The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

ICTP-IAEA Workshop
Non-adiabatic dynamics and radiation damage in nuclear materials

14 – 18 November 2011

ABSTRACTS OF POSTERS

Strada Costiera 11, 34151 Trieste, Italy - Tel.+39 040 2240 111; Fax +39 040 224 163 - sci_info@ictp.it

N. Afzal - Government college, Lahore, Pakistan

Phase Transformation Studies in Unirradiated and Proton Beam Irradiated Ni-Ti alloy between 25 – 100 ^{0}C

ABSTRACT

Phase transformation characteristics of unirradiated and proton beam irradiated Ni-Ti shape memory alloy have been investigated through its stress-strain behavior in the temperature range 25 to 100 ^{0}C. The wire shaped specimens were irradiated by 2 MeV proton beam at room temperature to a flux of 10^{15}/cm^2. Tensile tests of both unirradiated and irradiated specimens were conducted using universal testing machine at 25, 50, 75 and 100 ^{0}C. The results indicate that a direct stress induced transformation from austenite to martensite occurs in unirradiated specimens at all the test temperatures. However, in the case of irradiated specimens, an additional rhombohedral phase is observed between austenite and martensite phase at 25 and 50 ^{0}C. The rhombohedral phase however disappears with increase of test temperature to 75 ^{0}C and above. The martensitic phase transformation start stress and the plateau range in irradiated specimens are found to be lower than that of the unirradiated ones. These changes are attributed to the Ni_3Ti precipitates generated during irradiation. The formation of precipitates in irradiated specimens has also been confirmed by their XRD analysis.

Modeling of electron and lattice thermodynamics in swift ion semiconductor interaction by using semi-equivalent laser irradiation

T. Apostolova, M. Ivanov,
Institute for Nuclear Research and Nuclear Energy,
72 Tzarigradsko Shaussee, 1784 Sofia, Bulgaria
C. Kozhuharov , GSI
Planckstr.1, 64291 Darmstadt, Germany

In an attempt to use Fermi–Weiszäcker–Williams model that is based on the impact parameter picture to draw a parallel between ion and laser irradiation and to model the electron excitation in a semiconductor, we come upon its restrained range of applicability, namely regime of velocities where the semiclassical approximation is valid to describe the ion material interaction process. Moreover, the method requires the introduction of a lower impact-parameter cut-off, and is then restricted to distant collisions. Furthermore, the projectile must be considered as a small perturbation due to the fact that the different frequencies contributing to the spectrum are added incoherently. Finally, an important point is that, in principle, it is valid only in the ultrarelativistic case. Not taking into account charge transfer and ionization across the band-gap, and not resorting to the equivalent photon method, we have used an idea proposed in the literature to describe the electron excitation in bulk GaAs occurring during an ion–semiconductor interaction by employing the semi- equivalent process occurring during the irradiation of the semiconductor material with two orthogonal radiation pulses. The envelopes of the radiation pulses are chosen to simulate the electric field produced by the incoming ion during the ion interaction process. Intermediate non-relativitic velocities are considered.
The relative motion of electrons is studied by using the Boltzmann scattering equation including anisotropic scattering of electrons with phonons and impurities beyond the relaxation-time approximation. Deriving an expression for the rate of energy transfer from the electrons to the lattice per unit volume and an effective lattice temperature calculated from the obtained electron distribution function, we provide an equation for the lattice temperature evolution.
High-energy tail of a Fermi-Dirac distribution is predicted and the effect of pair scattering is analyzed. Moreover, the average kinetic energy (effective electron temperature) is calculated as a function of impact parameter, projectile velocity and charge number, so that the thermodynamics of hot electrons may be investigated.

E. Aradi - University of Witwatersrand, School of Physics, Johannesburg, South Africa

Role of Radiation Effect on Boron Nitride phase Transitions

The fascinating properties of cubic boron nitride (*c*-BN) such as extreme hardness, high thermal stability, and chemical inertness make it an important material for many applications such as coatings for reactor furnaces, and in high-pressure high-frequency microelectronic device fabrication. The work herein involves the use of radiation effect by the ion implantation technique to induce a phase transformation from the soft graphitic hexagonal boron nitride (*h*-BN) to ultrahard (*c*-BN) nanoparticles. Boron lithium and helium ions, at the energy of 150 keV and fluences ranging from $1x10^{14}$ ions/cm^2 to $1x10^{16}$ ions/cm^2, were implanted into hot pressed, polycrystalline *h*-BN. Analyses using Raman Spectroscopy showed that He^+, Li^+ and B^+ led to a *h*-BN to *c*-BN phase transition, evident from the longitudinal optical (LO) Raman phonon features occurring in the implanted samples' spectra. The nature of these phonon peaks and their downshifting is explained using the spatial phonon correlation model.

PREDICTING IMPURITY DAMAGE AND SWELLING OF WATER COOLED NUCLEAR REACTOR FUEL MATRIX

A. Ayensu
Graduate School of Nuclear and allied Science, University of Ghana,
Atomic Campus, P.O Box AE 1, Kwabenya, Accra, Ghana

ABSTRACT

An important consideration in the selection of a reactor fuel material is the problem of neutron irradiation damage. Irradiation effects in fuels are much more serious because of the generation of highly energetic fission products from neutron collisions with atoms in the fuel lattice. The average range of a fission-product atom in a reactor fuel is about 0.8 μm, and within this range there may be as many as one million atoms. As a result of primary and secondary knock-on collisions, fission products may produce a damaged region in the fuel referred to as fission spikes, which are rich in vacant lattice sites, vacancies and interstitials.

