSTALLINE POLYMER**  
U. Gafurov, Institute of Nuclear Physics, Tashkent 702132, Uzbekistan  
 In the model interconnection molecular chains in an oriented linear crystalline polymer were fastened on or near polymer crystallite surface by intermolecular bonds or cross-links. Simple cosine periodic potential as in Frenkel-Kontorova's dislocation model was used for intermolecular interaction and condition of balance of loaded chain in polymer crystallite. The dislocation formation is accompanied molecular chains slippage and local loads relaxation on their amorphous sections as well as by conformation regroupings of these sections in some conditions. In dependence on external load and amorphous region length different cases are realized. The first case takes place when the load is moderate. In this case the load on the amorphous section of a slipped out chain are completely relaxed and this section could change its conformation state. In the another case slipped out amorphous section of a macromolecule is in strained state but its strain is less than one of the macromolecule before its slipping out. The load relaxation value influences on dislocation behaviour. This behaviour depends except for of macromolecular chain parameters mainly from sizes of stressed amorphous section and of initial load on it. If after dislocation formation this amorphous section remains enough stressed, the dislocation remains in crystallite. In other cases the chain pulled into crystallite again with restoration of load value on amorphous section. The dislocation movement into crystallite and accordingly the further slippage of the passage macromolecule fastened by cross-link happens with increase of local load on crystallite boundary and with enhance of dislocation energy. While for the interconnecting macromolecules without cross-linking the slippage is accompanied by loss.
- H/P.59** **ATOMIC AND ELECTRONIC STRUCTURES OF THREADING SCREW DISLOCATION IN WURTZITE GaN**  
Imad Belabbas, SIFCOM UMR CNRS 6176, ENSICAEN, 6 boulevard du Maréchal Juin, 14050 Caen cedex, France, Mohamed Akli Belkhir, Groupe de physique du solide, Laboratoire de physique théorique, Université A. Mira de Béjaia, Algérie, Young Hee Lee, Center for Nanotubes and Nanostructured Composites, Institute of Basic Science, Department of Physics Sungkyunkwan University, Suwon 440-746, Korea, Gérard Nouet, SIFCOM UMR CNRS 6176, ENSICAEN, 6 boulevard du Maréchal Juin, 14050 Caen cedex, France  
 We have investigated atomic and electronic structures of the full-core screw dislocation in wurtzite GaN using a self-consistent density functional tight-binding calculations. Our calculations show that atoms located at the screw dislocation are severely strained in a hexagonal atomic core, and an extra charge transfer of 0.12e is occurred at the core atoms from Ga to N, in addition to the typical charge transfer of 0.56e of the bulk GaN. The gap states are spread over the entire band gap, indicating that the threading screw dislocation is electrically active as donors and acceptors. The tail states of valence and conduction bands are contributed by the p states of the core N-atom, whereas the deep levels are heavily localized at the core atoms of both Ga and N, contrary to the previous report that the deep levels were localized only on N atoms. The coexistence of acceptor and donor gap states in the vicinity of the screw dislocations could be an origin of the leakage currents observed in GaN-based devices.
- H/P.60** **OPTICAL AND PHOTOELECTRONIC PROPERTIES OF MELANIN FILMS**  
V. Capozzi(a,b), A. Gallone(a), G. Perna(a,b), R. Cicero(c), G. Guida(c), P. Zanna(c), M. Ambrico(d), V. Augelli(b,e), P.F. Biagi (b,e), T. Ligonzo(b,e) and L. Schiavulli(b,e), (a)Dipartimento di Scienze Biomediche, Università di Foggia, Viale Pinto, 71100 Foggia, Italy, (b)Istituto Nazionale di Fisica della Materia, Unità di Bari, Bari, Italy, (c)Dipartimento di Biochimica Medica e Biologia Medica, Sezione di Biologia Medica, Facoltà di Medicina e Chirurgia, Università degli Studi di Bari, Policlinico, Bari, Italy, (d)Dipartimento di Metodologie Inorganiche e dei Plasmi del C.N.R., Via Orabona 4, 70126 Bari, Italy, (e)Dipartimento Interateneo di Fisica dell'Università di Bari, Via Amendola 173, I-70126 Bari, Italy  
 Melanins are natural biopolymer which have recently become very interesting for different applications, as molecular electronic as well as biomaterials. We present a study of the optical and electrical properties of melanin films by means of absorption and photocurrent techniques. Melanin pigment was extracted from the liver of *Rana esculenta* L. and deposited as thin film on quartz substrate. The shape of the absorption spectra is similar to that of amorphous inorganic semiconductors, with an optical gap value of 0.5 eV. The model of the natural melanin film as a network of clusters of polymeric units based on the 5,6-indolequinone structure having different size is proposed to explain the absorption properties. Two silver points contacts have been deposited on melanin films: the contacts display a good ohmic characteristic in the 0-50 V voltage range. The obtained resistance has been of the order of 10<sup>12</sup> Ohm. Photosensitivity to sun spectra has been demonstrated by photoconductivity measurements under AM1 light source illumination. The role of a hopping model of conductivity is discussed.

