Invited Presentations

I1

Dynamic Simulation of Collision Cascades and Thermal Spikes in Ceramics

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keywords: *Fundamentals and Modeling; Defects Production; Oxides: Ceramics*

Classical molecular dynamics simulations have been employed to examine defect production by high-energy collision cascades in ZrO_2, UO_2, $Gd_2Ti_2O_7$, $Gd_2Zr_2O_7$ and $ZrSiO_4$. These atomistic simulations provide details of the nature and size distribution of defect clusters produced in collision cascades. In addition, electronic energy loss processes in these materials have been modeled in the form of thermal spikes to study the details of track formation and track structure. The results of our track simulations are in reasonable agreement with experimental observations of track characteristics. Track diameters were found to depend on composition and electronic energy loss, which affect both the maximum radial extent of the track formation process and the dynamic recovery processes that determine the final track radius. These results will be discussed in light of experimental observations.

I2

Response of $A_2B_2O_7$ Pyrochlore to Irradiation and Pressure: a New High-Pressure Phase

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keywords: *Swift-Heavy Ions; High Pressure; Ceramics; Phase transformations*

Pyrochlore, $A_2B_2O_7$, exhibits a variety of properties that find application in a number of different technologies, from electrolytes in solid oxide fuel cells to actinide-bearing compositions that are used as nuclear waste forms and inert matrix fuels. Ion beam irradiations (energy: GeV) have been used to systematically modify the $Gd_2Zr_{2-x}Ti_xO_7$ binary at the nanoscale by radiation-induced phase transitions that include the crystalline-to-amorphous transition and an order-disorder structural transformation to a defect-fluorite structure. Synchrotron XRD, Raman spectroscopy, and TEM provide a consistent understanding of these results of the pure electronic excitation and ionization caused by the heavy ions. When pressure is included as an additional parameter, the response of the pyrochlore structure to these extreme conditions differs significantly. We show that the combination of relativistic heavy ions and high pressure can result in the formation of a new metastable pyrochlore phase, which cannot be obtained by irradiation or pressure applied separately. TEM and quantum mechanical calculations suggest that these novel structural modifications are caused by the formation of nanocrystals and the related modified energetics of the material.

I3

Study of defects in implanted silica glass by Depth Profile Positron Annihilation Spectroscopy

Roberto Brusa, *University of Trento, IT*

keywords: *Defect profiling in silica; Positron Annihilation Spectroscopy*

Positron Annihilation Spectroscopy (PAS), carried out with pulsed and continuous slow positron beams, allows to depth profile samples from few nanometer to 3 micron depth. Open volume defect distributions can be measured and the defects can be characterized in size (from vacancies to cavities of few nanomerters). Moreover, the neighbor atoms or the decoration of the open volume defects can be probed.

Four PAS techniques (Doppler Broadening Spectroscopy, Coincidence Doppler Broadening Spectroscopy, Lifetime Spectroscopy, three gammas positronium spectroscopy) will be presented.

Examples of PAS measurements will be selected to show the potentiality of the technique in studying and characterizing silica glass implanted with different ions at different fluences.

I4

Ion tracks and density fluctuations in swift heavy ion irradiated silica

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keywords: *Swift-Heavy Ions; Small Angle X-ray Scattering; Ion Tracks; Silica*

Swift heavy ion irradiation (SHI) of a solid can produce narrow trails of permanent damage along the ion paths, so called ion tracks. These nanometric objects are interesting in a variety of disciplines including materials science and engineering, nuclear physics, geochronology, archaeology, and interplanetary science. Though average structural properties of ion tracks can often be inferred from macroscopic measurements, the inner track structure remains extremely difficult to retrieve due to the lack of sufficient contrast inherent with most techniques. Small angle x-ray scattering (SAXS) provides an interesting tool to study structural details of ion tracks. Using a combination of synchrotron SAXS, molecular dynamics simulations and calculations using a transient thermal spike model, we have recently observed a fine structure in the radial density distribution of ion tracks in amorphous silica comprising a cylindrical core-shell configuration with a lower density core and a higher density shell as compared to un-irradiated material [1]. This structure is consistent with a frozen-in pressure wave originating from the centre of the track. Irradiation of the material with high ion fluences, i.e. where the material experiences multiple coverage with ion tracks, leads to an in-homogeneous steady state of density fluctuations consistent with an ion track “annihilation process”. The presentation will give an overview of the utilization of synchrotron SAXS for the study of SHI tracks and present our recent results obtained on tracks in insulating materials with a focus on amorphous silica.