Given the large number of variables that are likely to affect fission solid products and fission gas behaviour, and the variety of elementary processes considered simultaneously, a comprehensive model for fission products swelling in operating fuel rods has not yet been developed. The research seeks to investigate some of the key processes and critical parameters required to develop or set up swelling prediction equation and thereby estimate the total swelling from the contributory processes. In this respect, the occurrence and nature of swelling (of fuel element) for various burn-ups in water cooled reactor (Light-water moderated reactors; Boiling Water Reactor (BWR), Pressurized Water Reactor (PWR), and Miniature Neutron Source Reactor (MNSR)) through the generation of solid fission products, fission gas release and voids during fission were investigated.

The physical and mathematical models of irradiation swelling were analysed to develop predicting equations for swelling in the fuel matrix of water cooled reactor by quantifying the amount of solid fission products, fission gas release and void formation in correlation with fuel burnup. Mathematical formulation of neutron irradiation damage, Burnup calculations and equations for prediction of swelling were developed. The total swelling strain could be modeled based on contribution of various swelling mechanisms and process as shown in the equation;

$$\varepsilon_{fuel}^{s} = \left[\left(\frac{\Delta V}{V}\right)_{solid\ fp} + \left(\frac{\Delta V}{V}\right)_{gaseous\ fp} + \left(\frac{\Delta V}{V}\right)_{void} - \left(\frac{\Delta V}{V}\right)_{hp}\right]$$

Swelling due solid fission products was proportional to burnup, i.e. $(\Delta V/V)_{sfp} = 0.3\beta$, where the coefficient of prediction depended on fission product yields and partial volumes of the fission products. The gaseous fission product term was related to the size and concentration of fission gas bubbles. The void swelling strain was due to void formation in as fabricated fuel and irradiated fuel due to formation of vacancy clusters. The hot pressing contribution to fuel swelling was negative in as much as porosity was removed by the process. The porosity was interpreted as the cavity volume due to pores which did not contain gas, rather than the total porosity.

The total gas swelling at steady state reflecting only swelling due to fission gases was 6.2 %, while swelling due to solid fission products in oxide fuel was 0.32 % per atom percent burn up.

Abstract-SMR 2260-Joint ICTP-IAEA workshop on Radiation Damage in Nuclear Materials

50 MeV Li^{3+} ion irradiation induced modifications in structural and magnetic properties of Al^{3+}-Cr^{3+}substituted Cu-ferrites

M. C. Chhantbar[1*], U. N. Trivedi[2], S. Chattopadhyay[3], D. Jana[3], Ravikumar[4] and H. H. Joshi[5]

[1]*Shankersinh Vaghela Bapu Institute of Technology, Vasan , Gandhinagar, India*
[2]*Government Engineering College, Chandkheda, Ahmedabad, India*
[3]*Department of Physics, University of Calcutta, Kolkata, W.B. India*
[4]*Department of Material Science, National Institute of Technology,Hamirpur,India*
[5]*Department of Physics, Saurashtra University,Rajkot,India*

Email:*manisha_chhantbar@yahoo.com

50 MeV Li^{3+} ion irradiation induced changes on structural and magnetic properties of slow-cooled (SC) and quenched (Q) $CuFe_{2-2x}Al_xCr_xO_4$ (x =0.0, 0.2, 0.4 and 0.6) spinel ferrites have been studied. Polycrystalline samples were prepared by using standard double sintering ceramic technique and characterized by X-ray diffraction (XRD), Magnetization, ^{57}Fe Mössbauer Spectroscopy and AC susceptibility. The investigations on the influence of thermal history of the spinel system $CuFe_{2-2x}Al_xCr_xO_4$ showed that the slow cooled and quenched samples exhibit Jahn-Teller structural tetragonal deformation owing to the presence of Cu^{2+} and Cr^{3+} ions at octahedral sites of the spinel lattice. The study also showed that the distribution of cations is sensitive to the heat treatment of the materials. The swift heavy ion irradiation (SHII) reduces the tetragonal distortion in both the cases and significantly modifies the cation distribution in case of the quenched sample. The lattice parameters are found to decrease after the SHII in both the specimens indicated overall unit cell contraction after the SHII. The quenched samples show higher values of saturation magnetization compared to the slow-cooled ones. No remarkable change has been observed in the magnetization after the specimens subjected to the SHII. The Mössbauer parameters like linewidths and isomer shift values are influenced by both heat treatment and irradiation. Thus, the SHII affects the micro-magnetic properties like “hyperfine interactions” significantly compared to the bulk properties like saturation magnetization. The fluctuation in Curie temperature (T_c) values after the SHII in case of both the SC and Q samples are due to micro-structure disorder.

The study of the noble gas bubbles trapped in the UO_2 matrix

M. Colbert

IRSN, DPAM, SEMCA, LEC, 13115 Saint Paul lez Durance, France
CINaM, CNRS, Campus de Luminy, Case 913, 13288 Marseille Cedex 9, France

The aim of the present study is to improve the understanding at an atomic level of the behavior of Xe and Kr trapped in a UO_2 matrix.

In the first stage the variation of the elastic properties of UO_2 (bulk modulus, elastic constants, Young modulus) versus porosity is studied through atomistic simulations with semiempirical potentials. For this purpose the energy minimization is employed. In order to describe the interactions between the atoms three potentials available in the literature [1] are chosen: Basak, Morelon and Arima. A good agreement was found between the elastic properties calculated in the present atomistic simulations and those coming from the homogenization calculations [2].