- H/P.61** INFLUENCE OF GE AD-DIMERS ON THE CARBON INCORPORATION IN Si(001) SURFACES: A THEORETICAL STUDY  
 Ph. Sonnet, M. Habar, L. Stauffer, Laboratoire de Physique et de Spectroscopie Electronique, 4 rue des Frères Lumière, 68093 Mulhouse cedex, France, P.C. Kelires, Foundation for Research and Technology-Hellas (FORTH), P.O. Box 1527, 711 10 Heraklion, Crete and Physics Department, University of Crete, P.O. Box 2208, 710 03 Heraklion, Greece  
 We present an energetic ab-initio study of carbon incorporation in the Si(001) surface in presence of germanium ad-dimers parallel or perpendicular to dimer rows, located above or between the silicon dimer rows. In each case, a single carbon adsorption is considered. The influence of some parameters as the local stress before and after carbon adsorption and carbon-defect interaction is investigated. The local stress is calculated in the framework of semi-empirical Monte Carlo approach. We find that the presence of ad-dimer makes carbon incorporation easier, specially in the alpha sites of the third layer. A germanium ad-dimer in parallel orientation with respect to the silicon dimer rows, located just between the dimer rows, however makes the beta sites of the third layer markedly less disfavoured than in other ad-dimer models. This can be explained by taking into account the above parameters in a systematic and combined way. Finally, Monte Carlo simulations show that the germanium ad-dimers increase the carbon concentration in the subsurface layers more than silicon ad-dimers.
- H/P.62** FIRST-PRINCIPAL CALCULATIONS OF STRUCTURAL, ELASTIC AND ELECTRONIC PROPERTIES OF RO<sub>2</sub> (R = Zr, Hf and Ce) IN FLUORITE PHASE  
R. Terki, H. Faraoun, G. Bertrand and H. Aourag, Laboratoire d'Etudes et de Recherches sur les Matériaux, les Procédés et les Surfaces. LERMPS-UTBM, Belfort, France  
 Zirconium, hafnium and cerium oxides are important materials in ceramic engineering because they show high strength even at high temperature. In this study, we have performed calculations on structural, elastic and electronic properties of these materials in the fluorite structure using the full-potential linearized augmented Plane Wave (FP-LAPW) method, within the density functional theory (DFT). In this approach, the generalized gradient approximation (GGA) was used for the exchange-correlation potential. We first used the experimental lattice parameters as the starting point to investigate the structural properties of RO<sub>2</sub> (R = Zr, Hf and Ce). By calculating the total energy at different volumes and fitting the result with Murnaghan equation of state, we obtained the equilibrium lattice constant, the minimum of the total energy, the bulk modulus B and its first pressure derivative B'; the elastic constants were also calculated and our results are compared with the experimental and other theoretical works. On other hand, calculations of the charge densities were also performed to describe the nature of chemical bonding. The electronic structure calculations showed that the three compounds exhibit wide and indirect band gaps. Furthermore, the analysis of the density of state (DOS) allow us to discuss the features of orbital mixing and a comparison between the different results of ZrO<sub>2</sub>, HfO<sub>2</sub> and CeO<sub>2</sub> has been done in order to discuss the substitution effect in the fluorite structure.
- H/P.63** ELASTIC PROPERTIES OF BINARY NiAl, NiCr AND AlCr AND TERNARY Ni<sub>2</sub>AlCr ALLOYS FROM MOLECULAR DYNAMIC AND ABINITIO SIMULATION  
