SYMPOSIUM R

R: Radiation Effects and Ion Beam Processing of Materials

December 1 - 5, 2003

Chairs

Lumin Wang
Nuclear Engr Dept & Radiological Sciences
University of Michigan
2355 Bonisteel Blvd.
Ann Arbor, MI 48109-2104
734-647-8530

Lance L. Snead
Metals and Ceramics Division
Oak Ridge National Laboratory
Oak Ridge, TN 37831-6138
865-574-9942

Rainer Fromknecht
Institut für Festkörperphysik
Forschungszentrum Karlsruhe
P.O. Box 3640
Karlsruhe, D-76021 GERMANY
49-7247-82-3940

Heishichiro Takahashi
Ctr for Adv Research of Energy Tech
Hokkaido University
Nishi-8, Kita-ku, 060-8628 JAPAN
81-11-706-6767

Daniel F. Downey
Varian Semiconductor Equipment
35 Dory Rd.
Gloucester, MA 01930-2297
978-282-2226

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*Invited paper
SESSION R1 Radiation Effects in Metals and Alloys Chair: L. Shew and H. Takahashi
Monday Morning, December 1, 2003 Room 306 (Hynes)

8:30 AM R1.1

Irradiation of materials in a high energy (≥ 5 MeV) spallation neutron flux results in the production of hydrogen and helium as well as displacement damage in materials. Displacement damage modifies the mechanical properties and embrittles metals. The addition of helium may exacerbate this damage. Molecular dynamics simulations are utilized to understand the atomicity of the processes occurring during irradiation in a Fe-H system, thereby understanding the mechanical embrittlement of materials. This work is intended to model the Fe-H system, aid in understanding the mechanisms of embrittlement, and help in the development of materials with improved resistance to irradiation damage.

9:00 AM R1.2

Molybdenum and Molybdenum based alloys exhibit several properties that make them attractive for nuclear reactor applications. Unfortunately, these materials are susceptible to severe embrittlement due to irradiation damage. If Molybdenum is to be used in nuclear applications, the embrittlement mechanisms must be understood so that alloy engineering efforts can be directed. Toward this end, computer simulations at various length-scales are being applied to key aspects of the irradiation embrittlement problem in Mo. Electronic structure computations are being done to calculate defect and impurity atom interaction energies. Molecular dynamics simulations of damage cascades are performed to determine cascade structure and to investigate the morphology of cascade damage. Reaction rate theory is applied to monitor microstructural evolution as a function of irradiation and metallurgical conditions. Dislocation dynamics simulations are being developed to investigate the influence of irradiation induced defects on plasticity and failure related to dislocation channeling. The goal of the multi-scale modeling approach is to drive the development of embrittlement mitigation strategies. This presentation will review the computational efforts being made to improve the understanding of the irradiation problem in Mo with specific attention given to recent results of the molecular dynamics and rate theory calculations.

9:15 AM R1.3
Influence of Fe Alloying Additions to the Defect Structure of V under Irradiation. Seungwu Hong, Mikhail I Mendeleev, David J Srolovitz,1 and Roberto Carra;1,2 Princeton Materials Institute, Princeton University, Princeton, New Jersey; Department of Chemical Engineering, Princeton University, Princeton, New Jersey; Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey.

The addition of a wide range of solutes can have a pronounced effect on the swelling behavior of V under irradiation conditions similar to those for the first wall of a fusion reactor. In particular, addition of Fe to V at a few percent level drastically increases the rate at which V swells. In this study, we perform density functional calculations and molecular dynamics simulations to understand the influence of Fe on point defect behavior in V. We first perform density functional studies of the equilibrium structure of self-interstitials and their interaction with Fe impurities. This data is used to develop a set of interatomic potentials for V-Fe that properly reproduce the point defect structure of these materials and a wide range of other crystal, crystal defect and liquid properties. While self-interstitials are not present in V even at very low temperatures, molecular dynamics simulations show that iron atoms greatly modify self-interstitial migration. This is attributed to a strong attractive interaction between the interstitial and Fe solute atoms. The implications of these results for the void swelling behavior in V are discussed.

9:30 AM R1.4
Atomic Simulations of the Effect of Helium on the Irradiation Damage in bcc Iron. Maria A. Onnerfors,2 Simon van der Ven,3 Simon G. Simmons,2 Seungwoo Hong,2 Simon A. Makigami,2 Michael L. Dessau2, Michael R. James2 and James F. Stubbins5;1 Nuclear, Plasma, and Radiological Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois; 2Los Alamos National Laboratory, Los Alamos, New Mexico.

Irradiation of materials in a high energy (> 5 MeV) spallation neutron flux results in the production of hydrogen and helium as well as displacement damage in materials. Displacement damage modifies the mechanical properties and embrittles metals. The addition of helium may exacerbate this damage. Molecular dynamics simulations are utilized to understand the atomicity of the processes occurring during irradiation in a Fe-H system, thereby understanding the mechanical embrittlement of materials. This work is intended to model the Fe-H system, aid in understanding the mechanisms of embrittlement, and help in the development of materials with improved resistance to irradiation damage. The reduced activation martenitic (RAM) steel is presently the most realistic contender for application in fusion blankets near magnetically confined plasmas. The serious issues in its high burnup (an increase of 100% in fissile content) is the development of high temperature embrittlement and low reactivity. This presentation will review the computational efforts being made to improve the understanding of the irradiation problem in Mo with specific attention given to recent results of the molecular dynamics and rate theory calculations.

10:00 AM R1.5
Role of Irradiation in Stress Corrosion Cracking of Austenitic Alloys in High Temperature Water. Gary S. Walski, Nuclear Engineering and Radiological Sciences, University of Michigan, Ann Arbor, Michigan.

Irradiation is known to enhance the stress corrosion cracking susceptibility of austenitic alloys in high temperature water systems. The degree of irradiation assisted stress corrosion cracking (IASC) increases with dose, and the microstructure undergoes significant changes including the formation of dislocation loops, grain boundary segregation and hardening. Total dislocation loop length increases with increasing irradiation damage and with IASC susceptibility. Similarly, the amount of chromium depletion at grain boundaries scales with intergranular cracking propensity. Segregation of other elements at the grain boundary also correlates with IASC. However, these various changes can only be ascribed to comparable rates, complicating the attribution of IASC to specific components of the microstructure. Each of the principal effects of irradiation has been observed as a potential cause of IASC, but their relative contributions to the overall response are not yet agreed upon. The role of individual microstructural components in the determination of the mechanism, rather than the mechanism of IASC is...
more likely due to a combination of factors, or second order effects not yet considered. Among these effects is the change in deformation mode caused by the microstructure and BS, and the interaction of localized deformation with the oxide film and the grain boundaries. Current understanding and proposed mechanisms of ISACC will be reviewed, and recent progress to identify additional factors or combinations of factors affecting ISACC will be presented.

11:00 A.M. R1.1 The Irradiated Microstructure of Ferritic Steel T91 and and O-2 /RDS: J. C. Guo, James I. Cede, Todd R. Allen, Shigeharu Ueki, Shuji Shishini and Thevathasan; Nuclear Technology, Argonne National Lab-West, Idaho Falls, Idaho; 2Japan Nuclear Cycle Development Institute, Hiroaki, Japan; 3Pacific Northwest National Laboratory, Richland, Washington.

A ferritic steel T91 and an oxide dispersion strengthened alloy [SCODS] were irradiated with Ni ions at 500 °C to doses of 5 and 50 displacements per atom. Both alloys were aged with the high temperature irradiation at 500 °C in the absence of water, and then cooled in air. The high temperature irradiation in the oxide film and grain boundaries. Current understanding and proposed mechanisms of ISACC will be reviewed, and recent progress to identify additional factors or combinations of factors affecting ISACC will be presented.

11:15 A.M. R1.8 Defect Diffusion in hcp Zirconium: A kinetic Monte Carlo approach, Cristina Arevalo, 1 Marinh Catarino, 2 and J Maieu Perleber, 2 Instituto Fusion Nuclear, ETSI Universidad Politecnica de Madrid, Madrid, Spain; 2Departamento de Fisica Aplicada, Universidad Alcalá, Alcalá, Spain; Lawrence Livermore National Laboratory, Livermore, California.

α-Zirconium is currently used in nuclear reactor systems, in particular in fuel cladding and pressure tubes, and in the first barrier between the radioactive material and the environment. Its integrity needs to be maintained for safety reasons during operation as well as during transport and storage of spent fuel assemblies. Therefore it is important to understand the diffusion of defects at operating temperatures on the mechanical properties of these materials. Present approaches to high-temperature fusion reactor designs have focused on the structural aspects of these materials, while our recent work on high-temperature fusion fuel irradiation has been demonstrated to be effective in predicting the behaviour of these materials. Present approaches to high-temperature fusion reactor designs have focused on the structural aspects of these materials, while our recent work on high-temperature fusion fuel irradiation has been demonstrated to be effective in predicting the behaviour of these materials.

11:45 A.M. R1.10 In Situ TEM Study of Irradiation-induced Transformation in TiNi Shape Memory Alloys, Xiaodong Zuo, 1 F.R. Wai, 2 S. Zhu, 3 Z.G. Wang 4 and L.M. Wang; 1 Department of Applied Physics, University of Electronic Science and Technology of China, Chengdu, China; 2Department of Materials Physics, University of Science and Technology of Beijing, Beijing, China; 3Department of Nuclear Engineering and Radiological Sciences, University of Michigan, Ann Arbor, Michigan.

TiNi shape memory alloy (SMA) has potential applications for nuclear reactors and its phase stability under irradiation has been an important topic. Some irradiation-induced diffusion-dependent phase transformations, such as amorphization, have been reported before. In the present work, the behavior of diffusion-dependent phase transformations in TiNi SMA was studied under electron irradiation at room temperature. The effect of irradiation on the martensitic transformation of TiNi shape memory alloys was studied by Transmission Electron Microscope with in-situ observation and Differential Scanning Calorimeter (DSC). The results of TEM and DSC measurements indicate that the microstructure of samples is R phase in the room temperature. Electron irradiations were carried out using several different transmission electron microscopy (TEM) techniques to examine the effects of irradiation on the microstructure of TiNi SMA.

13:00 P.M. R1.9 Surface porosity development on metal substrates by helium implantation and annealing, R. Frick, 1 D. D. Flood, 2 H. Shuck, 3 J.H. Evans, 4 A.V. Pederson, 1,4 P.Y. Hou 5 and J.T. M. De Hosson; 1Defects in Materials, III, University of Delft, Delft, Netherlands; 2Camrose Consultants, Abingdon, United Kingdom; 3Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California; 4Materials Science Centre, University of Groningen, Groningen, Netherlands.

In this work we study the development of porosity at the surface of metals in a controlled way using ion implantation under blistering threshold and subsequent annealing. The samples were examined using Scanning Electron Microscopy (SEM) and Scanning Confocal Microscopy (SCM). Polycrystalline copper substrates were implanted with 34 kV He+ ions up to doses of 3 and 5 x 1016 cm-2. In order to avoid the release of gas during annealing thin films were deposited on the substrates. Therefore W-C films with a thickness of 2 μm and an adhesive intermediate layer of Chromium layer of 200 nm and TiAl with a total thickness of 6 μm and a periodicity of approximately 20 μm were deposited by PVD on the copper substrates. Finally the samples were annealed afterwards in vacuum at temperatures from 725 to 1073 K for 30 minutes. After a post-deposition annealing, the implanted gas is collected as bubbles at the coningament interface. These bubbles are confined by the presence of the coating and developed to equilibrium bubbles with an equilibrium pressure P = s t which is the surface tension of the bubble. In the case of TiAl multilayers this leads to the formation of faceted structures in the substrate implanted with the highest dose. Low index facets develop. For the lowest dose no faceting is observed but each copper grain develops a different surface porosity. This faceting and surface porosity causes dewetting and final flaking of the coating after annealing at T=573 K. In the case of W-C films, samples were annealed at 753 K some blistering is observed but almost all the coating remains intact. Further annealing at 1073 K provokes blistering and flaking of the coating. Contrary to the multilayer coating no development of any cellular structure with crystallographic facets was observed in the flaked areas. A small scale substructure was observed probably related to the presence of the Cr adhesive interlayer. The heating can also be performed by laser irradiation of the pre-implanted sample. An iron aluminate sample coated with a thermally grown alumina layer 300 nm thick was implanted with helium ions at 1200 °C with a fluence of 3x1023 cm-2. After irradiation with a high power Nd-YAG infrared pulsed laser beam [maximum 500 mJ in 5 ns] the alumina layer was removed and the alloy surface developed a cellular structure similar to the case observed for the copper coated with TiAl multilayers. Similar procedures have been applied to titanium and aluminum deeply pre-implanted with helium at 1400 °C. Samples were subsequently heated both by annealing in vacuum oven at 1000 °C and by laser irradiation. The role played by the helium concentration, the confinement by the coating layer and the annealing method will be discussed in detail.

SESSION R2: Radiation Effects in Ceramics, Glasses and Polymers I

Chairs: Y. Watanabe and L.M. Wang
Monday, December 2, 2003
Room 306 (Hynes)

1:30 P.M. R2.1 Radiation Effects in Nuclear Waste Forms: A Review, R. Fagin, Department of Nuclear Engineering and Radiological Sciences, University of Michigan, Ann Arbor, Michigan.

During the past decade, there have been important advances in the understanding of radiation effects in the complex ceramics that are
proposed for the immobilization of a wide variety of fission products and actinides that result from reprocessing spent nuclear fuels and the Pu from the dismantlement of nuclear weapons. The challenge was to predict the response of material to radiation damage over periods of tens to hundreds of thousands of years over different thermal regimes. Much of the recent information has come from systematic studies using ion beam irradiations, as more and more recent results from actinide-doping experiments. This presentation will review the state-of-the-art for two structure-types, zircon and pyrochlore, with a special emphasis on the relationship between ion beam experiments and the results of actinide-doping experiments.

200 PM R2.2

Chloride-Induced Toxicity Of The Damage Induced In Ion-Irradiated Ceramic Oxides. Lionel Thorne and Frederico Garrido. CNRS Orsay, Orsay, France.

The safe and long-term control of radioactive waste arising from nuclear power plants is generally considered as the major challenge to future development of nuclear energy. Due to the emergence of increasingly sources of nuclear waste, there is a strong interest in the selection of new fuel materials for ionizing radiation studies and the development of inert fuel matrices for actinide burning. Among the materials of potential use to this purpose, a particular attention was recently focused on crystalline single-phase ceramic oxides. The evaluation (radiatively and in a few cases chemically) of the main parameters concerning the physico-chemical properties of the selected materials, such as high melting point, good thermal conductivity, oxidation resistance, low solubility in water, stability against irradiation, the latter latter, which has become the object of intensive investigation in the past years, is the subject of this presentation. The topic that I am attempting to cover easily requires a whole book to do it justice. I will thus focus my talk on the description of recent results concerning the study of the kinetic parameters of the damage induced by ionization in ceramic oxides. After having presented the basic principles which dominate the damage creation in a broad energy range (from keV to GeV), I will give illustrative examples taken from well-studied and relatively well-understood materials.

230 PM R2.3

Radiation Effects on Hollandite Ceramic Materials for Radioactive Waste Immobilization. A. Alam, 1 Adeline Damoun, 2 Daniel Courrèges 2, Didier Gourrier 2, Noël Bisfield 1, Thierry Advouet 1 and Jean-Marc Costantini 3. 1LCES, CNES, ONESCP, Paris, France; 2DEN/DIEC/SCDV Marcoule, CEA, Bagnols-sur-Ceze, France; 3DEN/DMM/RMA Sacy, CEA, Gif sur Yvette, France.

Progress on separating the long-lived fission products from the high level radiolytic liquid waste (HLW) has led to the development of specific host matrices, notably for the immobilization of cesium. Hollandite (NaCaAl12(PO4)12(OH)2) one of the main phases constituting Syros - an assemblage of ceramics designed for the conditioning of unseparated HLW - receives renewed interest as a specific Ca-host transform. The radioactive cesium isotopes consist of short-lived 137Cs (t1/2 = 30 years), and long-lived 134/135Cs (t1/2 = 2.1 and 88 years), with cesium being one of the most important actinide elements in waste. 1Cs and 137Cs have high fission yields and 134/135Cs have long lifetime (halflife of 15 years). All decay according to Ca(134/135) + Bb(137) + e(+) + (0.51 MeV) + γ (0.6 MeV). Therefore, Ca-host forms must be both heat- and (β+γ)-resistant. Nevertheless, the amount of work reported on the radiolytic degradation of the hollandite under extended ionizing radiation, simulating the decay of Cs, is very limited. This is the topic of this study. Several materials having the B2a-Cs2C2H6Tib=2−δO6=O (Cs = Al12, Gd12, Ga12, Pr12, Mg12, Sm12, Sc12) composition type (1.10 ≤ c = 1.28, 0.05 ≤ c = 0.28) synthesized by oxide route were essentially irradiated by 1 and 2.5 MeV electrons with different doses to simulate the β and X-ray irradiations. These irradiations were also performed. As all these irradiations imply mainly electronic excitations, the generation of point defects was then followed by Electron Paramagnetic Resonance (EPR). The nature, concentration and thermal stability of these defects were studied. For instance, all electron irradiations carried out on B2a·Cs2C2H6Tib=2−δO6=O sample generated defects of the same nature (oxygen centers and Ti3+ ions) but in different proportions varying with electron energy and dose. The annealing of irradiated samples lead to the disappearance of the latter defects but give rise to two other types of defects. It is necessary to heat at relatively high temperature to recover the initial material. The stability of hollandite phase under cesium irradiation is discussed in the light of these EPR-detected point defects.