The effect of the temperature on the stability of the voids (diameters ranging from 0.8 nm to 2.0 nm) is then studied through molecular dynamics simulations in the NVT and NPT statistical ensembles. Only the Basak form of potential is used to treat the interactions between the atoms. For the pressure P=0 atm and temperatures lower than 1200K the voids are stable but for T>2000K they crumble. The solid-liquid phase transition as calculated with this method occurs between 3400K and 3500K (the experimental value is T=3150K). Since the system has to cross a potential barrier associated with the creation of the solid-liquid interface, one may expect the NPT molecular dynamics simulation to give a higher temperature for this transition for the perfect UO_2. The presence of voids induces a decreasing of the solid-liquid transition temperature.

In the second stage Xe bubbles are created by filling the voids with Xe at constant temperature. This is achieved through Grand Canonical Monte Carlo simulations. Then, molecular dynamics calculations in NVT ensemble help to give an estimation of the stress induced in the UO_2 matrix by the Xe contained in the bubbles. In these simulations the Xe-Xe interactions are described by a Buckingham potential as parametrized by Brearley and MacInnes [3]. For the Xe-UO_2 interactions two kinds of potential are used: one proposed by Geng and al. [4] and another one which we have computed. Some preliminary results of this study will be presented.

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Szymon Daraszewicz and Dorothy Duffy

Department of Physics and Astronomy and London Centre for Nanotechnology,
University College London, Gower Street, London, WC1E 6BT, United Kingdom

Extending the inelastic thermal spike model for band-gap materials: a molecular dynamics study

Classical molecular dynamics (MD) simulation methods have traditionally been used to model radiation damage in materials, with some notable success. However these models are limited in their application due to their neglect of the effects of excited electrons. Radiation deposits energy in a material by interactions with both the atomic nuclei and the electrons and the relative amount of energy deposited in each subsystem depends strongly on the type of radiation. In ion irradiation, for example, the ion moving through the material loses energy to the atoms (elastic collisions) and to the electrons (inelastic collisions) and the proportion of energy lost to the electrons increases with increasing velocity. Swift heavy ions of typical energies of several MeV/u penetrate matter interacting mainly with the electrons, i.e. fall into the so-called electronic regime, where, at least in the early part of the track, electronic energy loss dominates. Modifications in the material structure caused by swift heavy ions include formation of cylindrical regions of ~10nm cross-section called latent or radiation tracks - typically of defect-rich or amorphous structure. Latent tracks are primarily observed in insulating materials, but there is also evidence that they are formed in metals at very high ion energies.

The inelastic thermal spike model (ITSM) is based on a two-temperature (TTM) approach, where two different temperatures are assigned to the atomistic and electronic systems with the incident particle depositing energy in the electronic system. The temperatures evolve via heat diffusion and the energy exchange is realised by the electron phonon coupling. ITSM has been successful in producing quantitative results, such as examining the latent track diameter dependence on stopping power. Nonetheless, we argue that the application of the ITSM, previously employed to describe swift heavy ion interaction with metals, to band-gap materials is limited, since it does not treat the evolution of carriers explicitly. I discuss the extended thermal spike model [1], which incorporates an additional conservation equation for carrier density.

A continuum model cannot elucidate the structure of ion tracks at an atomistic level; it can only be used to calculate the region of the material that has exceeded the lattice temperature at some point during the simulation. Furthermore, continuum models neglect superheating, lattice straining and the emission of shock waves. Therefore, a predictive and a reliable modelling framework providing atomistic-level description of the transient non-equilibrium processes induced by swift heavy ions is required to incorporate the effects of electronic excitations at the simulation level of molecular dynamics.

The poster will describe the coupling of the extended inelastic thermal spike model to MD via a modified (scaled to the electronic temperature) Langevin thermostat – a mechanism for the electronic energy transfer to the atomistic lattice. It will compare and contrast the results obtained using the extended model with those obtained using the standard TTM-MD model developed for metals [2,3]. The results for swift heavy ion irradiation of an exemplar semiconductor - Silicon - allow us to determine the transient phononic and electronic systems temperature in an ion irradiated

material and to describe the phase change processes, which elucidate the mechanisms of latent track creation.

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Zr-H Study using Tight-Binding Formalism

A. Dufresne - Centre Interdisciplinaire de Nanoscience de Marseille, France

In the context of zirconium hydrides study using atomistic modelling, this poster will describe what have been done up to now using the tight-binding approach. The first part of the results is the parametrization of zirconium, which was not straightforward as expected. In fact, the tabulated values show strong discrepancies with the data available in the litterature for the band structure. A new parametrization was thus derived for pure zirconium.

The accuracy of tight-binding methods depends on two parameters: the amount of neighbouring atoms taken into account in the model and the number of atomic orbitals modeled. To determine the modelling precision we need, we compare the energy of fcc with the one of hcp structure, while filling the atomic orbitals. The favourable/predicted structure, for a certain electronic filling, is then compared with what is found in the nature (comparison with the periodic table). These comparisons give us the level of precision we need to obtain accurate results.

The second part is the development of a methodology to fit the potential. Two terms have to be clarified: the repulsive part of the potential, which is not in the framework of the tight-binding, and the potential dependency to the inter-atomic distance. The parameters are adjusted using the conditions for the equilibrium case and the Birch-Murnaghan equation of state. This methodology is now considered as being established and ready to be used to derive more accurate parameters during this PhD.

In the third and last part, some insights on the ZrH2 structure are given. The results are preliminary ones and further work is required for the H-H interactions parametrization.