[1] P. Kluth *et al.*, Phys. Rev. Lett.101 (2008) 175503

I5

Optical waveguides in Nd:YAG transparent ceramics produced by ion implantation

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keywords: *Nd:YAG Ceramics; Ion Implantation; Optical Waveguides*

Optical waveguides can confine light propagation to small dimensions of order of several microns, in which related properties of the substrate materials could be considerably improved with respect to those of the corresponding bulks. In the latest decade, highly transparent polycrystalline Nd:YAG ceramics have shown their strong potentials as excellent gain media for various high-power continuous-wave or pulsed solid state lasers. Particularly, the intriguing advantages of Nd:YAG ceramics over single crystals are multiple: larger size with same doping levels and lower costs, higher resistance to thermal shocks, and possibility for large-size multilayers for multifunctional lasers. The manufacture of active waveguides, maintaining the original or enhanced spectroscopic properties, on laser materials is one significant first step towards compact and cost-effective integrated lasers. For this purpose, the combination of excellent laser performance of Nd:YAG ceramics and waveguide technology is one promising solution to realization of high-power integrated lasers with stable output. In this work, we report on the fabrication of Nd:YAG ceramic waveguides by applying implantations of either protons or oxygen ions. The waveguides are with relatively losses no more than ~2dB/cm after annealing at 260°C in air. The reconstructed refractive index profiles of the waveguides are typical “barrier + well” type distribution. The microluminescence investigation shows that the fluorescence emissions of Nd^{3+} ions are pretty well preserved in the waveguide regions with respect to the bulk, implying further realization of Nd:YAG ceramic integrated lasers by using the ion implanted waveguides as gain media.

I6

Ion tracks in silica for engineering the embedded nanoparticles

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keywords: *Swift-Heavy Ions; nanostructures in insulators*

Swift heavy ions have unique feature of crating ion tracks in insulators of dimension from a few nm to about 10 nm. This particular feature of the swift heavy ions is used to engineer the size and shape of the particles embedded in silica matrix. On the basis of several experiments, it is shown that the embedded particles either grow in size or reduce in size, if they are smaller than the ion track size. The shape transformation from spherical to elongated along the beam direction occurs, when the particle size is larger than the ion track in silica. Results of these experiments on Au particles embedded in silica matrix will be discussed.

I7

Nano-patterned Ion Implantation into Insulators with Porous Alumina Masks

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keywords: *Oxides; Nanostructures in Insulators; Patterning*

Heavy-ion patterned irradiation is promising to directly control nanostructures in insulators for optical waveguides or plasmonic/photonic devices. Although the ion irradiation has merits such as good spatial controllability, one of the most serious concerns is radiation damage. In order to conduct the nano-patterned irradiation, the key is to prepare nano-featured stencil masks with radiation resistance. Usage of self-organized porous alumina is an attractive option to obtain regular nanopore arrays over a wide area. Since the stencil mask is subjected to high-energy ion irradiation, dimensional stability of the nanopores against the ion irradiation is requisite. Radiation-induced effects of the substrate insulators should be studied as well.

In this paper, we study radiation effects of insulators, both the porous alumina masks and the SiO_2 substrates. Negative Cu ions of 60 keV were irradiated into either amorphous or crystalline SiO_2 by using an anodic porous alumina mask. The usage of negative ions, without surface charging, is important to avoid Coulomb repulsion. The porous alumina masks had radiation tolerance up to an ion fluence of 1×10^{16} ions/cm^2 and demonstrated successful patterned implantation of nano-sized periodic spots, down to 100 nm in diameter. Above the tolerant fluence, the nanopores became narrower with increasing ion fluence. The cross-section of the alumina side-wall showed significant swelling of a mushroom shape near the beam entry. The lateral swelling becomes pronounced due to the absence of lateral constraints. The irradiation into the crystalline SiO_2 substrate demonstrated the patterned swelling. The pore-size dependence of swelling showed that the swelling height increased with decreasing the pore size. In this case, the lateral constraint in the substrate led to the increase in swelling. As the feature size becomes smaller down to a submicron scale, the radiation effects characteristic in a nano-scale emerge in these insulators.

I8

Radiation Tolerance of Fluorite-structured Oxides Submitted to Swift Ion Irradiation

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keywords: *Binary metal oxides; fluorite-type structure; radiation tolerance*

Binary metal oxides possessing the fluorite-type crystal structure are well known to be amongst the most radiation tolerant materials. Such a crucial property led to the early use of uranium dioxide as nuclear fuel and to the recent development of the so-called inert matrix fuels for in-reactor actinide transmutation (actinide cations partially substitute regular cations). Whilst radiation-induced structural modifications due to low-energy ions, i.e. in the nuclear stopping regime, were extensively investigated, specific irradiation effects due to electronic stopping of penetrating ions are still much debated. This work focuses on the radiation stability of fluorite-type canonical systems, namely urania and yttria-stabilized cubic zirconia single crystals, irradiated with high-energy heavy ions. Several analytical techniques, which probe the material at various depth scales, were used (e.g. RBS in the channelling mode, XRD, TEM, AFM) to gain information on the nature of the created damage (depth distribution, disordering kinetics, occurrence of structural and micro-structural modifications) at fluences ranging from the formation of isolated ion tracks up to complete surface recovery. Damage formation is interpreted in terms of the huge electronic excitations created in the wake of the ion's path. The melting of the material in the core of tracks, via a thermal spike mechanism, leads to the creation of large hillocks at the surface of the crystals. The overlapping of ion tracks at high fluence induces a severe transformation of the microstructure of single crystals. The formation of nanometer-sized domains slightly disoriented from the main crystallographic direction occurs, with a mean size decreasing with increasing irradiation fluence.