2:45 PM R2.4

Damage Evolution and Annealing of Au-Irradiated Samarium Titanate Pyrochlore. Yewen Zhang 1, Vaibhav Agnihotri 2, Shuttin Wannapun 3, Ramanrampi Devnamthan 3, Sunitamthukulpa Thevathamby 1, William J. Weber 1, Jonathan Andrews 3, Geetha Balakrishnan 1. 1Physics Department, Pacific Northwest National Laboratory, Richland, Washington; 2Physics Department, Northwestern University, Evanston, Illinois; 3Department of Physics, University of Warwick, Coventry, United Kingdom.

Damage evolution and thermal recovery of Au28+ irradiated samarium titanate pyrochlore [Sm3Ti2O7] single crystals were studied by Rutherford backscattering spectroscopy and nuclear reaction analysis using 18O(d,p)17O and 16O(p,α)12C. The damage evolution follows a nonlinear dependence on dose that is well described by a disorder accumulation model, which indicates a predominant role of defect-atom stabilized amorphization processes. The critical dose for amorphization at 170 and 300 K is ~0.14 dpa, and a higher dose of ~0.22 dpa is observed for irradiation at 700 K. The amorphization doses are in agreement with previous in-situ transmission electron microscopy (TEM) data for polycrystalline Sm3Ti2O7. Based on on-going TEM observations; however, the present results provide quantitative details on the damage accumulation processes that could not be obtained in the TEM studies. Annealing in a 18O environment after damage recovery stage at ~850 K coincides with a significant increase in 18O exchange due to vacancy mobility. This thermal recovery stage is also consistent with the critical temperature for amorphization measured by in-situ TEM in polycrystalline samples.

3:00 PM R2.5


Alkaline ion-exchange reactions play a significant role in the release rates from low-level vitrified waste and may be dominate in determining release mechanisms over an extended period of time [M.I. Ojoam et al, J. Nucl. Mat., 298, 174 (2001)]. However the role of irradiation in the kinetic of ion exchange is not clearly understood. This paper develops a kinetic model (using Monte Carlo simulation) to incorporate radiation-induced changes in the kinetic of alkali-exchange. Rates of alkaline ion-exchange have been calculated depending on irradiation dose D (Gy) and dose rates (Gy/h). Derived rates depend both on D and P illustrating that some effects cannot be simulated by external irradiation and consequent analysis but require in-situ experiments. The higher D and P the higher decreases of ion-exchange rates. The most significant changes are in the activation energies. Sodium ion-exchange energy barriers have been revealed for glasses Na2O. 10H2O to 12H2O to decrease from 4 to 6 times depending on glass composition, e.g. from 48.5 kJ/mol without irradiation to 7.9 kJ/mol in radiated fields.

Radiation-induced changes are most pronounced at relatively low temperatures being diminished by the increase of glass temperature. Hence described effects are most important in performance assessment of vitrified low-level waste, non-host-generating nuclear waste, and high-level waste after its cooling to ambient temperature. Numerical estimations show that changes in alkaline ion-exchange kinetic are notable already at D far below damaging doses of waste forms.

3:30 PM R3.2.6

Radiation-Induced Defects in Nanocrystalline Natural Minerals: mineralogical and environmental significance. Georges Calas, Thierry Allard, Etienne Balan and Guillaume Morin; Mineralogy, University of Paris, PARI, France.

Short-lived radionuclides, formed by radioactive decay of natural U and Th, generate a background radioactivity, which will influence the mineral structure. The radionuclides are mainly in minerals. These minerals are mostly electronic, with the presence of trapped electrons and positive holes, often associated to element impurities, which act as final traps over geological periods. Two main examples will be illustrated, based on spectroscopic measurements (EPR, UV-visible spectroscopy). Natural fluorites (CaF2) are a typical example of a nominally colourless common mineral, which exhibits a wide range of original colors. By contrast to artificial alkaline and alkaline earth halides, natural fluorites do not exhibit native F-centers. Positive holes may be trapped on rare earths (Sm3+) but, most defects consist in an association between the point defect and an impurity located nearby, such as the V-associated F-center. Finally, Ca colloids may be formed under severe irradiation conditions. Other minerals, of apatite, confirm the importance of impurities in the trapping of radiation-induced defects in geological systems. In the second example, we will review the present knowledge on the most important point defects in kainite. The high clay minerals sensitive to the geochemical radiation background and provides a record of the past occurrence of radionuclides in geosystems. Point defects in kainite are hole centers associated to oxygen or silicon. They have different thermal/time stabilities, and indicate distinct formation periods. An experimental dosimetry, based on a simulation of natural irradiation, allows to derive mean past U-concentration. The detection of past minerals in radionuclides in high clay minerals may be used in the safety assessment of radioactive waste disposal.
4:00 PM R3.7
Coupling Between Order Parameter and Compositional Fluctuations in the Irradiation Induced Monoclinic to Tetragonal Phase Transition in Pure Zirconia.
David Sirringue, Esaunne, CEA; Gif sur Yvette, France;
CEA/DMN/SIRMA/ILMS, CEA, Gif-sur-Yvette, France.

Zirconia has been the object of extensive investigations and therefore it is a textbook example for describing the phase transition mechanism within the Landau theory approach. This material exhibits many phase transitions and the temperature-pressure phase diagram of pure zirconia is very complex. The first order phase transition between the monoclinic and tetragonal phase occurring at about 1200 K prevents the use of pure monoclinic zirconia at room temperature as a structural material. The sensitivity of zirconia phase transitions to radiation exposure also suggests that zirconia can be a good paradigm system for modeling the effects of radiation damage on the stability of the instabilities unutilized in the theory of Landau.

In this paper, we try to build a simple microscopic model explaining the monoclinic to tetragonal phase transition observed in pure zirconia samples exposed to radiation damage, pointing out the key role of the compositional fluctuations induced by the radiation exposure and the way they couple to the order parameter field (M point phonon).

4:15 PM R3.8

Halogen or chalcogen ions (Cl, Br, I, S, Se) were implanted in silica glass at energies of the order of MeV, followed by the MeV Cu ion implantation. Structure of Cu ions in the ion-implanted glasses was investigated by XAFS. It was found that Cu ions were incorporated with oxygen ions in the implanted glasses. Heat treatment at 600 degree C caused the formation of Cu-O bonds (X=Cl, Br, I, S, Se) in the glasses without forming crystalline compounds. Taking account of the atomic concentration, it was deduced that Cu ions form Cu-O bonds preferably to the Cu-O bonds. Compounds of implanted ions were formed after heating at above 900 degree C. These findings imply that Cu-O bonds were formed in silica glass prior to the formation of crystalline compounds.

4:30 PM R3.9

Crystalline damage created by ion-implantation of dopant impurities in ZnO (0001) substrates was characterized as a function of atomic mass of implanted species using triple-axis (2θ,ω) x-ray diffraction and Rutherford backscattering (RBS). The former revealed the presence of implantation-induced strain throughout the broadening of the isometric and symmetric (2θ,ω) reflections. However, RBS indicated that the damage introduced during implantation of these ions was insufficient to transform the (0001) lattice into a completely amorphous state. Additional XRD characterization as a function of annealing temperature of the implanted materials showed a reduction in the broadening of the isometric reflections, indicating that structural recovery of implanted ZnO crystals can be achieved.

4:45 PM R3.10
Space Environment Effect on Fluorinated Polymers. Mircoa Chipara, Marc L. Edwards, Ted Zaleski1, and Barbara Ferenski1. 1Indiana University Cyclotron Facility, Bloomington, Indiana; 2Environmental Effects Group, Marshall Space Flight Center, Huntsville, Alabama; 3Space System Loral, Palo Alto, California; 4Chemistry Department, Indiana University, Bloomington, Indiana.

The excellent thermooxidative stability of fluorinated polymers justifies the wide range of applications of fluorinated polymers and copolymers. While the radiation stability (in vacuum) of fluorinated polymers is good, the competition between the radiation induced degradation and the oxidative degradation leads to a rapid deterioration of fluorine bonded polymers. Accordingly, the space applications of these polymers have to be considered with caution. As ionizing radiations trigger the degradation of fluorinated polymers, opening the route for their fast and accelerated oxidation. The effects are expected to be stronger at low Earth Orbits where the synergism between singlet oxygen induced degradation and radiation induced degradation is expected. The extreme temperatures of the space environment may limit the lifetime of polymers in space. Electron spin resonance spectroscopy was used to identify the nature of free radicals induced by ionizing radiations in model fluorinated polymers [polytetrafluoroethylene and polyvinyl fluoride] and composites based on fluorinated polymers [graphite-polytetrafluoroethylene and Teflon], and to quantify the time and temperature evolution of these free radicals. The resonance spectra were obtained by using a Bruker spectrometer operating in X band. The temperature dependence of resonance spectra has been investigated. The samples have been irradiated with gamma rays (60Co), accelerated electrons (accelerated up to 1.0 MeV), and accelerated protons (accelerated up to 205 MeV) in air, at room temperature at doses ranging between 10 KJy and 100 KJy. Additional mechanical and electrical tests on these materials are analyzed. It was observed that the irradiated spectra present immediately after irradiation an incompletely resolved hyperfine structure due to the delocalization of the unconnected electron over the fluorine nucleus. Gradually, these primary radicals are converted into peroxy like radicals, with no resolved hyperfine splitting. The combined effect of radiation and oxygen (including singlet oxygen) decreases the average molecular weight of fluorinated polymers, after plasma cleaning process used to remove the native oxides. Their lifetime. The role of oxygen diffusion and the glass transition related anomalies due to the rapid increase of the oxygen diffusion coefficient within fluorinated polymers above glass transition temperature, are discussed. A critical review of the space applications of fluorinated polymers is presented.

SESSION R3: Poster Session: Radiation Effects
Chairs: H. Takahashi and L. M. Wang
Monday Evening, December 1, 2010
5:00 PM
Exhibition Hall D (Hynes)

R3.1
Diffusion Contrast Image Analysis on the Defects of the GaAs Crystals Caused by ECR Cleaning Process.

Cross-sectional and plan-view TEM techniques were used to study the defects on (110) facets of GaAs crystals caused by ECR hydrogen and argon plasma cleaning process used to remove the native oxides. It is found that the densities of the defects are dependent on the ECR gas type, mode voltage and the etching time. By TEM diffusion contrast image analysis, the crystal defects are determined as Frank dislocation loops at the (111) planes of the GaAs crystal. The details of the TEM analysis procedures are described in the paper. In order to obtain a damage free and oxygen free (110) surface of the GaAs crystal, the control of the ECR process parameters is critical.

R3.2

Irradiation effect of low-energy nitrogen ion beam on carbon nitride (CNx) thin films has been investigated. The CNx films were prepared on silicon single crystal substrates by hot carbon filament chemical vapor deposition (HFCVD). After deposition, the CNx films were irradiated by the nitrogen ion beam in the energy range from 0.1 to 2.0 keV. Irradiation effect on the film microstructure and composition was studied by SEM and XPS. Surface and cross-sectional observations by SEM reveal that the deposited films show a densely distributed columnar structure and the films change to a sparsely distributed one like configuration after irradiation. It is suggested that the films are selectively etched out by the nitrogen ion beam irradiation. It is found from the XPS analysis that the atomic ratio of nitrogen to carbon (N/C) in the films jumps from approximately 0.05 to 0.2 after 10 minutes irradiation by 0.1 keV nitrogen ion beam and then it increases gradually to 0.3 with the irradiation time of 300 min. Depth profiles of nitrogen in the films observed by XPS show that nitrogen incorporation into films is more prominent after irradiation by low-momentum nitrogen ions compared to MeV high-energy ions such as 2.0 keV. These results provide a clue for understanding of the basic processes during nitrogen ion beam irradiation on CNx thin films.

R3.3
Destruction of Multival Carbon Nanotubes Under the Influence of Ion Bombardment. Mariya M. Brzoziakowska1, Evgeniy M. Brzoziakovski2, and Shintetsu V. Vladimir2. 1Physics, Chelyabinsk State Pedagogical University, Chelyabinsk, Russia.
The conception of crystal structure as a system of precise order of atoms or ions is an aesthetic abstraction. The utmost of raw materials' purification and specific conditions of synthesis of one or other material are always reasons for non-uniformity of structure affecting the material's performance. The present work is dedicated to study structure defects on optical and luminescence properties of rare earth (RE) activated garnet (YAG) and orthoaluminate (YAP) crystals. Due to fast neutron irradiation the Frenkel defects concentration was increased. The experimental results were practically homogeneous so that the whole sample body was excited evenly by light-energy photons. The main results are as follows. Self-trapping of intrinsic electron excitons at a fundamental center playing a key role in scintillation mechanism. The temperature dependence of RE luminescence intensity, which is stimulated by gamma-rays (GSL), is considered from the standpoint of holes self-trapping. Due to the hot holes' ability to migrate for a long distance during thermal activation, non-complete RE luminescence quenching occurs even at low temperatures. Fast neutron bombardment creates a deep coloration of the sample, and several additional wide absorption bands appear in the whole spectral range of 200-1100 nm. Actinor GSI intensity decreases with the fast neutron fluence although this decrease is substantially larger than that which was expected due to emission redshifting (passive losses) enhanced by taking into account the self-trapping phenomenon at the corresponding wavelength. Both actinor and Frenkel defects (displacement defects) are responsible for the mechanisms of the energy transfer to activator luminescence centers (active base). Frenkel defects themselves are recombination luminescence centers, which are emitting in the same spectral range as the cerium-doped scintillators. This circumstance as well as the principal feature in decay characteristics of defects' luminescence can make changes in the main scintillator parameters such as light output and decay time.

R3.4
Gamma-Ray Detectors Based on AIBSCO Semiconductors. Galina Klymen, General Physics, State Pedagogical University, Drogodych, Ukraine; 2General Physics, State Pedagogical University, Drogodych, Ukraine.

Composite semiconductors AIBSCO due to their unique structural and electro-physical properties are used as the attractive materials for design of gamma-ray detectors operating at the room temperature under external electric field. There are no literature data concerning the problem. The abstract reports first experimental data on electrical parameters of p-type single crystal AIBSCO structures based on AgGaS2 material after gamma-irradiation at the room temperature. Numerical algorithm used for electric processes simulation is also presented. Electric-field measurements were shown drastically changes in charge carriers transport. Detailed numerical analysis showed the field-current characteristics similar to the ones of the p-n-homjunctions; at the same time, three different tunneling modes were observed. The experimental and numerical results made it possible to propose a simple gamma-sensitive active element.

R3.5
Effects of High-Energy Ion Irradiation in Bismuth Thin Films at Low Temperature. Hiroshi Hashimoto, Akiko Iwane; 2Department of Materials Science, Japan Atomic Energy Research Institute, Tokai Research Establishment, Tokai-mura, Naka-gun, Ibaraki, Japan; 3Research Institute for Advanced Science and Technology, Osaka Prefecture University, Sakai-shi, Osaka-fu, Japan.

We have studied high-energy ion irradiation effects in bismuth by measuring the electrical resistivity at low temperature in relation to its structural change. Bismuth thin films (300-600 Â thick) were irradiated below ~10 K with several kinds of energetic (100-2000 MeV) heavy ions. The resistivity of the specimen is measured in-situ at ~7 K during the irradiation. After irradiation the resistivity is observed up to ~35 K. The temperature dependence of the resistivity during annealing shows an abrupt increase around 20 K, implying re-crystallization of irradiation-induced amorphous region. Since amorphous bismuth also shows a superconducting transition below ~0.5 K, high-density electronic excitation due to energetic heavy-ions irradiation may induce columnar region of superconducting amorphous bismuth in normal crystalline bismuth. We are trying to detect the superconducting transition as a result of irradiation-induced amorphization.
In recent years, great attention has been paid to investigations of stimulating optical properties of bandgap exciton in PWO crystals. It is the aim of this work to investigate the intrinsic electronic excitations in PWO crystals by studying the origin of color and emission centers through the measurements of the transition and luminescence spectra in the temperature interval 9-300K. Both undoped and Nb and La doped PWO single crystals were examined. Three additional absorption band at 360, 550 and 1300 nm were detected after the crystals had been UV-irradiated at 4K in the spectral range 0-250 nm. In PWO the electron transition for a shallow donor is the absorption edge. The latter one was studied in more detail. This significantly intense and wide IR absorption band seems to be complicated. Thus the sample heating to 300K causes a change in the IR absorption band in shape and replacing of peak position from 1300 to 1150 nm. This seems to be due to release the carriers from shallowest traps, which are responsible for the longest wavelength band at 1300 nm. The experiments on photo-stimulated color centers' transformation have shown that this band may be emitted at low temperature and might be identified as electron-like center (self)- trapped in regular site. The wide luminescence band in the blue-green spectral range can be observed under UV-excitation in the range of one-zero transitions of PWO crystal. Luminescence temperature dependencies measured at 420 and 520 nm are considerably different. That means two different luminescence centers at least exist. It should be noted that the blue emission in undoped and Nb doped PWO crystals is quenched partly in the temperature range of 9-70K, but the same quenching does not occur in the case of La doped crystal. This event is supposed to be due to electron self-trapping phenomenon, which is as mentioned above.