H. Faraoun(a), H. Aourag(a), C. Esling(b), J.L. Seichepine(a) and C. Coddet(a), (a)Laboratoire d'Etudes et de Recherches sur les Matériaux, les Procédés et les Surfaces. LERMPS-UTBM, (b)Laboratoire d'Etude des Texture et Applications aux Matériaux. ISGMP-LETAM, Belfort, France  
 Molecular dynamic simulation is used in order to investigate the structural and elastic properties of binary metallic alloys NiAl, NiCr, AlCr and ternary Ni<sub>2</sub>AlCr. The classical model is a Sutton-Chen like potential from the embedded atom method scheme, that we fitted to equilibrium properties of the three binary phases. First principle calculations based on density functional theory and the full potential linear augmented plane waves method were carried to determine the binary phases properties used in the classical potential fitting procedure. The classical calculations carried in an NVT thermodynamical ensemble leads to the determination of lattice parameters, bulk modulus and elastic constants in a temperature range from 300 to 900°K for the four systems. The AlCr binary alloy was found to have the lowest strength and the largest thermal expansion, when NiCr has the largest hardness and Ni<sub>2</sub>AlCr the lowest thermal expansion. The elastic constants variation with temperature was found to follow the physical behavior of the metallic alloys and to be consistent with the calculated thermal expansion coefficients.
- H/P.64** AB INITIO INVESTIGATION OF THE ORDERING EFFECTS ON THE ELECTRONIC STRUCTURE OF AlN/GaN, InN/GaN AND InN/AlN SUPERLATTICES  
 A. Lakdja and B. Bouhaf, Modelling and Simulation in Materials Science Laboratory, Physics Department, University of Sidi Bel-Abbes, 22000 Sidi Bel-Abbes, Algeria, P. Ruterana, SIFCOM, UMR 6176 CNRS-ENSICAEN, 6 Boulevard Maréchal Juin, 14050 Caen Cedex, France  
 We report the electronic structure of short-period m×n AlN/GaN superlattices (with m, n ≤ 3) calculated in wurtzite [with (0001) orientation] structure using a first-principles full potential linearized augmented plane waves method within the local density approximation (LDA). The calculated gaps range from 3.1 for Al-rich to 2.6 eV for Ga-rich m×n (001) AlN/GaN systems.  
 We predict also that ordering affects significantly the 1×1 (001) InN/GaN and InN/AlN electronic band structures compared to 1×1 (001) AlN/GaN. The 1×1 (001) InN/GaN and InN/AlN are found to have direct smaller band gaps of 0.4 and 1.1 eV, respectively. The origin of the reduction in the band gaps in InN/GaN and InN/AlN is discussed, as well as the effects of increasing the monolayer number in AlN/GaN superlattices.
- H/P.65** FIRST PRINCIPLES SEARCH FOR MULTIFERROISM IN BiCrO<sub>3</sub>  
Pio Bättig and Claude Daul, Department of Chemistry, Université de Fribourg, 1700 Fribourg, Switzerland, Nicola A. Hill, Materials Department, University of California, Santa Barbara CA 93106-5050, USA  
 We present results of first-principles density functional calculations for the candidate multiferroic magnetoelectric, bismuth chromite. Although little is known experimentally about BiCrO<sub>3</sub>, its chemical neighbors BiMnO<sub>3</sub> and BiFeO<sub>3</sub> are known to be ferromagnetic and ferroelectric respectively, with structural distortions driven by the strongly polarizable Bi ions. Our calculations reveal, as expected, a Bi-induced distortion, and an octahedral Cr<sup>3+</sup> ion which resists off-center displacement. We predict a G-type antiferromagnetic ground state, with an antiferrodistortive or antiferroelectric structural distortion, similar to that seen in PbZrO<sub>3</sub>.