Molecular dynamics simulation of atomic structure in the vicinity of point defects in FCC and BCC metals

Alexander Germanov, Irina Valikova, Andrei Nazarov
SSC RF "Institute for Theoretical and Experimental Physics",
Bolshaya Cheremushkinskaya, 25, 117218 Moscow Russia
a_germanov@yahoo.com

Behavior of structural materials under extreme conditions is generally defined by point defects. Many features of point defects such as vacancy relaxation volumes are defined by atomic structure in their vicinity. For the theoretical description of temperature dependence knowledge of atomic structure at finite temperatures is needed. Thus the aim of our work is a detailed study of temperature-defined changes of atomic structure surrounding vacancies and self-interstitials, as the changes in structure do affect these features. In this work Molecular Dynamics (MD) is applied to determine atomic structure in the vicinity of point defects at different temperatures. This enables the calculation of temperature dependence of these features, based on atomic structure obtained via Molecular Statics (MS) [1].

Atomic structure of different FCC and BCC metals is studied by MD using velocity Verlet algorithm. The computational cell has free-boundary conditions and a spherical shape. To decrease surface effects up to 40000 atoms are used. Various pair and many-body potentials for Al, Cu, Ni, Fe, V are used. Coordinates of the central atom and its neighbors are averaged during a simulation, which time (400 and up to 1000 atomic vibrations) is considered sufficient enough. We use the obtained mean positions of atoms to directly calculate interatomic distances. Thus as the result of calculation we get the temperature dependence of lattice parameters. At the next step in the system containing monovacancy we obtain distances between atoms inside its six nearest lattice shells in a system with the point defect. As a result of our simulation we found that distances for the nearest neighbor (NN) shells in a defect system starting from the forth NN shell change with the temperature the same way as the lattice parameter in perfect lattice. Thus we can state, that the ratio of relaxation volume to the atomic volume at the same temperature remain constant. This result allows to calculate the temperature dependence of the relaxation volume for different metals in a simple way.

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Electronic Stopping Power of Ionic Crystals from Small Clusters Models

P. Gonzalez-Morelos[1], A. Arnau[1,2,3], D. Sánchez-Portal[1,2].
[1] *Donostia International Physics Center, Paseo Manuel de Lardizabal 4, 20018 San Sebastian, Spain*
[2] *Centro de Física de Materiales, Centro Mixto CSIC-UPV/EHU, Apartado 1072, 20080 San Sebastian, Spain*
[3] *Departamento de Física de Materiales, Facultad de Química, Apartado 1072, 20080 San Sebastian, Spain*

Abstract

The electronic stopping power of slow ions in materials with large band gaps, such as LiF, shows a velocity threshold. In this work, we analyze this behaviour for proton projectiles moving through different ionic crystals. These are described by small clusters of the AB compounds where, A=Li,Na, K and B= F, Cl, Br. Our results show that this simple model captures the essential features of the stopping process, as far as the threshold behaviour is concerned. We use time dependent density functional theory as implemented in SIESTA and a simple two-level model that permits understand the physics in the system. We find a direct relation between the width of the energy band gaps and threshold velocity of the stopping power, although the shape and strength of the interaction potential felt by the moving particle as it travels through the medium with constant velocity also plays a role.

Thermal and Mechanical properties of Thorium from First Principles and Lattice Inversion Method

Sebastián Jaroszewicz[1a], Hugo Mosca[1b] , Jorge E. Garcés[2]

[1]Centro Atómico Constituyentes, CNEA, Buenos Aires, Argentina.
[2] Centro Atómico Bariloche – CNEA, S.C. de Bariloche, Argentina.
[1a] jaroszew@tandar.cnea.gov.ar, [1b] hmosca@.cnea.gov.ar, [2] garces@cab.cnea.gov.ar

The structural and thermal properties of fcc thorium have been calculated through a free-parameter pair potential deduced by computing only the cohesive energy from first principles calculations, the Chen-Mobius lattice inversion method and the Debye-Gruneisen model. The computed elastic constants, shear modulus, Young's modulus, Poisson's ratio and termal properties of fcc Th are found to be in a very good agreement with experiments and previous theoretical results. The interatomic pair potential derived in this work will be used as a starting point to develop a n-body free-parameter potential suitable to be used in molecular dynamic calculations for predicting the microstructure, thermal properties and radiation damage in Generation IV nuclear reactors based on the Th-cycle.

3D Thermal Spike Model: Ion Shaping Application

V. Khomenkov, Ch. Dufour
CIMAP (UMR CNRS, CEA, ENSICAEN, UCBN)

Irradiation with swift heavy ions (SHI) is powerful technique used to modify the material properties.
To describe SHI dissipation and material state modification we developed 3D thermal spike model, which allows simulation of several material composition of any geometry.
In particular, we studied magnetostrictive multilayers interdiffusion. Combination of layers with different thermal properties increases the irradiation effect.
Another application is elongation of metallic nanoparticles (NP) confined within an amorphous matrix due to SHI. Dependence of molten and vaporized phase on NP shape and size has been studied for central and non-central SHI impact. Performed simulations explain surface melting effect which can cause NP shaping.

Spin-Lattice Dynamics for Iron and Magnetic Alloys

Pui-Wai Ma[1], S. L. Dudarev[1], C. H. Woo[2] and Terry Haohua Wen[2]
[1]EURATOM/CCFE Fusion Association, Culham Centre for Fusion Energy, Abingdon, Oxfordshire OX14 3DB, United Kingdom
[2]Department of Electronic and Information Engineering, The Hong Kong Polytechnic University, Hong Kong, SAR, China

Molecular dynamics (MD) is a well known numerical method for simulating finite temperature effects and non-equilibrium dynamics of atoms. Spin-lattice dynamics (SLD) [1] extends MD to magnetic materials, which treats both magnetic and atomic degrees of freedom. It allows one to consider the correlated dynamics of magnetic moments (spins) and atoms.