R3.10 Abstract Withdrawn

R3.11 Order Patterning Induced by Cascade Size in Irradiated Metallic Alloys. Jin Ye and Pascal Bellow; Materials Science and Engineering, Univ. ofIllinois at Urbana-Champaign, Urbana, Illinois.

Heavy ion irradiation leads to the formation of dense displacement cascades in the host material. These cascades are characterized by two length scales: the atomic relaxation range and the size of the cascades. We showed that, when the atomic relaxation range exceeds a critical value, the composition field of an alloy may spontaneously form dynamically stable patterns [1]. Here we identify a new patterning reaction in the case of ordered alloys: when the cascade size is large enough, the degree of chemical order develops patterns, under appropriate irradiation flux and temperature. This order patterning is observed in kinetic Monte Carlo (KMC) simulations for an A/B alloy that forms an L12 ordered phase at equilibrium. A dynamical phase diagram is built that yields the stable steady state in a function of the cascade size and the irradiation flux. Three possible steady states are identified: long range ordered, disordered and order patterning. In the order patterning phase, highly ordered domains of the four variants of the L12 structure coexist in equal proportions. All of these domains, however, remain of finite size, and thus the material is not long range ordered. An analytical mean-field continuum model is introduced to describe the role of the cascade size on the evolution of the degree of order in an irradiated alloy. The dynamical phase diagram built from this analytical model is in very good agreement with the KMC one. It allows us to firmly identify the physical origin of the order patterning reaction, and to conclude that cascade-induced order patterning is a general phenomenon that can take place in any ordered phase. Experimental tests of these predictions are proposed, and potential applications for the controlled synthesis of nanostructures are outlined. [1] R.A. Enriquez, P. Bellow, Phys. Rev. Lett. 85, 1819 (2000).

R3.12 Electron Irradiation Induced Evolution of Transformation Characteristics in TiNI, TiNiCu and CuZnAl Shape Memory Alloys with Different Mechanisms. z.g. wu1, Xiaoqin Zuo2, s. zhu3, j.h. wu4 and l.m. wang2. Department of Applied Physics, University of Electronic Science and Technology of China, Chengdu, sichuan, China. Department of Nuclear Engineering and Radiological Sciences, University of Michigan, Ann Arbor, Michigan.

Ti-50.8 at%Ni, Ti-42at%Ni-7at%Cu and Cu-21.5Fe-7.5at%Zn-5.85%Al shape memory alloys were irradiated by 1.7 MeV electrons using an electron accelerator. The evolution of microstructure and transformation temperatures was studied by transmission electron microscopy (TEM), differential scanning calorimeter (DSC), X-ray diffraction (XRD) and positron annihilation technique (PAT). Different mechanisms of the effect of the electron irradiation on the transformation temperatures are found. In TiNi shape memory alloys some point defects created by electron irradiation migrate to the stressed borders of the TiNi precipitates modifying the local atomic configuration, and reducing the elastic energy of stress fields around

the Ti3Ni4, thus lead to the decreasing of martensite transformation start temperature [Ms] after irradiation. In TiNiCu shape memory alloys, electron irradiation leads to the increase of the interface energy between parent and martensite phase and decrease of the elastic energy between the martensitic variants, thus cause the shift of austenite transformation start/finish temperature [As/AF] to higher temperature. The ordering degree of electron irradiation in the martensite state leads to martensite stabilization, i.e. the shift of austenite transformation start/finish temperature [As/AF] to higher temperature in CuZnAl alloys. According to the results we can conclude that the electron irradiation in the Ti3Ni4 in TiNi alloy, the interface energy between parent and martensite phase and the elastic energy between the martensitic variants in TiNiCu alloy and the ordering degree in CuZnAl alloys have significant effects on the transformation characteristics.

R3.13 Effects of Dose Rate on End-of-Range Dose Defects Induced by Si and Implantation. Yi-Sheng Lin1, J. S. Chen1, Y. S. Hsiao, H. L. Sun2 and K. B. Huang3; Materials Science and Engineering, National Cheng Kung University, Taiwan, Taiwan; 2Diffusion, Taiwan Semiconductor Manufacturing Company, Taiwan, Taiwan.

Extended defects formed by amorphous implanted Si(100) followed by spike annealing are investigated. The end-of-range (EOR) defect density is reported to be influenced by the implant species, energy, ion dose, dose rate, and solubility. In addition, the creation of EOR damage that is present in the depletion region of the n+-p junction will lead to the increase in leakage current. As a result, engineering of the radiation damage has become the challenge to ion implantation technique. Given the dose of 1×1014 cm−2 in our study, the threshold energy for EOR defects formation is found to be more than 50 keV to induce the visible defects imaged by transmission electron microscopy (TEM). The cross-sectional view manifests an amorphous layer (a-Si), a transition region and the undamaged crystal [a-C(u-Si)]. The EOR defects are located near the lower bound of the transition region. Since high-mass Si ions used for ultra shallow implantation usually exhibit a low amorphization threshold density. The a-Si layers formed during deep ion implantation are decayed by oxygen vacancy/interstitial distribution and interface morphology are affected by dose rates. Therefore, in this work, 70 keV Si ion implantation with various dose rates were conducted to induce the amorphization/crystallization structure, which was examined by cross-sectional TEM, ultraviolet-visible spectroscopic ellipsometry, and thermo-IR. The location, density and size of EOR defects related to the amorphization/crystallization structure will be addressed.

R3.14 Mossbauer Studies of 50 MeV Li++ Ion Irradiated Mg56Mn34In8Fe26O19Ferrites. M. Singh, Rithi Sharm Kumma2 and Anjanu Dogra Kumar1; 1Physics, I.I. University, Shimla, India; 2Physical Science, National Institute of Technology, Hamirpur, India.

A series of samples of Mg56Mn34In8Fe26O19 was irradiated with 50 MeV Li++ ions for X = 0, 0.03, 0.05; 0.5 were prepared by conventional technique. Radioactivity of these ferries were confirmed by X-ray Diffraction technique. The samples were irradiated with 50 MeV Li++ ions with fluence 5×1013 ions/cm2. The Mossbauer studies were performed on unirradiated as well as irradiated samples by using Fe57 nuclear resonance. The spectra of unirradiated samples show insignificant variation of isomer shifts between both the tetrahedral and octahedral sites. On irradiation isomer shift changes from negative to positive values. This anomalous character of isomer shift after irradiation is due a change in the electronic configuration of Fe+++ ions. The Quadrupole splitting of unirradiated samples are negligibly small, shows the presence of Cubic symmetry at both the sites. On irradiation appreciable changes were observed in Quadrupole splittings. Hyperfine field of unirradiated and if unirradiated (50 MeV Li++) decreases with the substitution of In+++ ions. However, decrease in hyperfine field after irradiation is slow as compare to unirradiated samples.

R3.15 Modification of lattice structure and magnetic properties of Fe-Rh alloys by using energetic particle irradiation. Masanobu Fukumizu1, Ryoshib Taniguchi1, Fuminori Hori1, Seiji Komma2, Yasuo Chini3, Tadashi Kamburu4, Fumihisa Ono5 and Akhiro Inwe6; 1Materials Science and Engineering, Osaka Prefecture University, Sakai, Japan; 2Okyama University, Okayama, Japan; 3Japan Atomic Energy Research Institute,Okayama, Japan; 4The Institute of Physical and Chemical Research, Saitama, Japan.

In the near equiatomic ordered Fe-Rh alloy, the magnetic and structural transitions take place at several temperatures. It is well known that the magnetic transitions are very sensitive to composition, heat treatment, magnetic field and external pressure. Recent studies
have also shown that lattice structure of Fe-Rh alloys is changed by high speed deformation. The above results suggest that the magnetic properties and the lattice structure can be modified by high energy particle irradiations, because such irradiations realize lattice expansion, high temperature state and high pressure state in materials. In the present study, we irradiate Fe-50 at. %Rh alloys with 1 MeV 4He, 10 MeV 4He heavy ions (6H, Xe, and so on), and with 8 MeV electrons at room temperature. After the irradiations, the effects of irradiation on the magnetic properties and the lattice structure are investigated by using XRD, positron annihilation and magnetic susceptibility measurement. The lattice parameter for 8 MeV electron irradiated specimen is about 0.3 % larger than that before irradiation, suggesting a large change in temperature of the transition from antiferromagnetic phase to ferromagnetic phase.

R3.16 NMR study of proton beam irradiated TiH2PO4. S-Han Kim, Kyu Won Lee and Cheol Eui Lee, Physics, Korea University, Seoul, South Korea.

We have investigated the proton beam irradiation effect on TiH2PO4 (TDP) showing an antiferromagnetic phase transition and a ferromagnetic phase transition. The samples were irradiated by 0.51 MeV proton beams and studied by means of 1H NMR measurements. The NMR line shape and the rotating-frame spin-lattice relaxation time were measured as a function of temperature, and analyzed in order to understand the proton motions and the order parameter reflecting the structural changes caused by the proton irradiation.


Carbon nanotubes are one of the preferred fillers for polymer composites due to their exceptional electrical and mechanical properties. In this work, we present the detailed study on reinforcement effects of polymer thin films against high energy radiations when the various amount of CNT fillers are introduced. By the irradiation of short wavelength ultraviolet (UV) light with ozone and electron beam of low energy, carbon nanotube/matrix composites are fabricated. The changes on their CNT/PDMA thin films are studied as a function of weight % of CNT in PMMA matrices. The experimental evidence indicates that the presence of CNT in PMMA matrix lowers significantly the stripping rate in the composite material. The results are correlated with systematic study of the rheological and chemical properties of PMMA/CNT composites by thermal analysis (i.e. TGA and DSC), and spectroscopic techniques. Part of this work was supported by the Ministry of Science and Technology of Korea through Proton Accelerator User Program (No. M1.02KS01001-02K1901-01810).

R3.18 The evolution of chemical states of MgO surface at the initial stage of aging in ac-PDP. Yeojin Y1, Sungwan Cho1, Myungkeon Noh2, Myeong Chang Sung1, Chung-Nam Whang1, Kwanhong Jeong3 and Hyeon-joon Shin3, 1Institute of physics and applied physics, Yeonsei university, SEOUL, South Korea; 2Yonsei Center for Nanotechnology, Yeonsei university, SEOUL, South Korea; 3Pohang accelerator laboratory and department of physics, Pohang university of science and technology, Pohang, South Korea.

We investigated the detailed chemical information of MgO surface at the initial stage of panel aging in ac-PDP via x-ray photoemission and corresponding photoemission spectra study. Spectroscopic image showed the lateral distribution of chemical states on MgO surface, which clearly indicated the surface modified by the plasma damage during the panel operation. The spatially resolved photoemission spectra obtained on a initial MgO layer revealed MgO, Mg2O3, Mg(OH)2, and Mg(OH)2 phases. As the aging proceeded, the rapid disappearance of Mg(OH)2 and Mg(OH)2 phase and the sharp increments of Mg2O3 phase were observed. Our experimental results successfully revealed the surface chemical status of a thick insulator in pixel-by-pixel by overcoming the trivial surface charging-related problems on insulator.

R3.19 Vacancies in electron irradiated 6H silicon carbide studied by positron annihilation spectroscopy. C. H. Lam1, 2, C. C. Ling1, H. M. Weng1, 2, Deng Sheng Hong3, 4, C. D. Beling4 and S. Huang1, 2, 1Physics, The University of Hong Kong, Hong Kong, Hong Kong; 2Physics, University of Technology of China, Hefei, China; 3Physics, Nanjing University, Nanjing, China.

Positron annihilation spectroscopy PAS is a very useful technique to study vacancy type defects in semiconductors, in which the concentration and the microstructure of the vacancy are possibly deduced. PAS was employed to study electron irradiated n-type 6H-SiC. A variety of defects were involved and their annihilation properties were investigated. Implications on the microstructure of the deep level defects Si-V (1) and Si-V (2) will also be discussed. ACKNOWLEDGEMENT This project is supported by the RGC, Hong Kong (project no.: 0788/01P).

R3.20 Location of As in MeV irradiated Si:As investigated by positron annihilation of Rutherford backscattering-channeling spectra. Alessandra Sutti1, 2, 3, Eros Albertizzani1, 3, Simone Balboni1, 3, Marco Bianconi1, Luciano Colombo4 and Giorgio Lulli4, 1IMM, CNR, Sezione di Bologna, Bologna, Italy; 2CSEIA - Settori Reti e Comunicazioni, Università di Bologna, Italy; 3INFN-Dipartimento di Fisica, Università di Cagliari, Monserrato (CA), Italy.

Both theoretical and experimental studies of the interaction between As and point defects in silicon suggest that As electrical deactivation mainly occurs through the formation of As-vacancy complexes. The exact nature of these defects and their kinetics are still matter of investigation. This work reports Rutherford backscattering-channeling (RBS-C) analysis of As in heavily doped Si:As exposed to 2 MeV Si+ irradiation, a process believed to induce vacancy supersaturation in a ~1 micron thick surface Si layer. In order to interpret RBS-C spectra, we used stochastic modeling of ion-channeling, which includes the ab-initio calculated structure of As-vacancy clusters. Results indicate preferential relocation of the As contained in As-vacancy complexes upon irradiation, possibly due to the relatively low energy of displacement of dopant atoms in these defects. Upon rapid, low-temperature annealing the relocated As appears to almost fully recover its configuration, probably by capture of vacancies and re-formation of the complexes dissociated by irradiation.


An iron phosphate glass with a composition of 4mol% Fe2O3 and 5mol% Fe3O4 was irradiated under electron and ion beams. High-resolution electron microscopy (HRTEM) and selected-area electron diffraction (SAED) as well as energy-filtered transmission electron microscopy (EFTEM) and high-angle annular dark-field (HAADF) imaging were used for the study of the microstructure evolution of glass under irradiation. Results indicated that many nanoparticles have formed even after a small dose of low energy (several keV) ion beam irradiation. These nanoparticles show a bimodal size distribution, one around 10 nm and another around 20 nm in diameter. EFTEM indicated that they consist of Fe without any P. SAED further confirmed that they have a bcc-Fe structure, i.e. iron irradiation resulted in the formation of bcc-Fe nanoparticles in the glass. On the contrary, after a small dose electron beam irradiation, there was no nanoparticle formation. After electron doses higher than 4x1026 e/m2, phase separation occurred with P-rich phase separated from Fe-rich phase. At much higher dose of electron irradiation (about 1x1027 e/m2), some amorphous fragments were formed which were confirmed to be a P-rich phase. The formation mechanisms for the two different crystalline nanoparticles were discussed.

R3.22 Influence of High Fluence Neutron and/or Proton Irradiation on the Optical Properties and Microstructure of Rutile. Tiecheng Liu1, 2, Xiang Liu1, 2, Xiaobo Sun1, 3, Sha Zuo1 and Lumin Wang1, 3, 4, Department of Physics, Sichuan University, Chengdu, China; 1Key Lab for Radiation Physics and Technology of Ministry of Education of China, Sichuan University, Chengdu; 2Department of Nuclear Engineering and Radiological Sciences, University of Michigan, Ann Arbor, Michigan; 3National Center for Material Physics, Chinese Academy of Sciences, Shenyang.

Rutile (TiO2) single crystals with (110) and (100) orientation were irradiated with high-fluence neutron and proton beams of 1x1019 n/cm2, 2x1019 n/cm2, 4x1019 n/cm2, and with the fluence of 1x1015 to 1.9x1017 n2/cm2+, respectively. UV-VIS-IR, LRS and IR-FETEM were used to analyze the optical properties and microstructure of rutile samples. The UV-VIS-IR results showed that high-fluence neutron irradiation and proton irradiation induce similar variation of optical properties of samples. LRS results showed that the relative strength of common vibration modes did not change for different plane. Both high-fluence neutron irradiation and proton irradiation induce the variations of the frequencies and strength of vibration modes of different oriented samples. Moreover, new vibration modes are shown in irradiated sample. It looks like high-fluence irradiation induce recrystallization phenomenon, which is demonstrated by...
HIETEM observation. In addition, the difference between neutron-induced irradiation effect and proton-induced irradiation effect has been also discussed.