**H/P.66** MODELLING OF ANISOTROPIC EXCHANGE COUPLING IN RARE-EARTH-TRANSITIONMETAL PAIRS: APPLICATIONS TO  $\text{Yb}^{3+}\text{-Mn}^{2+}$  AND  $\text{Yb}^{3+}\text{-Cr}^{3+}$  HALIDE CLUSTERS AND ITS IMPLICATION TO THE LIGHT UP-CONVERSION

M. Atanasov(a), C. Daul(b), H.U. Güdel(c), (a)Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, Acad. G. Bontchev Str. Bl.11, 1113 Sofia, Bulgaria, (b)Departement de Chimie, Université de Fribourg, Perolles, 1700 Fribourg, Switzerland, (c)Departement für Chemie und Biochemie, Universität Bern, Feiestrasse 3, 3000 Bern 9, Switzerland

A procedure for calculating magnetic exchange coupling constants in rare earth (RE)-transition metal (TM) dimmers is presented. In a first step RE-TM transfer (hopping) integrals between orbitals carrying unpaired (magnetic) electrons on RE and TM are determined from a MO-calculation utilising the concept of orbital exchange pathway and effective Hamiltonian theory. In a second step, many-electron wave-functions for ground or excited electronic states on RE and TM are constructed in which spin-orbit coupling (which dominates for the RE) is fully (variationally) taken into account. Finally, the data from steps 1 and 2 are combined to obtain numerical values for kinetic exchange integrals (within Anderson's super-exchange theory) utilising a non-Heisenberg (orbital dependent) exchange operator. The MO's corresponding to the d(Mn) and f(Yb) magnetic orbitals have been used to also calculate ferromagnetic exchange integrals. The model is applied to  $\text{Yb}^{3+}\text{-Mn}^{2+}$  dimmers with corner, edge and face shared octahedra and  $\text{Cl}^-$  and  $\text{Br}^-$  bridging ligands. For that purpose we utilise a spectroscopically adjusted (to spectra of single nucleus  $\text{MnCl}_6^{4-}$  and  $\text{YbCl}_6^{3-}$  complexes) parameterisation of the Extended Hückel theory. The expediency of the approach is discussed based on a comparison between calculated and experimental (available from inelastic scattering experiments) anisotropic exchange parameters in  $\text{Br}_3\text{Cr}^{3+}\text{-}\mu(\text{Br}_3)\text{Yb}^{3+}\text{Br}_3$  dimmers. Ferromagnetic exchange parameters for the ground state and the lowest emitting excited state increase from corner to edge to face Mn-Cl-Yb sharing thus lending support to a exchange mechanism of the up-conversion.