Temperatures for the spin and lattice degrees of freedom are introduced using Langevin thermostats. Temperature-dependent magnetism is shown to have a significant effect on mechanical properties of iron and iron-based alloys [1, 2 and ref. therein]. Furthermore, we are able to derive an explicit formula for the dynamic spin temperature [3], which is analogous to the Dalton equation for the lattice temperature expressed in terms of the kinetic energy of atoms. The fact that spin temperature can be defined and evaluated for an arbitrary configuration of magnetic moments makes it possible to apply SLD to modeling a broad range of non-equilibrium processes involving magnetic excitations.

In order to perform large scale simulations involving millions of atoms and spins, we developed numerically efficient parallel programming technique [4] and numerical integration algorithms [5]. They are based on the Suzuki-Trotter decomposition of spin evolution operators, and have been proven to accumulate little numerical error in the limit of long time scales, due to their symplectic nature. The computer code for SLD is now available in both CPU/C++ and GPU/CUDA implementations.

The application of SLD is not limited to perfect crystals, but is also applicable to the dynamics of defects. We simulated self-diffusion in iron

using both MD and SLD [6]. SLD simulations show a visible change of the self-diffusion coefficient near the Curie temperature, similar to that observed in experiment, whereas conventional MD simulations show no feature in the Arrhenius plot that can be associated with the Curie temperature. This confirms that magnetism affects diffusion of vacancies in iron even at high temperatures approaching 770°C.

This work, part-funded by the European Communities under the contract of Association between EURATOM and CCFE, was carried out within the framework of the European Fusion Development Agreement. The views and opinions expressed herein do not necessarily reflect those of the European Commission. This work was also part-funded by the RCUK Energy Programme under grant EP/I501045, and Grant 532008 from the Research Grant Council of Hong Kong.

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Charge localization in Co-doped Ceria with oxygen vacancies

G. E. Murgida[1,2,3], V. Vildosola[1,2], V. Ferrari[1,2] and A. M. Llois[1,2,3]

[1]*Centro Atómico Constituyentes, GIyANN, CNEA, San Martín, Buenos Aires, Argentina*
[2]*Consejo Nacional de Investigaciones Científicas y Técnicas, Buenos Aires, Argentina*
[3]*Departamento de Física Juan José Giambiagi, FCEyN, UBA, Buenos Aires, Argentina*

The search and development of novel materials, ferromagnetic beyond room temperature, is currently a subject of intense work with the driving force of its potential technological applications. In this regard, Cerium oxide with diluted magnetic impurities is a natural candidate for spintronics as it offers a good integrability with the current electronic devices. However, this material still poses several questions being the main one to find a consensed explanation for the observed room temperature ferromagnetism.

There is experimental evidence supporting the idea that the free electrons left behind by oxygen vacancies localize themselves in specific Cobalt and Cerium atoms, changing their oxidation states (Co4+ -> Co2+ and Ce4+ -> Ce3+, respectively) and turning the Cerium atoms into magnetic ones. The study of this charge localization is crucial to aproach an understanding of the magnetic properties in these materials.

Using the framework of the Density Functional Theory, we evaluate the relative stability for different configurations of vacancies in Co doped Ceria and we show that the vacancies tend to locate close to the Co impurities. In addition, we address the issue of the charge localization that takes place due to desoxygenation processes, finding that the excess electrons reside at Ce atoms which are next nearest neighbours of the vacancy sites.

Application of maximally localized Wannier functions for understanding magnetic and ferroelectric materials.

Matías Núñez

Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET). Avda. Rivadavia 1917, CP 1033 AAJ, Buenos Aires, Argentina

Centro Atomico Bariloche, U-A Tecnologia de Materiales y Dispositivos, Division Materiales Nucleares, Av.E.Bustillo 9500 - (8400) - S. C. de Bariloche - (RN). Argentina

Instituto de Ciencias Basicas,Universidad Nacional de Cuyo Mendoza,5500 Mendoza,ARGENTINA

We show two examples of the use of density functional theory and maximally localized Wannier functions for understanding the physical properties of i) a stereotypical ferroelectric material (BaTiO3) and ii) a metastable magnetic material (CrSe2). For the case of BaTiO we have elucidated the nanoscale organization and local polarization of the material as a thin film between metallic contacts. The profile of the local polarization for different film thicknesses unveils a peculiar spatial pattern of atomic layers with uncompensated dipoles in what was originally thought to be a ferroelectric domain. This effectively *ferrielectric* behavior is induced by the dominant roles of the interfaces at such reduced dimensionality and can be interpreted using a simple classical model where the latter are explicitly taken into account. For the case of CrSe2 we calculated the band structure using two different exchange correlations functionals and analyzed its influence on the associated maximally localized Wannier functions.

Ab-initio studies of diffusion-related point defects in Ti and Zr

Roberto C. Pasianot(1,2,3)

(1) Dto. Materiales, CNEA-CAC
Avda. Gral. Paz 1499, 1650 San MartÌn
ARGENTINA
(2) CONICET
(3) Instituto Sabato, UNSAM/CNEA

Electronic structure calculations, carried out with the SIESTA code (pseudopotentials coupled with numerical atomic orbitals), are performed in order to study point defects structure relevant to diffusion in hcp Zr and Ti. This includes the vacancy and the ultra-fast diffuser Fe impurity, always present in commercial samples, and shown long ago to dramatically enhance self-diffusion, even if present as a trace element.
Within the framework of transition state theory, the difficulties to obtaining quantitative agreement with measured diffusivities are highlighted. The latter stem from both, entropic and energetic contributions.