R3.23
The role of crystallinity on the blistering of GaN layers using hydrogen implantation. Sumiko Hayashi,1 Benjamin Ponte2
Benjamin Heying1 and Mark Gerszten1
1University of California, Los Angeles, Los Angeles, California; 2Northrop Grumman, Redondo Beach, California.

The exfoliation of thin GaN layers from 600 nm GaN layers grown on sapphire substrates was achieved using H2 implantation and subsequent annealing. We demonstrate that the extent of exfoliation depends on the crystallinity of the GaN layer. Extensive defects are not uniformly distributed over the wafer, so certain areas showed more pronounced exfoliation. Previous studies of hydrogen-implanted GaN have demonstrated that the onset of blistering depends strongly on the implant conditions, although there is some disagreement about those conditions. The required implant temperature has been reported to be >250°C for blistering to take place during subsequent annealing,3 whereas blistering was reported for lower implant temperatures (20°C) but only at somewhat higher doses (≈1017 cm−2).2 Given the literature concerning the interaction of extended defects in GaN with hydrogen and the range of "effective" implantation value reported in the literature, the issue of the crystallinity of GaN on blister formation is an important one.

The wafers consisted of 600 nm GaN layers grown on an AlN buffer layer on sapphire substrates by molecular beam epitaxy. Some wafers also included a 20 nm Al0.2Ga0.8N, 7 nm GaN cap layer. With an implantation energy of 60 keV (to penetrate 200 nm depth of about 500 nm of hydrogen defects lower than 2.5×1016 cm−2 were employed); the wafers were held at room temperature during implantation. Changes in the strain and mosaic tilt in the GaN layers were determined using x-ray scattering and topography, the blistering was observed using AFM microscopy and Nomarski microscopy. We observed blistering for all implant doses. For example, blistering was observed for a much lower implant dose (2.5×1016 cm−2, the lowest employed in this study) than had been previously reported.2 The onset of blistering under these conditions occurred upon annealing at 425°C for less than three minutes. Longer annealing times at temperatures lower than 425°C did not produce blistering. A compressive strain was observed in the GaN layers after implantation for even the low doses. After blistering, the strain was relieved. However, for some of the wafers that did not show blistering (e.g. dose of 2.5×1016 cm−2 annealed at 300°C), the implant-induced strain was not relieved. The crystalline quality (as measured by layer peak FWHM) varied across the wafer with better crystalline quality at the perimeter than the center. Interestingly, a "blistering gradient" was typically observed with no blistering at the center of the wafer, light blistering observed about half-way between the center and edge and heavy blistering at the edges under annealing conditions for which blistering did occur. The interaction of extended defects and implanted hydrogen is proposed to account for these differences.1, 2


The development of low energy neutral beam scanning systems combined with time-of-flight impact collision ion scattering spectrometry. Kenji Umezawa,1 Shigemitsu Nakashima,1 Walter M Gibson2 and Shigo Okamura1
1Dept. of Materials Sciences, Osaka Prefecture University, Suita, Osaka, Japan; 2Physics, The University at Albany, SUNY, Albany, New York.

We have been developing the low energy ion beam scanning systems combined with time-of-flight ion scattering spectrometer for the analysis of insulators and semiconductors surfaces. Insulator surface structural analysis has difficulty in measurements, because of change up using conventional electron or ion beams. Structural analysis of insulator surfaces are very attractive in the fundamental research as well as technological fields. In our scheme, charged ion beams, He+ and Ne+ are converted into neutral beams by charge exchange with He, Ne gas in a small cell. Other features of this system are pulsed beams, time-of-flight measurements, and a detector of MCP is coaxially mounted along the primary beam. This system is quite useful for the measurements of defect, surface stericity of ion beam synthesized insulator materials.1, 2, 3


R3.25
Proton Beam Irradiation Effects on Magnetic Nanocomposites. Mirena Chipara4, David Huia,2,3, Jeffrey Zalewski3,2, Sephimi Balasubramanian1, and Dimitris Leslie Fletcher1
1Indiana University Cyclotron Facility, Indiana Department of Mechanical Engineering, University of New Orleans, New Orleans, Louisiana; 2Chemistry Department, Indiana University, Bloomington, Indiana; 3Physics and Astronomy, University of Nebraska, Lincoln, Nebraska.

Magnetic nanocomposites have potential applications in future ultra high-density data storage media. Little attention has been paid to the effect of ionizing radiation on magnetic nanocomposites. Such investigations are of particular interest to NASA, due to the potential adverse effect of the radiation component of the space environment on nanomaterials and devices based on nanomaterials. Magnetic nanocomposite materials have been obtained by dispersing barium ferrite (BaFe) nanoparticles in a dilute solution of styrene-isoprene-styrene block copolymer (SIS) in toluene. The magnetic nanoparticles were obtained by mechanical milling. From these synthesis lines, the magnetic character of the magnetic nanoparticles was estimated to be about 20±4μm. BaFe-SIS solutions were sonicated 50 hours, at room temperature. Thin films of BaFe-SIS were obtained by spin coating. The films were held one day in vacuum at room temperature to completely remove the solvent. AFM studies showed that both BaFe-SIS and BaFe nanoparticles exhibit a cylinder like nano-morphology. The nanocomposites were irradiated with proton beams accelerated up to 200 MeV, at various fluences up to 2×1017 protons/cm2. The irradiated samples have been measured after one week since the irradiation was stopped. The magnetic properties of pristine and irradiated magnetic nanocomposites in the temperature range 5 K to 250 K were measured by SQUID. The temperature dependence of the magnetic susceptibility in the presence of an ac field was investigated. The temperature dependence of the average magnetocrystalline anisotropy has been estimated from the temperature dependence of the magnetization on the applied magnetic field, for individual crystalline fields. The magnetic properties of magnetic films as measured by UV-VIS spectroscopy was excellent for both pristine and irradiated samples. Ferromagnetic resonance spectra have been recorded by using a Bruker spectrometer, operating in X band. The angular dependence of ferromagnetic resonance spectra in the out of plane configuration (magnetic field perpendicular to the plane of the film) in the temperature range 300 K to 450 K has been investigated. The resonance spectra of irradiated nanocomposites showed a narrow resonance line located near g=2.00. This result suggested that the free radicals concentration was relatively low after a recombination time of one week. The ferromagnetic resonance spectra indicated that the proton bombardment of the nanocomposite material is affecting the features of the resonance lines and their angular dependence. A detailed analysis of the radiation induced modifications in BaFe-SIS nanocomposites is presented.

R3.26
Electrically Active Defects In Electron-Irradiated and Annealed CVD Diamonds. Vasily Polynov1, Alexander Rukovshikov2, Victor Ralchenko2 and Igor Vlasov2
1Microelectronics, Institute of Radio Engineering & Electronics RAS, Moscow, Russian Federation; 2General Physics Institute, Moscow, Russian Federation; 3General Physics Institute, Moscow, Russian Federation.

Electrically active defects in the undoped and boron-doped microwave plasma CVD diamond films subjected to electron-irradiation and/or vacuum annealing to high, up to 1300K, temperatures were investigated. Charge-trap Deep Level Transient Spectroscopy (Q- DLTS) was applied to determine the density, activation energy Ea, and capture cross-section of intrinsic and boron-induced defects in the samples. The undoped samples before the treatments displayed the acceptor point defects with a continuous energy spectrum while the B-doped samples showed two discrete boron-induced levels with Ea of 0.37 and 0.25 eV near the valence-band top. It is found that the electron irradiation changes the parameters of boron-induced levels, decreases the density of point defects with a continuous energy spectrum, and strongly, by four orders of magnitude, reduces electrical conductivity. It is found also that after annealing at high temperatures the B-doped films show only one boron-related level with Ea = 0.37 eV that corresponds to Ea value for substitutional boron. Along with stabilization of boron atom position (recovery effect), an increase in abundance of acceptor defects with low activation energy was observed. The information on the defects got with Q-DLTS is analysed in conjunction with photoluminescence spectroscopy data obtained for the same samples. This work was supported by the Russian Foundation for Basic Research Grant No 03-02-16406 and Grant INTAS-00-2123.

R3.27
MAS NMR Study on the Structural Changes of Zeolite-NaY under Electron Irradiation. William Gu and Rodney C Ewing, Dept. of Nuclear Engineering and Radiological Sciences, University of Michigan, Ann Arbor, Michigan.

Previous studies indicated that zeolites are susceptible to solid-state amorphization under energetic particle irradiation or upon thermal
treatment at high temperatures. In the present work, strontium ion exchange experiments have been conducted for neutron irradiated, thermally treated, natural zeolite. It is found that ion-exchange ability of a neutron irradiated zeolite is between the original and heat-treated zeolite. This implies that the ion-exchange sites begin to lose due to the structure changes in the framework under neutron irradiation. The results of high-resolution X-ray magic-angle spinning nuclear magnetic resonance (MAS NMR) indicate the bond angles of both Al-O-Si and Si-O-Si decrease with the increase of neutron-irradiation dose levels, but the changes in the former are larger than the latter. The decreasing of bond angles of Al-O-Si results in more resistant to neutron irradiation damage. It is also found that [AlO6] formed at higher dose level, which means the mild demetallization occurred during neutron irradiation. The contract of the frame work under neutron irradiation by the decrease of Al-O-Si and Si-O-Si bond angles and the formation of [AlO6] is responsible for the ion-exchange ability variation of zeolite after neutron irradiation.

R3.28 Study on Proton-Irradiation Effects upon the Optical Behavior of Transparent MgAl2O4 Ceramics. Lihai Lin, 1, 2, Je He 1, 2, Taocheng Lu 1, and Peng Wang 1 1Department of Physics, Sichuan University, Chengdu, China; 2Key Lab for Radiation Phys. & Technol. of Education Ministry of China, Sichuan university, Chengdu.

The transparent ceramics samples of MgAl2O4 were irradiated by proton beams with energy of 7.5-6.6 MV and flux from 1 x 10^{10} /cm^2 to 2 x 10^{11} /cm^2. After irradiation, the samples were annealed at different temperatures from 350 to 550°C. The measurements of ultraviolet-visible-infrared absorption spectra were performed before and after irradiation and annealing. It is found that there is an absorption peak at 237 nm of F color centers and absorption band at 370nm of V color center after irradiation with the flux of 1.5 x 10^{11} /cm^2 and energy of 18-MeV proton beams. V centers and part of F centers were eliminated. In order to explain these processes, positron lifetime spectrum is measured. It is shown that while F centers disappeared after annealing, some V centers were accumulated during the annealing.

R3.29 Ion Beam Irradiation Effects on Polymers. Mircen Chopra, Indian University Cyclotron Facility, Bloomington, Indiana.

The physical and chemical modifications induced in polymers under the effect of ion bombardment result from the energy deposited within the target by the incident ion. This energy induces excitation and ionization processes that finally result in scavenges reactions. The products of these reactions (ions, radicals and radical like molecules) are non-equilibrium species that are not stable in the environment. The crosslinking and scission reactions modifies both the molecular mass distributions and the average molecular mass of the polymer, affecting the physical properties of the polymeric target as well as its behaviour upon further bombardment. Thermal spikes model assumes that the high amount of energy deposited within insulating polymers by accelerated ions leads to a large local heating, which is responsible for the formation of free radicals. Our experimental data [1-3], obtained by electron spin resonance investigations on different polymers irradiated with various accelerated ions such as O, N, F, and Ne revealed a significantly lower average temperature within the incident particle track than predicted by the thermal spike description [1-3]. The ESR studies revealed that for polyethylene terephthalate and polycarbonate films the local heating is relatively modest and that a big fraction of the latent heat is not heated above the melting temperature, that the free radicals are captured by extreme exchange interactions in clusters along the incident particle track, that the exchange interactions are monotropic, and that the anisotropies associated with the onset of segmental motions above the glass transition temperature are affecting the chemical structure as well as the latent track features. Based on these results, a model for the latent track and for the interaction between incident ions and insulating materials is suggested. A critical review of ion beam induced decomposition processes is presented. 1. M. Chopra, J. Reyes-Romero, Electron spin resonance investigations on polycarbonate irradiated with U ions, Nucl. Instrum. and Meth. B, 185-186, 7582, 2001. 2. O. Puglisi, M. Chopra, W. Eage, G. Congiu, and J. Reyes, J. Phys. Chem. B, 104, 3651, 2000. 3. M. Chopra, J. Reyes-Romero, Spectroscopic investigations on ion beam irradiated polycarbonate, Nucl. Instrum. and Meth. B, 166-167 (1-4), 944-948, 2000. 3. M. Chopra, ESR investigations on ion beam irradiated polymers, Nucl. Instrum. and Meth. B, 131, 85-90, 1997.

R3.30 Influence of ionizing radiation on montmorillonite, Stephanie Soulard, Thierry Alonso, Geza Czablat, Lamine Wang and Rodney C. Ewing, 1, 2Mineralogy, University of Paris, PARIS, France; 2Laboratoire des Solides Irradiés, Ecole Polytechnique, Palaiseau, France; 3Nuclear Engineering & Radiological Sciences, University of Michigan, Ann Arbor, Michigan.

Smectites, such as montmorillonite, are a major component of bentonite, a material considered for engineered barriers in high level nuclear waste repositories (HLNWR). In order to predict the long-term performance of the barriers, knowledge of the chemical factors such as, e.g., thermal gradient, redox potential or mechanical stresses are currently considered. By contrast, little is known about radiation effects in smectite, although it might affect the properties of this mineral through cumulative radiation damage produced by ionizing radiation. The present study focuses on radiation damage in montmorillonite considered as a simplified model of bentonite. Two clay types have been selected, one from Licinian (China, CHI), an iron-poor smectite containing native radiation-induced defects, and the other (MX) separated from the MX80 reference bentonite (Wyoming, USA). In order to simulate ionizing radiation effects, irradiations with electron and helium ions have been performed, using a large dose range consistent with HLNWR, up to 3.5 10^9 Gy Radiation effects have been determined by combining X-ray diffraction, Fourier Transform Infrared spectroscopy, Electron Paramagnetic Resonance (EPR) and Mössbauer spectroscopic methods. Two main effects are induced by irradiation. The first one concerns the formation of different trapped holes located on oxygen atoms of the smectite structure. They are characterized by different thermal stabilities, according to their origin. The second effect concerns a modification of the oxidation state of structural Fe and hydrogen, detected by Mössbauer spectroscopy. The type (reduction or oxidation) and intensity of redox modifications are sample- and dose-dependent and vary with the nature of the interlayer cation. Changing its nature also has a consequence in the influence of the water content on the redox effects: each irradiated montmorillonite presents a specific response to irradiation with and without thermal treatments. Results will be compared for α and β irradiations and with data on radiation effects in montmorillonite and kaolinite. As the redox modifications strongly modify the layer charge, the discussion will focus on their influence on smectite properties relevant for HLNWR.

R3.31 Ion Irradiation of Metallic Nanoclusters in SiO2: Compositional and Structural Modifications. Giovanni Matti, 1, 2Valentina Bello, 1 Giovanni De Marchi, 1, 2Chien Muzcio, 1, 2Philo Muraski, 1 Cinzia Suda 1 and Giancarlo Battaglini, 1, 2Dept. of Physics, University of Padova, Padova, Italy; 1Dept. of Physical Chemistry, University of Venice, Venice, Italy.

Composite materials made by monocolonetal or metallic alloy nanoparticles embedded in SiO2-based matrices exhibit peculiar nonlinear optical properties which are function of the cluster size and composition. Sequential ion implantation in glasses has demonstrated to be a very effective technique for such composite. In this work we report on the use of ion beam irradiation to induce transformation (either compositional or structural) on metallic nanoclusters in SiO2. An elementselective de-alloying in bimetallic Au-Cu and Au-Ag nanoclusters prepared by sequential ion implantation has been found upon ion irradiation or thermal annealing in oxidizing atmosphere. For instance, in the Au-Ag system, irradiation with He, Ne, Ar or Kr ions promotes a preferential extraction of Au from the alloy, resulting in the formation of Au-enriched "satellite" nanoparticles around the original Au-Ag nucleus. For a proper comparison, all the irradiations were performed keeping constant the energy density and the power density related to the samples, while varying the nuclear (S) vs. electronic (Se) fraction of the energy loss by using different ions. A systematic investigation on the role played by the irradiation parameters (i.e., dose, dose-rate, energy of the implanted ions) has been carried out. A correlation between the nuclear component of the energy released by the irradiating ions and the size and density of the satellite clusters is found. On the contrary, thermal annealing is found to promote preferential extraction of the less noble metal: in the case of Au-Cu system the preferential interaction of the incoming ions with copper promotes CuO formation, therefore extracting Cu from the alloy. Effect of ion irradiation on other systems (like In nanoclusters in SiO2) will be presented, showing a strong influence on the nanocluster size distribution.