**H/P.67** KINETIC MONTE CARLO MODELLING OF HIGH-K ATOMIC LAYER DEPOSITION

G. Mazaleyrat, L. Jeloica, A. Estève and M. Djafari Rouhani, LAAS-CNRS, France

**H/P.68** DENSITY FUNCTIONAL THEORY OF HIGH-K REACTION MECHANISMS ON  $\text{SiO}_2/\text{Si}$  SYSTEM

L. Jeloica, A.Dhkissi, G. Mazaleyrat, A. Estève and M. Djafari Rouhani, LAAS-CNRS, France

12:45

LUNCH

Thursday, May 27, 2004

Afternoon

Session VIII: Oxide materials II

Session chair: P. Hyldgaard

- H-VIII.01** 14:00 -Invited- HIGH-K DIELECTRICS: DEFECTS DYNAMICS FROM AB INITIO CALCULATIONS  
**Jacob Gavartin**, Department of Physics and Astronomy, University College London, Gower street, London WC1E 6BT, U.K.
- H-VIII.026** 14:30 -Invited- PREDICTIVE PROCESS DESIGN: FIRST PRINCIPLES MODELLING OF ATOMIC LAYER DEPOSITION  
**S. Elliot**, NMRC, Ireland
- H-VIII.03** 15:00 -Invited- MODELLING DEFECTS IN AMORPHOUS MATERIALS: AN EMBEDDED CLUSTER APPROACH  
**P.V. Sushko**, S. Mukhopadhyay, S. Mysovsky, A. Taga, A. Shluger, Department of Physics and Astronomy, University College London, Gower St., London WC1E 6BT, U.K.  
Understanding the effect of structural disorder in amorphous materials on defect structure and properties is important fundamentally and for many technological applications. Predicting defect properties and relative abundance of different defect configurations generally requires considering a statistical ensemble of structural sites. Yet additional factors include the history of the sample and the mechanism of defect formation. This provides new challenges for both theoretical and experimental analysis of defects in amorphous materials. We develop an ab initio embedded cluster method and study the structure and properties of E' centers at different sites of a model amorphous silica structure generated using a classical molecular dynamics technique. We form a statistical distribution of neutral oxygen vacancies in different sites and then calculate relaxed configurations of these vacancies after trapping a hole using quantum mechanical embedded cluster technique. In this way we create a distribution of centers with structures ranging from a dimer to a dangling bond configuration. We correlate the properties of defects with bond lengths, ring size, and dihedral angles. We verify our findings by comparing the calculated optical absorption energies and hyperfine and super-hyperfine EPR parameters with the experimental data.
- H-VIII.04** 15:30 HOW MOLECULAR OXYGEN REACTS ON SILICON  
**N. Richard**, A. Estève and M. Djafari Rouhani, CEA-DAM, Paris, LAAS-CNRS, Toulouse, France
- H-VIII.05** 15:45 FULLY COORDINATED SILICA NANOCLUSTERS : BUILDING BLOCKS FOR NOVEL MATERIALS  
**S.T. Bromley**, M.A. Zwijnenburg, E. Flikkema, Lab. of Applied Organic Chemistry and Catalysis, DelftChemTech, 136 Julianalaan, Delft University of Technology, Delft 2628 BL, The Netherlands  
All-silica materials span a remarkably large spectrum of different polymorphs and densities unknown to any other single class of solids. Furthermore, largely due to this diversity of form, silica has a large range of important applications including gate dielectrics and subwavelength photonics. The structural basis for the vast majority of silicas is a 3D network of corner-sharing SiO<sub>4</sub> tetrahedra. However, silica tetrahedra can also participate in edge-sharing, giving rise to closed rings containing two silicon atoms and two oxygen atoms. Such two-rings provide one way in which fully-coordinated silica nanoclusters [1] could be realised. Using a global optimisation algorithm approach to generate energetically low lying silica clusters, employing our recently developed nanoscale silica interatomic potential [2], and finally using high level density functional theory (DFT) calculations, we have generated a number of potential silica nanocluster building blocks. We argue, specifically, that fully-coordinated two-ring-containing nanoclusters could allow for the formation of a whole new class of stable silica materials with novel topologies and properties. Based on the properties of the two-ring-chain-based material silica-w, we speculate that SiO<sub>2</sub>-cluster-based molecular materials would be ordered, have a low refractive index (RI ~ 1.41), density (~ 1.97 g/cm<sup>3</sup>) and dielectric constant (k), and may also display liquid crystalline behaviour. Preliminary examples of such novel silica nanocluster-based molecular materials are reported using an empirically parameterised inter-cluster potential.  
[1] S. T. Bromley, M. A. Zwijnenburg, Th. Maschmeyer, Phys. Rev. Lett., 2003, 035502, 90, (2003). [2] E. Flikkema and S. T. Bromley, Chem. Phys. Lett. 378, 622, (2003).

16:00

**BREAK**

Session IX: Semiconductor materials

Session chair: S. Elliot

- H-IX.01** 16:30 -Invited- ATOMISTIC MODELING OF DOPANT IMPLANTATION AND ANNEALING IN SI: DAMAGE EVOLUTION, DOPANT DIFFUSION AND ACTIVATION  
**Lourdes Pelaz**, Departamento de Electrónica, Universidad de Valladolid, E.T.S.I. de Telecomunicación, 47011 Valladolid, Spain