Linear-scaling first-principles calculations of point defects in the MgO ceramic

Oscar Paz (1), Alberto Garcia (1) and Pablo Ordejon (2)

Affiliations:
(1) Institut de Ciencia de Materials de Barcelona (ICMAB-CSIC), Campus UAB, E-08193 Bellaterra, Spain
(2) Centre d'Investigacio en Nanociencia i Nanotecnologia (CIN2-CSIC), Campus UAB, E-08193 Bellaterra, Spain

We have used the order-N functional minimization methods implemented in the SIESTA code to perform ab initio supercell computations of native point defects in bulk magnesium oxide. We investigate the energetics, structural and electronic properties of a vacancy and interstitial atom with different charge states, and of several atomic arrangements of neutral interstitial pairs and Schottky defects.
For the isolated defects, we find minimum formation energies corresponding to the full formal charge state, except for the O interstitial and vacancy cases showing charge transition levels (0/2-) and (2+/0) at electron dopings around 4 and 2.5 eV respectively.
Defect pair arrangements of 1st-, 2nd- and 3rd-neighbor configurations for divacancies and up to 5th-neighbor geometries for di-interstitials were evaluated. We obtain an overall lowest formation energy for the nearest neighbor configuration in both defect types.
Interestingly, interstitial atoms in the 2nd- and 5th-neighbor configurations move towards lattice sites of same species during relaxation, displacing lattice atoms to otherwise form a 1st-neighbor di-interstitial defect in the supercell.
Computationally, the O(N) approach yields accurate results (~0.01 eV/atom) even at relatively short localization radii (~10 Bohr), which will make it the method of choice for studies of larger defect aggregates.

ION BEAM IRRADIATION INDUCED MIXING AND CHEMICAL MODIFICATIONS AT THE METAL/POLYMER INTERFACE

Abstract: - The interface mixing in Ni/Teflon and Au/Teflon systems, have been investigated as a function of the morphological and chemical modifications induced by 120 MeV Au ions with fluences ranging from $1x10^{12}$ to $5x10^{13}$ ions/cm^2. Rutherford Backscattering Spectroscopy (RBS) and Atomic Force Microscopy (AFM) were used to analyze atomic transport at the interface and the resulting roughness and morphology changes at the surface of the samples. Modifications are observed in both the systems, Ni/Teflon system exhibits strong ion beam induced interface mixing, as compared to Au/Teflon system as analyzed by RUMP simulation code. It is found that the observed mixing is not due to the surface roughness and found to be driven by a solid-state chemical reaction. The changes in the chemical structure at the interface were studied by Fourier Transform Infrared (FTIR). The formation of new bonds (Ni-F) as a result of mixing, chain scissoring and cross-linking of the normal chain (-CF=CF_2, -CF=C<) by irradiation is confirmed by FTIR. The role of swift heavy ion (SHI) in mixing mechanism of the metal/polymer systems has been discussed.

* author: Jai Prakash, Department of Chemistry, M.M.H.(P.G).College, Ghaziabad -India. Phone No. +91-9910533582, E-mail address: jpg1983@gmail.com

Nonlinear evolution of creep under irradiation

P. Selyshchev
University of Pretoria, Department of Physics

The problem of material's creep inside reactor plants, where in spite of force and thermal factors, the important role plays continual irradiation, it keeps actual in nowadays in condition of intensive development of nuclear power energy.

In this papers there is theoretical research, which illustrate non-linear characteristics (bend and breaks) of the dose-depend creep's speed of impurity materials under irradiation. These characteristics have been seen experimentally over and over again.

The dynamics of transfer creep of pure materials is studied in [1]. The analysis of the influence on the creep the presence of impurity atoms, which are always in the real metals, is an accent here.

The investigation was taken within the framework of the model "slip-creep over". It was supposed that the speed of creep is proportionate the module of difference of flux of interstitial atoms and vacancies. The part of admixture is defined in connection of free vacancies and interstitial atoms in slow-moving complex.

During the work it found that depending on irradiation's conditions and behaviours of the irradiated specimen, it can be realized one or two stationary creep's states. The concrete stationary creep's state is defined by reference states of the sample. The creep's speed tend to the stationary value monotonically or passing the extreme. In the moment, when the flux on the vacancy's location and interstitial atoms is becoming equal, then the creep's speed will be zero. It brings to appearance of breaks of the dose-depended creep.

The change of impurity concentration is reduced to the modification of stationary value of the creep's speed at the concentration of the defect. But it doesn't result to the qualitative modification of the dynamics of non-stationary creep. The phase portraits are deformating, but there are topologically similar. All qualitative effects (breaks, bend, hysteresis, collapse of creep's speed) are particular to the creep in irradiated materials, it has a place as in pure, as in materials with an admixture.

Acquired results allow to forecast conduct of materials and to determine optimal conditions of their exploitation.

1. Selyshchev P.A. Samoorganizatsia v radiatsionnoi fizike// Kiev: Aspect poligraf, 2004, p.240

Radiation-induced diffusion of interstitial atoms under heavy ion irradiation.

A.I. Ryazanov, E.V. Semenov, E.V. Metelkin

National Research Center "Kurchatov Institute", 123182, Moscow, Kurchatov Sq.1, Russia

Kinetic energy of fast heavy charged particles with energies of 1 MeV/nucleon during their slowing down in materials by interaction with atomic nuclei and electrons is transferred to the electronic subsystem in general and only a small part is transfered to the ionic subsystem. Knocked out electrons (δ - electrons) of the target atoms by heavy charged particle can have a significant influence on various processes occurring during the formation of areas of radiation damage in different materials. This model is based on the solution of Boltzmann kinetic equation to calculate the distribution function of slowing down δ - electrons produced by impact of heavy charged particle. Then the effect of electrons in the process of radiation-induced diffusion of interstitials is calculated on the basis of this solution. To do this, the the collision frequency of electrons accompanied by interstitial knocking and producing its movement through the crystal is determined using the found distribution function. Both relativistic and nonrelativistic cases are considered. An analytical solution is obtained for diffusion coefficient of interstitials atoms in nonrelativistic case. It's shown that taking account of the scattered radiation increases the frequency of collisions accompanied by knocking interstitial atom and consequently the coefficient of radiation-induced diffusion by about two orders of magnitude. The results are analyzed and compared with results of other authors.