R3.32 Influence of Hydrogen Plasma Treatment on He Implantation-Induced Nanocavities in Silicon. A. Vengurlekar, 1
He implantation followed by thermal anneal is a well-established technique for creating layers or bands of cavities in silicon. This process is a consequence of the interaction between He and ion-implant-induced vacancies. Applications of such cavity layers include gettering and localized minority carrier storage. Despite differences in the formation mechanisms, compliant substrates for lattice-mismatched heterostructures. Studies have shown that the presence of interstitial-type defects can lead to the shrinkage of He cavities due to the interstitial capture by the cavities. However, the details of the interaction of the cavities with vacancies. Here we present results on the formation of He-cavities in Si in the presence of vacancies produced by electronic cyclotron resonance (ECR) high-density hydrogen plasma treatment. Epitaxial Si (111) samples were first implanted with 1.56 MeV He to a dose of 5.6 x 10^16 cm^-2, with or without (control) follow-up ECR plasma hydrogenation (with deuterium) at 600 W microwave power, 5 sccm deuterium flow rate, 30 min. duration and 350 °C substrate temperature. A subsequent 800 °C - 30 min anneal produces a band of cavities (~210 nm) around the He projected range (~5.6 μm). The band is mainly made up of big elongated cavities in the middle surrounded by a high density of smaller ones. Other defects (mainly dislocations) have also been observed beneath the cavity band. With the hydrogen plasma treatment, however, the morphology of the He-cavities changes significantly. Both the width of the cavity band and the cavity size are found to increase, while the area density of cavity defects decreases. Such effects can be explained in terms of the vacancy-type defects introduced by the hydrogen plasma, and thus its interaction with He-cavities. We have confirmed the generation of high concentrations of vacancies by hydrogen plasma treatment through positron annihilation spectroscopy (PAS) measurements. Additional results using lower energy (40 keV and 160 keV) He implantations following ECR hydrogenation pretreatment shed further light on the role of hydrogen-induced vacancies in He-cavity generation.

R3.33 Density Fluctuations in α-Decay Self-Irradiated Zircon.

Minerals containing uranium and thorium undergo amorphisation over geologic periods of time, providing us with fundamental data to assess the extraplated behaviour of nuclear waste forms experiencing self-irradiation during long periods of time. α-decay induced amorphization in natural zircon, ZrSiO₄, is accompanied by 18% volume swelling. The origin of the enormous macroscopic swelling is believed to be a consequence of the non-uniform structure of α-radioactive cascades. As found in molecular dynamic simulations (MD), these cascades densify and form Si₂O₅ polymers, vortices of a depleted matter. While the prediction of polymerization agrees with

ρ-NMR results, no direct experimental evidence exists so far concerning the existence of depleted regions or nanoscale voids. Even in the case where such density fluctuations are produced after the release of the recoil nucleus, these might remain away over long periods of time. On the other hand, if depleted regions do exist, they provide the structure with pathways for enhanced leaching of the encapsulated radionuclides. Smaller-scale swelling measurements were performed in a series of natural zircons with various degrees of damage. A one-dimensional position-sensitive detector was used for this purpose, providing us simultaneously with the small- and the wide-angle scattering regions. In the wide-angle region the "first sharp diffraction peak" characteristic of amorphous zircon was observed. The corresponding integrated intensity matched well with the degree of damage. Simultaneously, a signal in the small-angle region was present and it indicated that a degree of damage increased, indicating that the structural features producing the signal are located within the amorphous phase. These electron density fluctuations were found to be spherical or randomly oriented, having a characteristic size ~ 6 Å, in good agreement with nanovoid sizes found at the interior of MD cascades.

SESSION R4: Poster Session: Radiation Effects: Theoretical Modeling and Simulation
Chair: R. Fromknecht
Monday Evening, December 1, 2003
8:00 PM
Exhibition Hall D (Hynes)


Defect accommodation in 3C-SIC has been simulated by molecular dynamics using a Brenner-type potential connected smoothly to the Ziegler-Himpsel-Litmark potential. This combination was chosen because it provides a better description of equilibrium properties, as well as point defect properties, compared to previous SiC potentials, and presents a reasonable model of the repulsive interaction at distances less than 0.1 nm. Defect simulations were performed in a deformation-controlled framework to consist of point defects, vacancy and interstitial clusters and antisite defects, modelled by exchanging Si and C atoms at random or in a predefined random Frenkel pair. SiC. The system was allowed to relax with the NPT ensemble and defect accommodation was analyzed. The results provide insights into the relative importance of Frenkel pairs and antisite defects in the radiation damage of SiC.

R4.2 Atomic simulations of defect production in Si02 by neutron irradiation. Fernando Olaya, J. Marín and Jose Cuesta. Instituto Fusion Nuclear (DENIM), Madrid, Spain; & J. Esteban Domingues. Universidad de Alicante, Alicante, Spain; Lawrence Livermore National Laboratory, Livermore, California.

Silica is one of the candidate materials for future focusing mirrors in inertial fusion reactors. These materials could be exposed to high neutron doses with high energy and intensity neutron fluxes during operation. Radiation damage results in point defects and new defects that can lead to changes in the optical properties of these materials. Currently, the threshold displacement energies of Si and O atoms have been calculated using molecular dynamics simulations with the parallel code MDCAK. This study was done simulating recoil energies in steps of 10 eV starting at 50 eV until the final analysis was performed. Two different simulation boxes containing 1336 and 13206 atoms. The coordination number of Si and O atoms and the displacement of the atoms are analyzed to look for defects in this amorphous system. We also present a study of primary recoil atoms with energies larger than 5 keV up to 20 keV in amorphous silica. Different types of defects will be searched and characterized. In particular, we will focus on oxygen deficient centers generated during irradiation since they will be converted into E' centers, optically active defects. Moreover, other defects will be searched that could be responsible of potential degradation under neutron irradiation. This work was carried out under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under contract W-7405-Eng-48.

R4.3 Ripening and dissolution of boron-interstitial clusters in boron-doped silicon. Marco Cogoni, Alessandro Marstoni and Luciano Colombi. INFN, Department of Physics, University of Cagliari, Monserrato (CA), Italy.

Boron-doped pre-amorphized silicon recrystallizes upon solid-phase epitaxy (SPE) so to incorporate strongly interacting boron defects, i.e. electrically active p-type dopants. It is however known that it exists a solubility limit for boron incorporation in substitutional sites. This is the key limiting factor for the realization of ultra-thin p+/n junctions with very high active carrier concentration. Recent large-scale molecular dynamics simulations [Marstoni et al., Europhys. Lett., vol.62, p.862 (2002)] have attributed the existence of such solubility limit to the formation of micro-boron/boride/interstitial clusters (BICs). Experimental evidence of BICs has been reported as well in thermally annealed boron-implanted samples [Jain et al., J. Appl. Phys. vol.91, p.8919 (2002)]. In particular, recent data [Mirabella et al., Appl. Phys. Lett., in press (2003)] seem to indicate that the typical activation energy for nanometerized BICs dissolution is about 3 eV. In this work we present a thorough computational investigation on BICs formation and dissolution, based on a combination of large-scale molecular dynamics (MD) and temperature-accelerated MD simulations. Present simulations turn out to be consistent with available experimental information and provide valuable physical insight on the relevant nanoscale mechanisms responsible for the formation of BICs during SPE. In particular, we pointed out the transition from boron-BICs (as observed just after SPE) to self-interstitial-rich BICs, driving such complexes to more stable configuration. Finally, we investigated several possible reactions ruling the dissolution of BICs by emission of interstitial defects. The theoretical prediction for BICs binding energy is about 3 eV, in close agreement with recent experiments. We
acknowledge illuminating discussions on temperature-accelerated dynamics with A. Voter (LANL, Los Alamos, NM).

R4.4 Simulations of Electron Diffraction Contrast Images of Nanometer-sized Dislocation Loops. Z Zheng 1,2, S. I. Datzner, M. L. Jenkins 1, A. P. Sutter 3, and M. A. Rooks 1 Materials University of Oxford, Oxford, Oxfordshire, United Kingdom; UKAEA, Culham Science Centre, Abingdon, Oxfordshire, United Kingdom; Laboratory of Computational Engineering, Helsinki University of Technology, Helsinki, Finland; 4Materials Science Division, Argonne National Laboratory, Argonne, Illinois.

Nanometered dislocation loops in crystals are usually investigated by using direct imaging and diffraction electron microscopy, particularly under weak-beam conditions. Image simulations obtained under the same conditions are necessary for a full analysis of such images. We have developed a new code for simulating electron diffraction contrast images by solving numerically the Howie-Basinski equations, which avoid the so-called column approximation. The code is capable of simulating rapidly and accurately diffraction contrast images of dislocation loops under both weak-beam and strong-beam diffraction conditions. A database of images has been built up, which includes images from dislocation loops with arbitrary orientation and under various diffraction conditions. This can be used to compare with experimental images quantitatively, for example to extract information on loop morphologies. Further simulations of images of defects of more complex morphology, such as the clusters seen in molecular dynamics simulations of displacement cascades, are in progress.


The controlled fabrication of a narrow layer of Si nanocrystals (NCs) in thin SiO2 films for multi-dot nonvolatile memories (NC memory) is still a considerable materials issue, which will be addressed in this contribution. The synthesis of NCs by Si implantation of SiO2 followed by a thermal treatment aims at an optimum NC density. A NC density being as high as possible is required in order to achieve a substantial threshold voltage shift of the MOS transistor. On the other hand, the advantages of the NC memory, as good scalability and data retention, are lost at too high NC densities. Then NCs change can spread over neighboring NCs by direct e− tunneling, i.e. due to electrical in-plane percolation. One single oxide defect could discharge several electrically percolated NCs. This contribution is devoted to the trade-off between these two optimization routes. The Si NC formation by nucleation, growth and Ostwald ripening in low-energy Si implantation SiO2 is simulated using a kinetic lattice Monte Carlo model [1]. On the basis of these atomistic simulations, the dependence of the Si NC density, the distribution of the NC spacing as well as the threshold for extended electron tunneling paths are predicted. Thus, process conditions could be identified, where NCs align in macroscopic density as high density as possible and are only isolated. The work was supported by the EU trough the growth project no. G5RD-2001800320. [1] T. Mueller, K.-H. Heinrich, W. Mueller, Appl. Phys. Lett. 81 (2002) 3049.

R4.6 Structural Stability of Ion Bombarded Thin Films. Alessio Lampedri and Paola Maria Ossi, INFN - Dipartimento di Ingegneria Nuclare, Politecnico di Milano, Milano, Italy.

We discuss the segregation-change transfer (SCT) atomistic model for the nucleation of crystalline or amorphous phases in binary compound films, irradiated under conditions suitable to the formation of dense collision cascades. The space and time evolution of a prototypical cascade lead to non-equilibrium compositional and electronic density profiles at the interface between the cascade and the surrounding crystalline matrix. The condition of the initial compound, mimetic system relaxation via formation of dimers of the effective compound. The energy cost to produce one such dimer, the difference of formation enthalpy between both effective compound and the corresponding initial compound and the local deformation associated to a CTR are calculated. We analyze a meaningful set of metallic and nonlinear compounds whose behaviour under ion bombardment is known. Threshold values are found in the above structure stability parameters; these allow for a qualitative separation, with a clear physical meaning, between compounds suitable retaining a structure upon ion bombardment, irrespective of their chemical nature.

R4.7 Molecular Dynamics Study of Surface Morphological Evolution By Cluster Impacts. Takashi Adachi 1,2 and Jiro Misra 1
1Quantum Science and Engineering Center, Kyoto University, Kyoto, Japan; 2Collaborative Research Center for Cluster Ion Beam Process Technology, Kyoto, Japan; 3Collaborative Research Center for Nano-scale machining with advanced quantum beam technology, Kyoto, Japan.

For the last decade, the surface modification processes utilizing the impact of large cluster ions have been proposed. One of the unique properties of cluster ion impact is that the low-energy and high-density atomic irradiation can be realized simultaneously. Therefore, when a cluster impact onto the solid target, some collisions between the target atoms at the shallow surface region are exposed by the abundant collisions with incident atoms, which results in local heating, large motion of and chemical excitation of the surface atoms. Many experiments have proved that cluster irradiation shows remarkable advantages in thin film formation, surface smoothing and high-rate and high-aspect etching. In order to understand the characteristics of surface modification process with cluster ion irradiation, molecular dynamics simulations of Ar cluster impacting on Si surface with various surface structures were carried out. It was found that the surface morphology is dynamically deformed with only one cluster impact and the impact process of cluster is different depending on the local surface structure. For example, when an Ar45 cluster accelerated with 20keV impacted on the convex point of the surface, the hill was compressed and the impact area was smoothed. On the other hand, at the impact on concave point, a deeper crater was formed compared with the impact on film surface. In this investigation, both the evolution of surface morphology with cluster irradiation will be discussed from these MD results of single and continuous impact of clusters. This research is supported by New Energy and Industrial Technology Development Organization in Japan.


Development of nanocluster defects in metals induced under high-energy environments significantly affects the mechanical behavior at microscopic lengths scales. Radiation also causes the change in deformation behavior in microscopic scales, which originates from interactions among defects such as defect clusters, dislocation, cracks, or grain boundaries. In this work, structural evolution of dislocations interacting with defect clusters is studied computationally using stochastic discrete dislocation dynamics scheme at room temperature. Simulations are run for single crystals of irradiated copper, palladium, and molybdenum under uniaxial loading condition, with randomly distributed Frank sessile faulted loops, stacking fault tetrahedra, perfect loops, <100> (100) type loops, and <111> (111) type loops. Simulation results indicate irradiation hardening behavior and enhancement of Portevin-Le Chatelier type mechanical instability as increment of irradiation dosage. This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48, and the support of the DOE (Grant No. DE-FG02-91ER45429).

SESSION R5: Radiation Effects in Ceramics, Glasses and Polymers II
Chair: D. Simone and S. Thvestham
Tuesday Morning, December 2, 2008
Room 306 (Hyres)

Experimental and computational results on ion-beam-induced defect production, damage accumulation, and thermal recovery in SiC are reviewed. The accumulation and recovery of disorder on the Si and C sublattices are determined experimentally by ion-channeling methods. Atoms-level simulations are used to determine stable defect configurations, defect production cross sections, energy transfer, and defect migration processes. These studies show that energetic C and Si collision cascades, with energies up to 50keV, primarily produce single interstitials, mono-vacancies, antisite defects, and small defect clusters. Overlapping of Si cascades results in the interaction of...
defects and clusters that stimulate cluster growth and produces long-range structural disorder. For energetic Au cascades, monolayer amorphous carbon produced disorder in the Au cascades, along with point defects and smaller clusters. Structural image simulations of the subcascades structures produced by energetic Si and Au recoils are consistent with experimental high-resolution transmission electron microscopy images. The disordering behavior and volume change observed experimentally and from molecular dynamics simulations are in good agreement, thus providing atomic-level interpretation of experimentally observed features. Multidimensional modeling measurements at 150 K indicate that Si and C interstitials are produced in both stable and higher energy configurations, and annealing above 150 K results in relaxation of the interstitials to be configurations that are not close to any of the Si and Si clusters in the stable 
recombination. Simulations of close-pair production and recombination in SiC indicate that the activation energies for recombination of most close pairs range from 0.24 to 0.38 eV. Several distinct dynamic and thermal recovery stages are observed over temperatures close to 870 K, and are consistent with interstitial and vacancy migration energies that have been determined by computational methods.

9:00 AM R5.2 Structural Disordering in Magnesium Aluminate Spinel Compounds under Ion-beam Irradiation. Syo Matsumura, Mikio Shimada, Kazuhiro Yaeda and Chiken Kinoshita, Applied Quantum Physics and Nuclear Engineering, Kyushu University, Fukuoka, Japan.

Atomic disordering of Mg$_2$Al$_2$O$_4$ was examined on specimens irradiated with 1 MeV Ne$^+$ (4.5, 10$^{16}$ ions/m$^2$), 500 keV He$^+$ (2.0, 10$^{16}$ ions/m$^2$) and 900 keV Fe$^{4+}$ (5.0, 10$^{15}$ ions/m$^2$) at an ambient temperature. High Angular Resolution Electron Channeling X-ray Spectroscopy (HARECSX) of analytical electron microscopy was utilized for the quantitative analysis of atomic configuration. Structural disordering takes place with progress of displacement damage under irradiation with 1 MeV Ne ions or 500 keV He ions. It proceeds dominantly with positional exchange between A$^+$ ions on octahedral (VI) sites and Mg$^{2+}$ ions on tetrahedral (IV) sites. Dispersion of O$_{2-}$ ions is also recognized in heavily damaged areas. Irradiation with 500 keV He ions causes less disordering than 1 MeV Ne ions irradiation does. The less disordering tendency is attributed to a higher ionizing rate under He irradiation, since recovery or recrystallization is accompanied with the regeneration of displaced ions. Ion tracks with structural disorder were observed in plan-view of a specimen irradiated with 200 MeV Xe ions. HARECSX X-ray profiles indicate that the disordering has taken place in some degree even at an extremely small amount of knocked-on displacements (less than 10$^{-3}$ dpa). Highly enhanced electronic energy deposition more than 20 keV/nm induces local displacement of ions significantly, resulting in the disordering. Discussion will be performed in terms of the roles of displacement damage and electronic excitation in the atomic disordering in spinel compounds.