- H-IX.02** 17:00 **FIRST PRINCIPLES MODELING OF INTERMEDIATE RANGE ORDER IN AMORPHOUS SiSe<sub>2</sub>**  
M. Celino(a) and C. Massobrio(b), (1aCP 2400, 00100 Rome AD, Italy, (b)IPCMS, 23 rue du Loess, 67037 Strasbourg, France  
 Amorphous materials are widespread used in technological applications even if the comprehension of their properties in most cases is still a challenge. Their properties are determined by the apparently disordered assembly of nanoscale atomic structures. A clear example of this effect is the amorphous SiSe<sub>2</sub> that shows spatial correlations giving rise to intermediate range order whose presence is observed in specific features of diffraction experiments. In this respect, intermediate range order is commonly defined as the level of structural organization involving distances well beyond nearest neighbor interactions. Chains of tetrahedra are responsible for network forming inside the structure. The atomic structure of the amorphous SiSe<sub>2</sub> has been completely described by performing extensive simulations based on first-principle molecular dynamics (FPMD). The calculated structure factor is in very good agreement with experiments, as well as the number of corner- and edge-sharing tetrahedra. By focusing on the sequences of Si atoms linked via intra and intertetrahedral bonds, we identify the predominant structural motifs. Moreover, an accurate methodology has been developed to produce by FPMD reliable amorphous samples from liquid systems with statistically significant number of nanoscale atomic structures.
- H-IX.03** 17:15 **AB-INITIO CHARACTERIZATION OF ELECTRONIC AND OPTICAL PROPERTIES OF NOVEL ALLOY SEMICONDUCTORS**  
P. Palacios, J.J Fernández, P. Wahnón and C. Tablero, Instituto de Energía Solar, ETSI Telecomunicación, Universidad Politécnica de Madrid, Madrid, Spain  
 The aim of this work is to study by first principle calculations at atomic level, the electronic and optical properties for a new type of photovoltaic material identified elsewhere<sup>1</sup> with semiconductor properties, characterized by an isolated metallic intermediate band located in the semiconductor energy band gap. This material may absorb photons of low energies that promote electrons from the valence band to a half filled intermediate band and from this one to the conduction band. In a previous work we have proposed several alloys semiconductors containing a transition metal atom, of the type: M<sub>1</sub>G<sub>m</sub>X<sub>n</sub> with X=As or P, and M=Sc, Ti... that present isolated half filled intermediate band and both direct and indirect band-gaps in their structures. The final objective is to produce a new photovoltaic device with a significant increment of the theoretical limiting efficiency of conventional solar cells. The promising properties of such materials encourage to develop a more sophisticated scheme in order to verify those properties. In this work we present an ab-initio study of such materials using the recently implemented Exact Exchange (EXX) framework for a localized basis set of functions. The calculations have been done using a modified version of the SIESTA code. Moreover we study the phonon dispersion diagrams and conductive coefficients of III-V alloys semiconductors TiGaX, where X= As or P. <sup>1</sup> P.Wahnón and C. Tablero, Physical Review B, 65 1651151-10 (2002).
- H-IX.04** 17:30 **SPATIALLY RESOLVED ELECTRICAL DEFECT SPECTROSCOPY WITH SCANNING PROBE MICROSCOPY TECHNIQUES**  
A. Krtschil and A. Krost, Institute of Experimental Physics, Otto-von-Guericke-University of Magdeburg, PO Box 4120, 39016 Magdeburg, Germany  
 At the example of threading dislocations in epitaxial GaN layers we present methods for spatially resolved electrical defect spectroscopy, i.e. for the determination of energy levels corresponding to these structural defects. These techniques base on scanning surface potential (SSPM) and scanning capacitance microscopy (SCM) which are sensitive to the Fermi level position and the carrier concentration with a spatial resolution in nanometer range. In extension to standard SSPM and SCM systems, we additionally equipped our microscope with a self-made temperature variable sample holder and a monochromatic irradiation facility via fiber optics for investigation of thermally and optically induced activation processes, respectively. Thus, it is possible to analyse the SSPM and SCM signals of structural defects at different temperatures between room temperature and about 70°C and to create an Arrhenius-plot according to a newly developed theoretical model which will be presented, too. Moreover, by varying the wavelength of the incident monochromatic light during the scans we can directly measure the local photo-excitation spectrum of the distinct defects. These techniques were successfully applied to dislocations in differently doped GaN layers grown by metal organic vapor phase epitaxy on sapphire substrates. As an example, we found that screw dislocations in p-type GaN are related to acceptor states with a thermal activation energy of 150-340 meV which are in good agreement with a broad band around 2.95 eV observed in optically excited SSPM scans. The results for other types of dislocations as well as the impact of the layer doping will be discussed in detail.
- H-IX.05** 17:45 **HALF-METALLIC Mn-DOPED SiGe ALLOYS: A FIRST-PRINCIPLES STUDY**  
 S. Picozzi, F. Antoniella, A. Continenza, Istituto Nazionale di Fisica della Materia INFM, Dip. Fisica, Univ. L'Aquila, 67010 Coppito (Aq), Italy, A. Moscaconte, INFM-DEMOCRITOS National Simulation Center, Trieste, Italy, and SISSA, via Beirut 2/4, 34014 Trieste, Italy, A. Debernardi and M. Peressi, INFM-DEMOCRITOS National Simulation Center, Trieste, Italy, and Dip. Fisica Teorica, Univ. Trieste, 34014 Trieste, Italy  
 First-principles pseudopotential calculations within density functional theory have been performed for SiGe alloys doped with Mn, focusing on the structural, electronic and magnetic properties as a function of the host matrix and distribution of Mn atoms. Our results show that half-metallicity, typical of most diluted magnetic semiconductors, is very sensitive to the local environment around the Mn impurity: for those systems where Mn is surrounded by Ge atoms, half-metallicity is preserved for all the considered composition range, whereas it is generally lost when Si atoms are first-nearest-neighbors of the Mn impurity. Remarkably, the calculated formation energies show that a local Ge environment around Mn impurity should be favored over a Si local environment: therefore, these systems, along with the desired half-metallicity, hold promise for spintronics applications.