Swift heavy ion induced modifications of Ag/a-C nanocomposite thin film

R. Singhal[1], D. C. Agarwal[1], D. Kabiraj[1], F. Singh[1], J. C. Pivin[2], A. K. Chawla[3], R. Chandra[3] and D. K. Avasthi[1]

[1]Inter University Accelerator Centre, Post Box No. 10502, New Delhi 110067, India
[2]CSNSM, IN2P3-CNRS, Batiment 108, F-91405 Orsay Campus, France
[3]Institute Instrumentation Centre, Indian Institute of Technology Roorkee, Roorkee 247667, India

Abstract

Metallic nanoparticles (NPs) exhibit unusual physical and chemical properties compared to those of bulk solid material due to increased surface to volume ratio. Therefore the synthesis of NPs has attracted a great deal of attention in recent years. NPs of noble metals are interesting especially due to their surface plasmon resonance (SPR) which occurs in visible region [1]. The Ag NPs have been synthesized in various matrices like SiO_2, Al_2O_3, ZnO, polymers etc [2]. However, the sensitivity of silver NPs to oxidation, especially when embedded in oxide matrices, is a problem of major concern. Carbon matrix is interesting in this respect for isolating the particles in non oxidizing environment. The Ag(17%)/a-C nanocomposite films, synthesized by atom beam sputtering setup [3] at IUAC New Delhi, were irradiated by 120 MeV Ag ions at different fluences. A blue shift of ~ 26 nm was observed in SPR wavelength of Ag NPs at a fluence of 3 $x10^{13}$ ions/cm^2. Transmission electron microscopy confirmed the growth of Ag NPs with ion irradiation. Raman spectroscopy was performed on the pristine and irradiated samples to understand this blue shift. An increase in the intensity of D band and shift of G band to higher wavenumber were observed with increasing fluence, which reveals the ordering of a-C with ion fluence.

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Analog of Rabi oscillations in resonant electron-ion systems

Lorenzo Stella, Rafael P. Miranda, Andrew P. Horsfield, and Andrew J. Fisher

Quantum coherence between electron and ion dynamics, observed in organic semiconductors by means of ultrafast spectroscopy, is the object of recent theoretical and computational studies. To simulate this kind of quantum coherent dynamics, we have introduced in a previous article [L. Stella, M. Meister, A. J. Fisher, and A. P. Horsfield, J. Chem. Phys. 127, 214104 (2007)]10.1063/1.2801537 an improved computational scheme based on Correlated Electron-Ion Dynamics (CEID). In this article, we provide a generalization of that scheme to model several ionic degrees of freedom and many-body electronic states. To illustrate the capability of this extended CEID, we study a model system which displays the electron-ion analog of the Rabi oscillations. Finally, we discuss convergence and scaling properties of the extended CEID along with its applicability to more realistic problems.

Theoretical modeling of shock wave formation and propagation in LHC collimator materials.

A.I. Ryazanov, A.V.Stepakov
National Research Center "Kurchatov Institute", 123182, Moscow, Kurchatov Sq.1, Russia

This study is oriented on the theoretical modeling of shock wave formation and propagation due to an interaction of 450 GeV proton beam with LHC collimator material (copper). The developed theoretical model of the shock wave propagation in irradiated materials is based on a so-called hydrodynamic approach produced by Ya.B.Zeldovich. The transmission of energy from the same high-energy protons is described here by the "thermal spike" theoretical model. For the solving of this problem it was developed the numerical algorithm based on the Godunov's scheme. This computer program solves a nonlinear system of differential equations, taking into account the conservation laws form with using of Eulerian variables, in which temperature, pressure and specific internal energy are calculated for ionic and electronic subsystems separately using nuclear data base FLUKA. The results of numerical simulations are presented here first for copper as graphs, which demonstrate the behavior of main physical parameters of irradiated materials (pressure (stress), electronic and ionic temperatures, density) in real space and time up to 500 bunches (14500 nanoseconds).

Ion guiding through nanocapillaries in PC foils

Jianrong Sun*, Yuyu Wang, Zhiguang Wang, Guoqing Xiao

Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou 730000, China

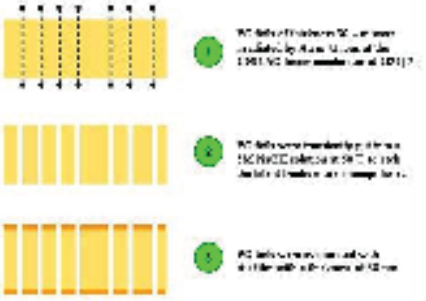
* Corresponding Author. E-mail address: sunjr@impcas.ac.cn

Abstract

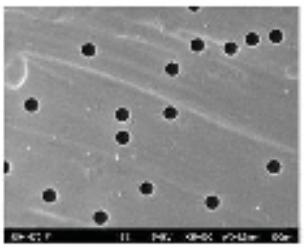
Nanocapillaries through insulating foils have received considerable interest as a target for beams of slow highly charged ions (HCI). Transmission of projectiles in their initial charge state has been measured for angles of incidence larger than the geometrical opening angle. Ions are guided along the capillary axis and do not closely interact with the inner walls [1]. New developments include e.g. polyethylene terephthalate (PET) [1, 2], SiO_2 [3], Al_2O_3 [4], polycarbonate (PC) [5] capillaries. Meanwhile, computer simulations have been carried out in consistency with the experimental results [6].