9:30 AM R5.3 Irradiated cubic single crystal SiC as a high temperature sensor. Alex A Volinsky and Lev Ginzburg, IPMCL, Motorola, Tempe, Arizona; "L.G. Tech-Link, Chandler, Arizona.

Radiation is known to cause point defect formation in different materials. In the case of cubic SiC, single crystal radiation flux on the order of 2x10$^{12}$ neutrons/cm$^2$x 0.18 MeV causes over 3% volume lattice expansion. Radiation-induced strain (measurable by X-ray diffraction) can be relieved when the annealing temperature exceeds the temperature of irradiation. Based on this effect the original technology of maximum temperature measurement was developed a while ago. Single crystal SiC sensor small size (10x30x300 microns), wide temperature range (100-1400 C), "no-lag" installation, and exceptional accuracy make it very attractive for use in small, rotating and "hard-to-access" parts, including, but not limited to gas turbine blades, Shuttle ceramic tiles, automobile engines, etc. With the advances in X-ray technology, micro and thin film growth techniques, it is the time to revise and update this technology. Modeling of the radiation damage, as well as annealing effects is also beneficial.

9:45 AM R5.4 He$^+$ ion damage in SiC studied by charge collection efficiency measurements. Roberta Nipoti, IMI Bolzano, CNR, Bologna, Italy.

Silicon Carbide (SiC) is a wide band gap semiconductor regarded with great interest for power electronic applications for space ambient too think to the good temperature showed by SiC against radiation damage. This work presents a study about the variation of the charge collection efficiency in a SiC diode used as an alpha-particle detector for increasing alpha-particle fluences. The micro-beam facility of the National Laboratory of Legnaro in Italy was used. The ion beam was He$^+$ at 2 MeV and had a spot diameter equal to 1.5 micron. The SiC diode was a large area n-type epilayer SiC Schottky diode. The diode was not biased. The pulse charge amplitude (PIA) per He$^+$ ion was recorded versus the beam spots. Above 50 keV about 75% of the diode was irradiated. He$^+$ fluences were studied in the range 1-500 ions/heavyspot, i.e. in the range 10E13-10E15 ions/cm$^2$. A statistics of about 1000 events per fluence value was constructed. The average values of these PIA distributions were almost constant from 1 ion/spot up to 10 ions/spot while they monotonically decreased with increasing fluence values above 10 ions/spot. The profile of the electron-hole (e-h) pairs and the damage in the SiC diode, both in the depleted and the neutral region, taking into account the SiC diode structure, the stopping power of the alpha-particles and the fact the SiC diode was not biased. The SiC diode charge collection efficiency was described by assuming a linear dependence between the charge recombination velocity at the damage plane and the ion fluency. (1) R. Nipoti et al., Nucl. Instr. and Meth. Phys. Res. B136-136 (1998) 1340-1344.

10:00 AM R5.5 Irradiation-Induced Recovery Of Disorder In Gallium Nitride AlGaN Carbyne, SiC,透露。Mitsunori Sato, Ken-En Hashi, Katsuhiko Inoue, Hiroyuki Matsuoka, Tohoku University, Sendai, Japan; "K. K. Ide, J. Tenshu, M. H. Fujii, K. Yamamoto, Fukuoka University, Fukuoka, Japan.

Both gallium nitride (GaN) and silicon carbide (SiC) are wide band gap semiconductors that have great potential for a wide range of electronic and optoelectronic applications, and SiC also has significant potential for future nuclear reactor power generation. In general, irradiation-induced atomic disorder is detrimental to the fabrication of devices and performance of the materials under high temperature or nuclear operating conditions. Recent studies indicate that thermal recovery of irradiation-induced disorder is not significant for annealing temperatures up to 1200 K, while SiC shows several thermal recovery stages over similar temperature regimes. The case of GaN, alternative methods of damage recovery that do not involve high temperature heating need to be explored. It is well known that ion-beam irradiation deposits energy into materials primarily through elastic and inelastic atomic collisions. The elastic collisions displace atoms, producing defects that can stimulate damage recovery and epilayer recrystallization processes, while the inelastic collisions can result in locally excited states that can affect local energy barriers to recombination and diffusion. These dynamic recovery processes may enhance or stimulate recovery of disorder that is not otherwise thermally recoverable at these high temperatures. In the present study, irradiation-induced recovery of damage states in GaN and SiC have been investigated. The results show evidence for irradiation-induced recovery in GaN at 873 K, which is far below any current temperature for thermal recovery. The dependence of recovery fractions on the preirradiation damage level and ion fluence for irradiation will be presented. Results for SiC indicate evidence for irradiation-induced recovery on both the Si and C orbitals near room temperature. Epilayer recrystallization in SiC under irradiation and ion-irradiation conditions will also be compared and discussed.

10:30 AM R5.6 Radiation Damage Tolerance In Complex Oxides. Kurt Edward Sickafus, Robin W Grimes, Mark R Levy, James A Vinkler, Ming Tang and Ping Lu, "Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, New Mexico; "Department of Materials, Imperial College, London, United Kingdom; "Dept. of Materials Science and Engineering, New Mexico Institute of Mining and Technology, Socorro, New Mexico.

We have used atomistic computer simulations and ion beam irradiation to examine radiation damage accumulation in single- and multi-component oxides. We have developed contour energy maps via computer simulations to predict the effects of oxide structure and chemical composition on radiation-induced atomic disorder, defect migration, and swelling. Ion irradiation damage experiments have been performed on fluorescent, pyrochlore, biloxite and perovskite-structured oxide ceramics to test the predictions from computer models. Our computer simulations predicted the radiation induced atomic disorder energies in 3.3 ABO$_3$ perovskite compounds are considerably lower than in A$_2$B$_2$O$_7$ fluorescent-structures compounds, as well as some A$_2$B$_2$O$_7$ pyrochlore compounds. After irradiation these disorder energies are considerably less favorable than those in the sesquioxi bicobate-structured compounds. These results may help to explain our observations of poor radiation damage behavior in 3.3 perovskites such as LaAl$_2$O$_3$ and YAl$_2$O$_3$ compared to more fluorescent-structured oxides as well as bixbyite-structured sesquioxide compounds such as Dy$_2$O$_3$ and Er$_2$O$_3$. This
presentation will examine theoretical predictions of radiation damage behavior and the results of experimental tests using ions.


The focus of this study is the development of hydrogen containing polyethylene burnable poison rod assemblies (BPRAs) surrounded by water as a moderator to reduce the energy of the neutrons for a high level of fission are important to control the neutron flux and maintain a constant power in a pressurized water reactor (PWR) which has been used to develop burnable poison rod assembly. Herein, a cross section has been used for a burnable poison in separate lattice pin or plate form of B4C and Al2O3 in a zirconium alloy cladding tube. Burnable poisons reduce the excess reactivity by capturing neutrons at the beginning of cycle (BOC). These burnable poison materials decrease their negative reactivity approximately at the same rate as the reactivity in fuel decreases and are only occupying space at the end of cycle (EOC). When this depleted burnable poison material is substituted for a polymeric material, the fuel cycle is improved by the extra moderation effect of the hydrogen in the polymer. Extended lifetimes of fuel batches and higher burn-up make nuclear power more cost-competitive. The following properties are required to use polymeric materials as the matrix of burnable poisons: 1) They should have at least 5% of hydrogen to show economic benefits (simulation study by K. S. Allen, 2) They must not melt or decompose if exposed to hydrothermal conditions (350°C and 3,000 psi), 3) They must have good thermal stability to withstand the operating temperature (above 350°C) in inert atmosphere during periods of fuel cycle 4) They must have a good radiation stability and proper thermal conductivity. Our research group has screened the polymeric materials by use of an auto clave test. High density polyethylene (above 300Mrad) and ultra-high molecular weight polyethylene (above 100Mrad) crosslinked by high gamma irradiation dosage were shown to have acceptable hydrothermal stability under 350°C and 3,000 psi of auto clave condition. All Samples were prepared by exposing to the gamma irradiation in a 60Co source to obtain a range of dosages between 70 and 700 Mrad. The samples both after and before auto clave test were characterized by Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), Thermogravimetric analysis (TGA), Differential scanning calorimetry (DSC) and Instron tensile tester in order to correlate the changes in the structure with the properties. The technique of solvent extraction was used to determine the gel content and the swelling ratio of the crosslinked PE.

11:15 AM R5.8 PS surface modification and influence of the ion irradiation on the metal adsorption probability, Jurgita Zekonyte, Ulrich Schuemann, Joern Eriksen, Vladimir Zaporojchenko and Franz Fasold, Chair for Multicomponent Materials, Christian-Albrechts University of Kiel, Kiel, Germany.

Changes in physical and chemical properties of a polymer film may be induced by exposing the material to a variety of surface modification techniques, such as chemical modification, treatment with physical gases, or with atomic or molecular beams, which allow to induce changes into polymer surface without affecting the bulk. In order to understand the underlying mechanisms XPS, TEM, AFM, FTIR techniques were used to study the alterations of the polystyrene (PS) surface after irradiation with Ar, N2, O2 ions at 1 keV energy under well controlled conditions with low fluences from 5 x 1012 to 1016 cm-2. The ion bombardment led to surface functionalization, loss of aromaticity, free radical formation, chain scission, and cross-linking. The work mainly focused on the induced changes in the surface glass transition temperature, Tg, and the condensation coefficient, C, of Cu and Au on the PS. The results of surface Tg (measured using the novel metal cluster embedding method[1]) on the surface. The Tg rose with increasing ion fluences. The ΔTg increased up to 20 K for the polymer treated with Ar ion fluence of 5 x 1013 cm-2. At this fluence the cross-linking density increased up to ~ 20%. It is known that metal cluster can also strongly change the polymer without removing the polymer, but form 3D-clusters during the vapor phase deposition. In the case of PS the incomplete condensation was observed on the untreated polymer at RT. The Cu clusters formed had a radius of ~ 1 in a density of 1015 cm-2. The Cu ion bombardment in the presence of a defined concentration of defects that acted as a new adsorption sites on PS, leading to the enhancement in the condensation coefficient and the chain density with increasing ion fluences. [1] V. Zaporojchenko, T. Steuerkus, J. Eriksen, F. Fasold, Macromolecules, 38(5) (2001) 1125.

11:30 AM R5.9 Diamond Synthesis from Organic Polymers using Electron Beam Irradiation, Sung-Oh Cho, Dept. of Nuclear and Quantum Engineering, Korea Advanced Institute of Science and Technology, Daejun, South Korea.

We have discovered that two different types of polymers, crosslinking type polyethylene and scission type polymethyl methacrylate, can be transformed into diamond crystals by electron beam irradiation. Since organic polymers contain molecular units with a periodic structure, they can serve as good carbon sources for the formation of diamond, which is composed of regularly arranged carbon atoms. In particular, polymers in powder form were used as experimental material. Burnable that each of the polymeric powder particles can be completely transformed into diamond crystals under irradiation of high-fluence electron beam. Single-crystal diamonds with the sizes ranging from several ten micrometers up to several millimeters were obtained from the polymeric powders. Besides the diamonds, a variety of carbon structures such as carbon nanotubes, carbon onions, intermediate carbon phases were produced, promising potential application of this technology in diverse scientific and industrial applications in addition to studying of unusual carbon phases.

11:45 AM R5.10 γ-Ray Irradiation Practical Conditions for Low Molecular Weight Chitosan Material Production, Rangrong Yoksan1, Mitsuuri Akashi2, Mikijii Miyata2, Biramonti Sirehatman2 and Shunioh, Chirosehnan2, 1The Petroleum and Petrochemical College, Chiangkong University, Bangkok, Bangkok, Thailand; 2Office of Atomic Energy for Peace, Ministry of Science and Technology, Bangkok, Bangkok, Thailand; 2Graduate School of Engineering, Osaka University, Osaka, Osaka, Japan.

Chitin-chitosan is the second most natural occurring polysaccharide with specific properties of biocompatibility, biodegradability, bioactivity, etc., which can be expected for the uses in biomedical field. However, due to the strong inter- and intramolecular hydrogen bond network, chitin-chitosan has the limitation about the solubility in most organic solvents to obstruct the derivatization. Thus, even various derivatives have been proposed, the commercial products are facing the problems of quality control and quantitative reactions. In molecular weight reduction can be considered as an alternative way to improve the solubility and reactivity. For the past decades, several pathways have been done to prepare low molecular weight chitosan (LMWC) and for oligo-chitosan such as chemical treatment, enzymatic degradation, and photoirradiation. Photoirradiation requires the expertise and operating system; the advantages about no chemical waste, simple process, and one step without extra purification are attractive for large-scale production. Although chitosan irradiations were reported in the past[5], the practical conditions have never been proposed. The utilization of irradiation should be acceptable only if the structural characterization of the irradiated chitosan has been done extensively. This will also assure us that the product obtained functions as a chitosan and can be used as a starting material for further derivatization. The present work focuses on a range of γ-ray doses for lowering molecular weight at the level that the current backbone is γ-ray on the conditions: (i) chitosan in; dry flake, dispersing in water, and dissolving in acid, (ii) chitosan with and without radical initiators, (iii) single and twice irradiation. The structure of the products clarified by FTIR, NMR, XRD, ESR, TGA, and HPLC including viscosity measurement will be reported.

SESSION R6: Computer Simulation and Modeling
Chairs: F. Guo and K.-H. Heing
Tuesday Afternoon, December 2, 2013
Room 305 (Hynes)

1:30 PM R6.1 Topological Identification of Defects and Amorphous Regions In Irradiation-Disordering Crystalline Structures, Lien W. Hohka1,2, Clark L. Allred1,2 and Xiong Kong Yuen1,2.

1Department of Materials Science & Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts; 2Department of Nuclear Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts; 3Charles Stark Draper Laboratory, Cambridge, Massachusetts.

Computer simulations of defect formation in irradiation cascades in crystalline structures typically require identifying defects more generally—disordered atomic arrangements within a matrix that becomes progressively strained and disordered. It is of great interest to know whether an atom is situated within an ordered array of other atoms (crystalline phase) or is part of a more disordered arrangement.
(amorphous pockets, specific families of defect clusters, or any of a number of single atomic defects). Currently, there is no simple, yet accurate, method to readily identify such disordered atomic configurations in simulations. The application of fiducial grids [referred to original crystal atom positions] is shown to be inappropriate and inaccurate for even modest defect content. In this presentation, we introduce instead a topological approach that considers structures as collections of nodes and bonds and evaluates the local topology associated with each atom in the simulation. "Crystalline atoms" (those belonging to an ordered crystallographic arrangement) are identified by comparing the GNs topologies to the topologies established for a known crystalline structure. Regions of radiation-induced phase transformation to other crystal structures can likewise be recognized. Various defects, including "amorphous atoms" (atoms belonging to amorphous regions), are similarly identified by their unique topological signatures, many of which have been catalogued for Si and Ge structures. The evolution of disorder can thus be followed through a complete range of inter- and final disordered structures. Examples are drawn from collision-cascade MD simulations in Si and Ge structures; however, it is relatively straightforward to extend this method to other simple crystalline structures, disordered mechanisms and simulation approaches. SiC is particularly interesting, because amorphization appears to require a threshold level of chemical disorder, which can likewise be identified locally using this topological approach.

200 PM *R6.2 Atomic Simulations Of Radiation Damage Effects In Ceramics, Kostya O. Trachenko, Earth Sciences, University of Cambridge, Cambridge, United Kingdom.

Several ceramics are currently used as waste forms to immobilize highly radioactive nuclear waste, with more being considered as potential waste forms. Our research talks have begun to provide insights about the radiation damage effects in several ceramics. The effects addressed are structural changes under irradiation that are important for the safe storage of highly radioactive nuclear materials, including polyenergetic, damage stability, large density fluctuations on the nanoscale, volume increase, and damage percolation. We discuss the implications of these changes for the safe storage, one of them being the observed percolation behaviour of diffusion. We also discuss the mechanism of "amorphization" and susceptibility of various ceramics to amorphization. We show how simulations can interact with experiments, by gaining insights into the experimentally observed behaviour, and then simulating new experiments.

230 PM R6.3 Abstract Withdrawn

245 PM R6.4 Molecular Dynamics Simulation of Displacement Cascades in Zircon, Ran Davenas1, L. Rene Corrales1, Constantin Meix2, Ahlin Chervish1 and William J Weber1. 1Fundamental Science Directorate, Pacific Northwest National Laboratory, Richland, Washington, 2CEA Saclay, GIrS-Valvette, 91191, France.

Displacement cascades in zircon, spanning a range of primary knock-on atom energies from 250 eV to 10 keV, have been simulated at 300 K. The interactions were modeled using the Coulomb potential over a long range, a partial charge model near equilibrium distances, and the Ziegler-Biersack-Littmark potential for distances less than 0.1 nm. In addition to fitting the potential to equilibrium properties, the melting behavior and diffusion coefficients in the molten state have been studied and found to agree well with experimental results. Si, Zr and U PIA have been simulated to study the effect of projectile mass on the primary damage. The nature of the primary damage state, the extent of Si-O-Si polymerization, and the statistics of damage production will be presented.