**H-IX.06** 18:00

**A NOVEL TECHNIQUE FOR THE STRUCTURAL AND ENERGETIC CHARACTERIZATION OF LATTICE DEFECTS IN THE MOLECULAR DYNAMICS FRAMEWORK**

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In recent years defect engineering has become an important issue in the fabrication of integrated circuits. Point and extended defects, amorphous pockets and even full amorphous layers can be formed during the implantation stage, which have been shown to influence dopant diffusion. To use process simulators with predictive capabilities it is essential to have detailed information about the properties of such defects. The molecular dynamics (MD) simulation technique has been shown to be a good tool for this study, since the small sizes and time scales often involved usually preclude direct experimental characterization. For the structural and energetic study of defects within the MD framework some relatively complex techniques have to be used, such as the conjugated gradient method, the cooling down to 0 K, and the nudge elastic band method. We present a novel technique which allows determining defect structures and energetics directly off the MD simulation, and thus monitoring the evolution of the defect properties as a function of time and/or temperature, without the need of using the methods previously mentioned. We have applied this technique to study the structure and energetics of the self-interstitial in the Tersoff model of silicon. We have observed that the Si self-interstitial can appear in different configurations, characterized by different formation energies. We have determined the relative probability of a self-interstitial being in a given configuration, which in turn has been found to depend on temperature.

**H-IX.07** 18:15

**NOVEL NONDESTRUCTIVE APPROACH X-RAY STANDING WAVE TECHNIQUE FOR INVESTIGATION OF Zn INCORPORATION IN III-V MATERIALS**

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Zinc is the common p-type dopant used in III-V semiconductors grown by MOVPE. However the unintentional zinc diffusion during MOVPE growth is very fast compared to n-type dopant. As a result the zinc profile distribution, which is has tremendous impact on device characteristics, is hard to predict. It is generally established that the zinc diffusion occurs through an interstitial-substitutional mechanism. However, an accurate knowledge of the interstitial-to-substitutional ratio is required to minimize the unintentional zinc diffusion in the device structures. We introduce a new nondestructive approach to control incorporation of p-type impurities in the doped layers of microelectronic device structures based on X-ray Standing Wave (XSW) technique combined with SIMS and CV profiling. Activation behavior of Zn in InP epitaxial layers grown MOVPE on InP(100) substrates has been studied. The XSW experiments were performed at the A2 beamline of CHESS. Angular dependences of the Zn-K fluorescence intensity excited by the XSW field inside the InP layer for symmetrical (4 0 0) and non-complanar (1 1 1) reflections have been measured along with the In-L and P-K fluorescence and X-ray reflectivity. Analysis of the XSW data based on the dynamical diffraction theory in layered crystal structures allowed us to determine the fractions of both Zn atoms incorporated into crystal lattice and interstitial Zn. These results were in good agreement with SIMS and CV- profilometry measurements.