We have measured the fraction of the ions transmitted through the nanocapillaries with their initial charge state for Xe^{26+} and Xe^{27+} ions impact on a polycarbonate (PC) foil with a thickness of 30 μm and a diameters of 150nm. Moreover, we tested the influences of charged inside-walls, charge state and incident current of ions through capillaries. These results are discussed within the models for the guiding effect.

Preparing capillaries

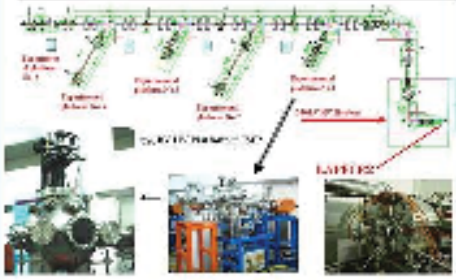


SEM image of the PC capillary with a diameter of 150 nm

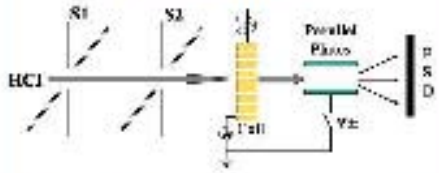


Experiments

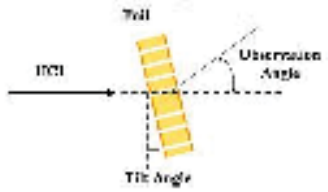
320 kV ECRIS Platform for HCI Beams in Heavy Ion Research Facility in Lanzhou (HIRFL)



Experimental setup

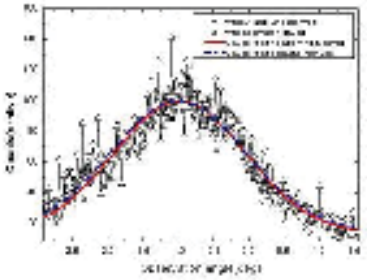


Definitions of the tilt angle and observation angle



Fraction of the initial charge state in the final charge state distribution

200 keV Xe^{26+}, current density ~0.08 nA/mm²



The majority of the transmitted ions have retained their initial charge state, the fraction is more than 97%

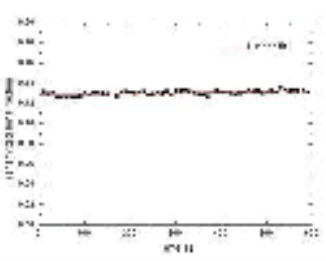
Angular distribution of the transmitted ion fraction

After determining the fraction of the transmitted ions remaining in their initial charge state, the PSD was replaced by a Faraday Cup to measure the transmitted ion fraction.

During the measurement, it is important to ensure that the intensity of the transmitted ions has reached equilibrium condition and that this condition can be kept in the whole experiment.

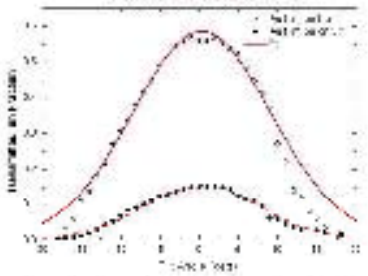
Time dependence of the transmitted ion fraction

0.5 nA/mm² 40 keV Xe^{27+} ions impact on f-h-PC



Influence of the charged inside-walls on the ion transmission

0.5 nA/mm² 40 keV Xe^{27+} ions impact on 150 nm f-h-PC and f-PC

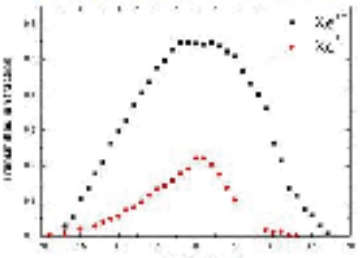


The tilt angle dependence of the transmitted ion fraction was fitted by a function of the form:

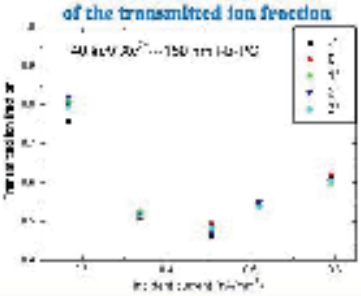
$$f(\varphi) = f(0)\, e^{-(\varphi/\beta)^2}$$

where the inverse of the parameter β is a measure of the guiding ability and φ is the tilt angle.

Comparison between Xe^{27+} and Xe^{26+}



Incident current dependence of the transmitted ion fraction



Conclusions

We have measured the transmitted ion fraction and the critical tilt angle for Xe^{26+} and Xe^{27+} ions impact on PC capillaries. Compared with f-h-PC, the maximum transmitted ion fraction of PC is nearly 4 times smaller and the critical tilt angle of f-PC is also slightly decreased. Moreover, comparison the transmitted ion fraction between Xe^{27+} and Xe^{26+} for the higher charge state the transmitted ion fraction is smaller for f-h-PC. Besides, with the increase of the incident current, the transmitted ion fraction decreases drastically and then increases slowly. A turning point appears between 0.5 nA/mm² and 0.8 nA/mm².

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Acknowledgements

This work was supported by the National Natural Science Foundation of China (Grant Nos. 10979010, 10979029) and the Major State Basic Research Development Program of China (973 Program, Grant No. 2010CB832905).