3:00 PM R6.5 Coupled Kinetic Monte Carlo And Molecular Dynamics Simulations Of Implant Damage Accumulation In Silicon. Gustav Otto and Gerhard Hofer: Institute for Solid State Electronics, Vienna University of Technology, Vienna, Austria.

Damage formation during ion implantation is a complex process that cannot accurately be modeled by binary collision simulations alone. Molecular dynamics (MD) simulations are suited to describe the quenching of collision cascades, while thermally activated processes may be treated with the kinetic Monte Carlo (KMC) method. Both phenomena need to be taken into account in order to predict the amount and type of defects depending on the implant parameters, such as ion species, energy, temperature, and dose rate. MD and KMC simulations have separately been used to investigate damage accumulation and annealing in silicon. Simulation of ion implantation at room temperature, however, requires both methods to be coupled. In this paper we describe for the first time a scheme of the coupling between MD and lattice KMC for damage accumulation. The transformation from MD to KMC is done for the smaller defects by classification into known types based on the atom positions determined by MD. Larger defects are defined by identifying neighboring empty lattice sites and assigning close interstitials to the nearest lattice site. The transformation from KMC to MD is done for the smaller defects by using their known coordinates. For the larger defects the empty lattice sites and interstitials are introduced into MD and relaxed to the energy minimum. Using this scheme we study the dynamic annealing behavior of implantation damage for light and heavy ions.

3:30 PM R6.6 Atom-scale Simulations of radiation effects in compound semiconductors and carbon nanotubes. Kai Nordlund, University of Helsinki, Helsinki, Finland.

The atom-level mechanisms of radiation damage production in III-V compound semiconductors have until recently not been well understood because of the lack of interatomic potentials which enable realistic simulations of damaging effects. We have recently developed potentials for the GaAs and GaN systems which enable description not only of the compound material, but also the pure constituent elements. Using these models, we have examined high-dose damage production and amorphization in GaAs and GaN. The models can correctly describe e.g. the onset of nitrogen bubble formation in GaN. Comparison of damage in the two compounds reveals three reasons why much less damage is produced in GaN than in GaAs; the high damage threshold, cascade damage recombination in single cascades, and subthermal amorphization of pre-existing damage by new recoils. There is a growing interest in examining how ion and electron irradiation can be used to modify the properties of carbon nanotubes in beneficial ways. We will present our simulation results and related experiments which show that carbon nanotubes can be used to make carbon nanotubes together, for ultrathin metal nanowires by using nanotubes as a mask, and produce links which strengthen the interaction between a nanotube and the surroundings.


Gallium nitride (GaN), together with other wide band-gap nitrides, holds substantial promise for advanced electronic applications. Despite the technological importance of GaN in future applications, there is very little information regarding the native defects and their properties in the material. Density functional theory (DFT) is used to study the formation, properties and atomic configuration of monovacancies, antisite defects and possible interstitial configurations in GaN. The relaxation around a vacancy is generally small, but the relaxation around antisite defects is large, particularly for a Ga antisite defect, which is not stable and converts to a N-N-C(1-2D) split interstitial. All N interstitials, starting from any possible sites, eventually transfer into the N-N-C(1-2D) split interstitial, forming N2 molecules. This defect is predicted to be the most favorable interstitial in GaN. In the case of Ga interstitial, the most favorable configuration is the Ga octahedral interstitial. However, it is found that the Ga-N-C(1-2D) split interstitial can bridge the gap between nonbonded Ga atoms along the <11-20> direction, which leads to the formation of GaNCN GaNCN with bond distance close to those noted in bulk Ga. In addition, two representative potentials, namely Stillinger-Weber and Tersoff potentials, have been employed to determine the formation of defects using molecular dynamics (MD) method in GaN. The MD results are compared to DFT calculations and to available experimental data. The present DFT and MD results provide guidelines for evaluating the quality and fit of empirical potentials for large-scale simulations of ion-solid interaction and thermal annealing of defects in GaN.

4:15 PM R6.8 Abstract Withdrawn

4:30 PM R6.9 Radiation Damage in Nanocrystalline Metals. Maria Samurs1, Peter M Derlet1, Helen Van Berghen2 and Max Victors3. 1Paul Scherrer Institute, PSI-Villigen, Switzerland, 2CPPF-Russia Technology Materials, EPFL, Villigen-PSI, Switzerland.

It is well known that grain boundaries can strongly influence the damage produced by irradiation in metals. Experiments in ion-irradiated samples have shown that the defect production is smaller than in polycrystalline counterpart, with the vacancy rapidly saturating in terms of dose. This contribution discusses the role of the grain boundary during cascade evolution with no Ni. Large-scale molecular dynamics of cascade production of the primary damage. 4/83
state have been performed in nc-Ni with average grain diameters of 5nm to 20nm. Primary Knock-on Atoms (PKA) with kinetic energies ranging from 100 keV have been investigated. The simulations show that GAs acts as a strong sink for self interstitial atoms/clusters (SIAs) via two possible mechanisms: replacement collision sequences and 1D/2D motion. In these processes, parameters characterizing the GB structure such as misfit, elastic constants and internal stresses are qualifying the sink efficiency for interstitials. The GAs initially play the role of a defect acceptor, and when the SIA cluster arrive within a few atomic distances from the GB, it starts to take over the dynamic structure and chooses an unoccupied area in the GB with a distinctive pressure and where there is enough free volume. This results in the observation of large clusters (up to seven SIAs) that move 1D/2D, something that has not been observed in single crystals. Furthermore, the nanosized GAs seems to have a flexible structure, that allows to accommodate a large amount of SIA.

4:45 PM R6.10
REACE: A New Algorithm for Low Energy Ion Implantation Simulation. Xinhong Shi, Min Yu, Ru Huang, Xing Zhang and Yangguang Wang, institute of microelectronics, Peking University, Beijing, China.

Simulation of low energy ion implantation is very important for ultra shallow junction technology. Cascade collisions and thus damage build-up not only influence the range profiles and come dose effect, so they dramatically affect the precision of the simulations. In addition, the damage build-up due to cascade collisions is amply necessary for further annealing simulations. To reduce the statistical noise, Bearden et al adopted Rare Event Algorithm (REA). However, cascade collisions cannot be simulated by REA, so dose effect is not included. To introduce damage build-up and reduce the statistical noise, 10000-20000 ions implantation should be simulated. Due to the very low computational efficiency of the previous method, the MD simulation is computationally inefficient. In this paper, a new MD algorithm, named REACE-Rare Event Algorithm with Cascade Effect, is developed combining REA and damage build-up together based on the MD technique. Differing from the existing methods, REACE can greatly enhance the computational efficiency, while retain the same precision. It separates dopant profiles simulation from implantation damage generation, in which two kinds of ions: "Real Ions" and "Virtual Ions" are defined. Real Ions generate damage build-up, and Virtual Ions are continually split out from Real Ions during the simulation process of Real Ions' moving without following the cascade collisions. In the simulation process of Virtual Ions, the influence of cascade collisions and moving defects can be involved for the special splitting methods. The dopant profile is calculated mainly by the distribution of Virtual Ions. With new splitting methods, not only damage build-up but some influence of cascade collisions can be simulated. Meanwhile, a linear splitting method is also developed to reduce the extra energy consuming of REA. The fluctuations of range profiles are analyzed and the depth of splitting layers is readjusted to make REACE more efficient. With the newly proposed algorithm REACE, simulation speed of MD technique is 5 to 60 times faster than before. Some data of simulation speed enhanced by REACE are shown in Table. REACE also makes it possible to simulate middle energy implantation using MD technique and build up the ion distribution simultaneously. All ions based on MD technique REACE can efficiently not only simulate cascade collisions and damage build-up but also reduce the statistical noise. 

9:15 AM R7.3

Cluster formation in high dose B, BF2, or BF3 implanted Si wafers is an important problem in silicon etching. It is due to the large electrical sensitivity of the junction profiles and the enhanced secondary electron yield. We have used high dose (1E16 cm^-2), as well as low dose (1E15 cm^-2) B, BF2, and BF3 implants to isolate the Ge as a pre-amorphizing implant. We have studied the Ge-profiles and cluster formation profiles. The cluster formation profiles are derived from Rutherford backscattering spectrometry (RBS) and transmission electron microscopy (TEM). The cluster formation patterns in the Ge-implanted wafers are consistent with the cluster formation patterns in the B, BF2, and BF3 implants. The cluster formation patterns in the Ge-implanted wafers are consistent with the cluster formation patterns in the B, BF2, and BF3 implants.

9:30 AM R7.4
Hydrogen-induced lattice damage of semiconductor layers for exfoliation. Sumiko Hayashi, David Bruno, Rajinder Sandhu1,2, Michael Wójcik and Mark Gogotsi, University of California, Los Angeles, Los Angeles, Illinois; Northrop, Redondo Beach, California.

Implantation of light ions such as hydrogen and helium is widely used to facilitate transfer by exfoliation of a thin layer from a semiconductor substrate onto a suitable adhesive surface. This process is widely employed in the synthesis of silicon on insulator structures and has been promoted as a technique to transfer III-V layers, especially InP to other substrates as well as for a variety of other applications. We compare the lattice damage induced to silicon layers and InP layers by hydrogen ion implantation (at a dose of 5x10^16 cm^-2 and energy ranging from 70 to 200 keV). In both cases, the hydrogen is implanted at -20°C. Wafers are polished at low temperatures (150°C) after an
oxygen plasma surface activation step. Next, etching through blistering (T ≥ 250 °C) leads to the transfer of large area silicon or InP films. The transferred silicon and InP layers are transferred to SiN / InP and SiN / GaN substrates. For comparison, unimplanted silicon structures were also wafer bonded. Transmission electron microscopy (TEM), triple axis x-ray reciprocal space imaging (RSM), and atomic force microscopy (AFM) are used to characterize the transferred layers. For the silicon case, the transferred silicon layer shows no signs of crystalline damage after the bonding and etching steps. The surface roughness, as determined using AFM, is approximately the implant depth. The TEM images show no signs of crystalline damage to the transferred layer and the crystal plane perfection of the layer - determined from the RSMs - matches that of the underlying silicon substrate. In the RSM, peaks from the Si substrate and the transferred Si layer can be distinguished, as there is a slight crystallographic tilt (≈ 0.1°) between the layer and substrate. These results confirm that silicon is an ideal candidate for layer transfer. InP transferred layer shows different behavior than the Si wafer. InP wafer without implant showed no crystalline damage. The implanted and transferred (annealed) structure, however, showed crystalline damage in both the TEM images and the reciprocal space maps. The surface roughness - similar to the silicon - was approximately the implant stage. The damage introduced to the InP layer was studied using a series of annealing sequences. The extent of damage was studied for different annealing sequences and the kinetics of the etching and damage recovery processes can be described using a model that includes the nucleation, growth, and subsequent recovery of crystallographic defects in the InP layer. Differences in InP and Si are attributed to the different nucleation sites. Post-implanted defects that are produced and the differences in the mechanical properties of the two materials.

0:45 AM R7.5 Formation of SiO2/SiC/Si Heterostructure in Si by C4 Implantation and Annealing in Controlled Atmospheres. Kai Sun, Xin Zhu and LuMin Wang, University of Michigan, Ann Arbor, Michigan.

SiO2/SiC/Si multilayer structure on a Si substrate was synthesized by high-dose C4 implantation and subsequent annealing in controlled atmospheres. The implantation was performed using a metal vapor arc ion source and an acceleration voltage of 16 kV. Subsequently, a furnace annealing at 1000 °C for 4 hours and an extraction voltage of 50 kV, the annealing was conducted in an atmosphere of 100% Ar gas for 2 hours in a 200 °C day. The as-received materials were then annealed at 1000 °C for 1 hour after cooling down to the intermediate temperature. The as-received materials were then annealed at 1000 °C for 1 hour after cooling down to the intermediate temperature.

11:00 AM R7.8 One- and Two-Dimensional Pattern Formation on Ion Sputtered Silicon. Ari-David Brown1,2, Henry Bola George3, Michael J. Aziz2 and Jonah D. Erlebacher2, 1Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, Maryland; 2Department of Materials Science and Engineering, The Johns Hopkins University, Baltimore, Maryland; 3Division of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts.

The evolution of surface morphology during ion beam erosion of Si (111) at grazing ion incidence (60° from normal, 500 eV Ar+, 0.75 mA/cm²) was studied over a temperature range of 300 to 800 °C. With all other experimental parameters fixed, it was found that one-dimensional sputter ripples oriented parallel to the projected ion beam direction form during sputtering at the lower end of the temperature range, and spatter ripples oriented perpendicular to the projected ion beam direction form during sputtering at the higher end of the temperature range. At intermediate temperatures (centered approximately at 530 °C), both parallel and perpendicular growth modes contribute to the surface morphology evolution, which leads to the formation of bumps ("dents") with quasi-rectangular symmetry. This variety of self-organized substrate morphologies may be used to template thin-film growth.

11:15 AM R7.9 New Electronic Devices Based on Ion Tracks in Insulators. Dietmar Fink1, Alexander Petrov1, Wolfgang Fink2, Kurt Hoppe3, Alexander Berdinsky3, and Amir Chandlers4, "Hahn-Meitner-Institut, Berlin, Germany; 2University Hagen, Hagen, Germany; 3Technical High School South Westfalia, Hagen, Germany; 4Novosibirsk State Technical University, Novosibirsk, Russian Federation; 5Panjab University, Chandigarh, India.

The etching and filling-up with (semi)conducting matter of track of energetic ions in polymer foils, Silicon dioxide and silicon oxynitride, eventually in combination with lithography, can be used to create new micro and nanoelectronic devices. We present as examples: miniaturized transformers, condensers, and sensors that were embedded in thin polyimide foils. Further we give the outline of the construction principle of a new family of ion track devices based on SiO2 or SiOxNy as the fluid in the between classical FETs, tunnel diodes, and vacuum diodes. Some 30 circuits have been designed and tested successfully with these new elements. They are in simple in design than classical electronics, suitable for high frequency applications, and presumably radiation-hard.
11:00 AM R7.10
Microstructure and He bubble effects on Al-Cu thin film interconnects. Cristiano Camacho1, Paulo F. Fichtner2, Fernando Claudio Zwaanski2 and Gerson Felldmann3,1 Institute of Physics, Universidade Federal do Rio Grande do Sul, Porto Alegre, RS, Brazil, 2Departamento de Metalurgia, Universidade Federal do Rio Grande do Sul, Porto Alegre, RS, Brazil, 3Departamento de Fisica e Matematica, UNIJUI, UIR, RS, Brazil.

The effects of film morphology (monocrystal or combination of grain structures) and of He bubbles on the redistribution of Cu as well as on the formation of Al-Cu precipitates in 200 nm thick Al/SiO2 films for microelectronic interconnects are investigated using advanced backscattering spectrometry, elastic recoil detection analysis and transmission electron microscopy. The grain size of the as-deposited Al-bamboo-like samples and monocrystal samples are 65 and 25 nm. After annealing (753 K, 2 h) the grain sizes change to 68 and 1500 nm, respectively. Al films were implanted with Cu and/or He ions in order to form concentration-depth profiles located 100 nm below the surface and with peak concentrations of about 2 at.%. Under such implantation conditions the Cu atoms form a supersaturated solid solution and the He atoms form a dense array of highly pressurized bubbles. Upon post-implantation thermal annealing at temperatures from 473 to 800 K, it is demonstrated that the presence of bubbles can significantly affect the vacancy fluxes inside the grains and therefore reduce or even inhibit the Cu redistribution as well as the nucleation and growth of ternary and tetra-prime Al-Cu precipitates in the Al matrix. It is also shown that monocrystal grain structures allow the control of grain size distribution within the 25 to 1200 nm size range, thus providing an additional microstructure engineering tool to improve device reliability against electromigration failures.

11:45 AM R7.11
Dynamic Amelioration in Group-III Nitrides under Ion Irradiation. Sergei O. Kuchayev1, J. S. Williams2, C. Jacobs1 and J. Zou3,1 Lawrence Livermore National Laboratory, Livermore, California, 2RSPS/ESE, Australian National University, Canberra, Australian Capital Territory, Australia, 3Division of Materials and Centre for Microscopy and Microanalysis, University of Queensland, Brisbane, Queensland, Australia.

Recently, there has been much interest in group-III nitrides (GaN, AlGaN, and InGaN). Such interest has been stimulated by important technological applications of these materials in (opto)electronics. In the fabrication of III-nitride-based devices, ion bombardment represents a rather serious and challenging source. However, ion-beam-produced lattice disorder and its undesirable consequences limit technological applications of ion implantation. Unlike the situation for mature semiconductors such as Si and GaAs, III-nitrides exhibit a strictly non-isotropic behavior involving, extreme property changes under ion bombardment. Here, we present a systematic study of the damage buildup behavior in wurtzite InGaAs (with x < 0.5) and Al,GaMgInN (with x < 0.6) films mounted on Si wafers as a function of ion energy, current density and ion species. By combining the in situ damage buildup experiments with the Rutherford backscattering spectrometry and cross-sectional transmission electron microscopy (XTEM) results were obtained, which indicate the In concentration strongly suppresses dynamic amelioration processes (i.e., defect migration and interaction processes) and, hence, enhances the buildup of stable lattice disorder in InGaN under ion bombardment. In contrast, an increase in Al content dramatically increases dynamic amelioration in AlGaN films. Based on this experimental data, we discuss physical mechanisms of the susceptibility of group-III nitrides to ion-beam-induced disordering and to the crystalline-to-amorphous phase transition. Work at LLNL was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-eng-48.

SESSION R8: Ion Beam Processing of Nanostructures
Chairs: R. Frömmel and A. van Veen
Wednesday Afternoon, December 3, 2003
Room 306 [Hynes]

1:30 PM R8.1
Metal Nanoparticle Formation in Insulators and Polymers by Ion Irradiation for Nonlinear Optical Applications. Naoki Kishimoto1, Hanna Boldyreffya2, Naoki Umeda3,4, Oleg A. Plaksin3,4 and Yoshiohiko Takeda1,1 Nanostructures Laboratory, National Institute for Materials Science, Tsukuba, Ibaraki, Japan, 2KMP, Charles University, Prague, Czech Republic, 3Institut of Materials Sciences, University of Tsukuba, Japan, 4SSSI RF, A. I. Leipunsky Inst. of Phys. and Power Eng., Obninsk, Russian Federation.

Nano-sized metal particles embedded in dielectrics are candidates for optical nonlinear materials with ultrashort response (~ps/ps-sec), due to surface plasmon resonance (SPR) of electrons confined in a nanoparticle. Ion irradiation is a superb tool to fabricate nanoparticles in insulating substrates, because of the spatial controllability and freedom from immiscibility of elements. Moreover, ion beam energy, primarily electron beam energy, is effective to make the metal precipitation via radiation-induced diffusion of implanted atoms. Since the precipitation process, more or less, is accompanied by post-irradiation atomic migration, understanding the kinetics becomes a prerequisite to use the ion-irradiation method for metal nanoparticle formation. In this paper, we study metal precipitation processes in insulators and polymers. Negative Cu ions of 60 keV, which eliminate the surface charging for insulating substrates, irradiated SiO2, MgO:2:4(A12O3), LiN2O3, and polymers of PMMA, polycarbonate and polyethylene up to 3x1017 ions/cm2. In-situ and ex-situ optical measurements were conducted to evaluate dynamic processes and resultant SPR, respectively. Nonlinear transient response at SPR was measured by laser induced fluorescence and the complete microstructure morphology was studied by cross-sectional TEM. An SPR peak around 2 eV appeared, more or less, at doses ~2x1017 cm-2 at the higher dose rate. The ion-implanted energy assisted spontaneous metal precipitation and the morphology significantly depended on insulator species and dose rate. The metastable nature of SiO2 and radiation resistance of MgO:2:4(A12O3) gave rise to characteristic morphologies. Nonlinear response of pico-sec was confirmed for the insulators, and especially LiN2O3 showed a sub-pico-sec response. Metal precipitation occurred in polymers but was more difficult to obtain a narrow SPR peak. Although radiation-induced diffusion may contribute to the precipitation of SPR, it also in polymer is occasionally hazardous to polymeric structures. The radiation-induced diffusion and radiation damage resistance are important to understand the nanoparticle formation processes in insulators and polymers.

2:00 PM R8.2
Ion Beam Manipulation to Fabricate Ordered Layered Structures and Amorphous Alloys in Some Highly Immiscible Bi-metallic Systems. X. Li1, R.P. Zhang and Qinlin Liu, Dept. Mat. Sci. & Eng., Tsinghua University, Beijing, China.

We developed a new scheme namely ion beam manipulation, i.e. ion-implantation-assisted ion beam mixing, for fabricating amorphous alloys and artificial solid-state microstructures in the metal-metal multilayers, in which the individual layer thickness was down to 2 nm, differing from the typical thickness of 5-8 nm in the conventional ion beam mixing [1,2]. We report, in this paper, some interesting results obtained in some immiscible systems by the scheme. In the Ag-W system, with a largest positive heat of formation among the transition metal alloys, amorphous alloys were obtained, for the first time, through a two-step structural transition, i.e. the initial polycrystalline Ag and W transformed into an intermediate state of bcc phase, which later transformed into the final amorphous state. While in the Ru-Pd system, the initial polycrystalline Ru and Pd transformed into a single polycrystalline face-centered-cubic (FCC) phase, which in turn was transformed into a well grown ordered structure, which, however, showed an apparent tendency to transform back to the same for phase upon overannealing [3]. For the Ag-Pt case, the intermediate phase was observed and identified to consist of two overlapping fcc lattice, corresponding to a new magnetic state of Co atom with an average magnetic moment of 2.84 μB, which was about twice the equilibrium value and probably the largest one ever observed [2]. The experimental observations are briefly discussed as a basic discussion concerning the associated mechanism were presented in this paper. References 1. B. X. Liu, W. S. Liu and Q. Zhang, Mater. Sci. and Eng.: Reports 29, 1-18 (2000) 2. Z. C. Li, D. P. Yu and B. X. Liu, Physical Review B 65, 245403 [1-6] (2002) 3. X. Y. Li, Z. C. Li and B. X. Liu, J. Physical Society of Japan 72 (1): 9-12 (2003).

2:30 PM R8.3
Formation of Nanocrystals in TiO2 and SrTiO3 by Ion Implantation in restricted volumes. Rainer Frömmel1, Gerhard Linker2, Kui Sun3, Shu Zhu3, Lumin Wang3, Marijn van Huis4, A. van Veen5, Jing Wang3, Joergen Niemeyer5, Thomas Weimann5, Tieshan Wang3 and Frank Eichhorn3, 1Forschungszentrum Karlsruhe, Institut fuer Festkoerperfysik, Karlsruhe, Germany, 2University of Michigan, Dept. of Nuclear Engineering and Radiological Science, Michigan, Michigan, 3University of Delft for Technological Interfaculty Reactor Institute, Delft, Netherlands, 4Physikaklisch-Technische Bundesanstalt, Quantenelektronik, Braunschweig, Germany, 5Forschungszentrum Rossendorf, Institute for Ion Beam Physics and Materials Research, Dresden, Germany.

Au-ions were implanted into TiO2 and SrTiO3 single crystals with doses ranging from 1x1015 to 1x1018/cm2 to 6x1016 Au/cm2 at RT and the samples subsequently were thermally annealed at temperatures of 550K to 1550K. The Au-atom precipitate to nanocrystals already during implantation at RT with an average particle size of 1.5nm.
HHTEM investigations revealed that the Au-nanocrystals, embedded in amorphous TiO2 and SiO2 regions, have a broad size and range distribution varying from large sizes in the new surface region to smaller sizes at larger depths. In the annealing process a reorientation of the Au-nanocrystal is observed, with the main effect of a decrease of the (111)-peak and an increase of the (200)-peak in the XRD spectra. After annealing the 1000K剡inside Au-implant was evaluated to ~6nm; this means that during annealing the particles grow, leading to a partially coherent orientation in the TiO2-matrix. Implantation performed through a metal mask with both 125nm and 6nm results in a displacement of the mixed arrangement of the Au-nanocrystals with a narrow size distribution of 2-nm in TiO2 and 3-nm in SiO2 in the new surface region. Au-ion implantation into microcrystalline TiO2 was performed in the amorphous structure of the mixed phase and, in this case, the microcrystalline TiO2 was formed after the implantation. In this study, the nanoparticles in the amorphous structure were formed through the dose-dependent local amorphization parameter, potential energy, volume, and inherent cluster bonding. The observed fluctuations obey a universal power law. Within the framework of the multi-Loaden picture, the resultant power law describes the distribution of multirelaxation times or cluster lifetimes. In addition, unified relation for the autocorrelation functions for such fluctuation phenomena has been derived. The behavior of the irradiated NiO system will be discussed.

2:45 PM R8.4
A multi-step process to manipulate the size distribution of nanocrystals by ion implantation has been described.\(^1\) Tony E. Hughes,\(^1\) Warren J. Mohler-Chang,\(^1\) and Michael J. Aziz,\(^1\)
\(^1\)Division of Engineering and Applied Science, Harvard University, Cambridge, Massachusetts; \(^2\)Condensed Matter Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

The broad size distribution of nanoparticles formed by ion implantation is a current limitation of this technique. Precipitates of uniform size can be obtained, in principle, by understanding and controlling the rate of metal ion incorporation, the degree of nucleation, and the state of the matrix. We have investigated the formation of nanoparticles of elements insoluble in SiO2, such as Au, by multiple implantation steps and intermediate anneals in order to control the nucleation and growth processes, thereby reducing the breadth of the size distribution. We have used cross-sectional TEM to compare samples implanted in multiple steps to samples implanted with the same dose in a single step. We discuss the effects of varying the initial nucleation dose and the growth temperature, and show that this methodology can be used to synthesize precipitates with improved size uniformity and spatial distribution.

3:00 PM R8.5
Ion-Irradiation-Induced Formation of Si Nanocrystals in Thin SiO2 Layers Sandwiched between c-Si/poly-Si.
Karl-Heinz Heinig,\(^1\) Horst Schmidt,\(^2\) Torsten Mueller,\(^1\) Lars Roestand,\(^1\) Karl-Heinz Stegemann,\(^1\) Michele Pereg,\(^3\) and Marco Fanciulli,\(^4\)
\(^1\)Inst. Ionen Technik Physik & Materials Research, Research Center Rosendorf, Dresden, Germany; \(^2\)ZMD AG, Dresden, Germany; \(^3\)Laboratorio MDM-INSF, Agrate, Italy.

Si nanoclusters (NCs) are fabricated in very thin (~10 nm) buried SiO2 layers by ion beam mixing and subsequent phase separation. This method is suitable for the formation of nanocrystals in planar and non-planar geometries. In contrast to the CVD synthesis, the NCs in SiO2 surface layers by ultra-low energy high-dose Si\(^+\) ion implantation. For instance, it has been shown recently that ambient humidity is absorbed in the as-implanted SiO\(_2\) surface layer [1] which oxidizes a large but not controllable fraction of the implanted Si during subsequent annealing. At present, great effort is devoted to Si NC formation in gate oxides for multi-portable memories. In this contribution we present experimental and computer simulation results on ion-irradiation-induced formation of Si NCs in thin SiO\(_2\) layers sandwiched between c-Si/poly-Si. SiO\(_2\) layers (8 to 15 nm thick) were covered by ~50 nm poly-Si and irradiated by [3 to 20]x10\(^{11}\) Si\(^{+}\)cm\(^{-2}\) at 50 to 100 keV. After annealing at ~1000°C for several seconds in N\(_2\) the SiO\(_2\) layer were analysed by XTEM and XRF. A combined computer study [2] of (i) ion beam mixing profiles using dynamical binary collision simulations (TRIDYN) and of (ii) Si phase separation from SiO\(_2\) using kinetic lattice Monte Carlo calculations were performed. The results of the computer simulations can be used as input for step (ii). It will be shown that under appropriate irradiation and annealing conditions NC layers form at the upper as well as at the lower SiO\(_2\)/Si interface. Using these NCs as charge storage centers in the gate oxide of MOS transistors, a promising nonvolatile memory behavior has been demonstrated. The work was supported by the EU through the GROWTH project no. GIRD/2000/08290 [1] B. Schmidt, D. Grumme, and F. Hermann, Nucl. Instr. Meth. B101 (2002) and K.-H. Heinig et al., EMRS2003 Meeting, Symp. E [2] T. Mueller, K.-H. Heinig, and W. Mueller, Appl. Phys. Lett. 81 (2002) 3049.

3:30 PM R8.6
Nanostuctural Fluctuations in Radiation-Amorphized Alloys.
Seiichi Watanabe,\(^1\) Hisashiroku Takahashi\(^2\) and Nghi Q Lam\(^3\)
\(^1\)Materials Science and Engineering, Hokkaido University, Sapporo, Japan; \(^2\)CARET, Hokkaido University, Sapporo, 060-8628, Japan; \(^3\)Materials Science Division, ANL, Argonne, IL 60439, Illinois.

Nanostructural fluctuations brought about by transient, metastable atom-cluster formation and the manifold nature of inherent atomic ordering in electron-irradiation-amorphized NiTi were investigated by using a combination of transmission electron microscopy and high-resolution high-voltage electron microscope and image analysis of molecular-dynamics-simulated atom configurations. Nanometerized clusters were found to appear and disappear in the irradiated region. The random formation and breakup of such clusters is believed to be responsible for nanostructural fluctuations which appear to be related to transitions among manifold inherent structural ordering phases in the NiTi. The calculated propagating temperature fluctuations in the amorphized structure were manifested through the dose-dependent local amorphization parameter, potential energy, volume, and inherent cluster bonding. The observed fluctuations obey a universal power law. Within the framework of the multi-Loaden picture, the resultant power law describes the distribution of multirelaxation times or cluster lifetimes. In addition, a unified equation for the autocorrelation functions for such fluctuation phenomena has been derived. The behavior of the irradiated Ni system will be discussed.

4:00 PM R8.7
Correlation of Kinetic MC Simulations and EFTEM Observations of Phase Separation in Si\(_2\) Implanted Thin SiO2 Films.
Torsten Mueller,\(^1\) Karl-Heinz Heinig,\(^2\) Caroline Bonafes,\(^3\) Hubert Coffin,\(^4\) Gerard Ben Assayag,\(^5\) Sylvie Schramm,\(^5\) Gerald Zanchi,\(^6\) Alain Chrise,\(^6\) Marcel Picte,\(^6\) and Christian Collie\x-
\(^5\)Institut de Physique Nucleaire de Lyon, Luminy, France; \(^6\)Laboratoire de Physique des Solides, Universite Paris-Sud, Orsay, France.

Studies on the ion beam synthesis of narrow Si nanocrystal (NC) layers in thin SiO2 films are presented. Very low-energy Si\(^+\) implantation into gate oxides for MOS transistors followed by thermal annealing allows for the fabrication of novel Si NC floating gate based non-volatile charge storage devices. Small and isolated Si NCs at high density are required to obtain a large threshold voltage shift of the memory transistor. However, recent work shows that the characteristic of the Si NCs embedded in SiO2 by conventional Transmission Electron Microscopy (TEM) is difficult. It requires careful considerations and special imaging conditions [1] due to the weak contrast between Si and SiO2. In this contribution, Energy Filtered Scanning Transmission Electron Microscopy (EFTEM) investigations on the morphology of phase separated Si in SiO2 are presented, which overcome the contrast limitations of the conventional TEM. Furthermore, a comparison of the observed Si pattern with predictions of kinetic lattice Monte Carlo (MC) simulations [2] is performed. The Si precipitates were synthesized by 1keV Si\(^+\) implantation into 10nm thick SiO2 and by furnace annealing in N\(_2\) (or N\(_2\) + O\(_2\)). Varying fluences from 5 × 10\(^{12}\) to 2 × 10\(^{13}\) cm\(^{-2}\) were used in order to adjust the Si excess in the SiO2. In this work, dynamical binary collision simulations (TRIDYN) of high-fluence implantation were combined with kinetic Monte Carlo simulations of NC formation by phase separations. For low Si excess, NCs are predicted to form by nucleation, growth, and Ostwald ripening. On the other hand, at high Si excess, phase separation proceeds via spinodal decomposition, which elongated NCs are found in our computer experiment. At even higher fluences, structural percolation occurs and a random connected Si mesh forms. Thus, the morphology of the phase separated Si changes with increasing ion fluence from isolated, spherical NCs to percolated structures as observed by EFTEM. The pattern of the phase separated Si predicted by kinetic Monte Carlo simulations and observed by Electron Microscopy agree remarkably well. The work was supported by the EU through the growth project no. GIRD/2000/08290 [1]. G. Ben Assayag, C. Bonafes, M. Carrada, A. Chrise, P. Nomand, and J. M. Lasials, Appl. Phys. Lett. 82 (2003) 2060; K.-H. Heinig, and W. Mueller, Appl. Phys. Lett. 81 (2002) 3049.

4:15 PM R8.8
Heavy Ion Interactions in New Nanoscale Materials.
B. W. Jundt,\(^1\) S. P. Song,\(^1\) V. M. Ayres,\(^2\) M. A. Crimp,\(^2\) R. M Ronningen,\(^3\) A. F. Zeller,\(^3\) H. C. Shaw,\(^4\) J. B. Bennawles,\(^5\) and J. Pham,\(^5\)
\(^1\)Electrical and Computer Engineering, Michigan State University, East Lansing, Michigan; \(^2\)Electrical Engineering and Computer Science, Michigan State University, East Lansing, Michigan; \(^3\)National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, Michigan; \(^4\)Code 562, NASA Goddard Space Flight Center, Greenbelt, Maryland; \(^5\)Dynamic Range Corporation, Bowie, Maryland.

We report first experiments on the effects of heavy ion interactions with carbon nanotubes and silicon nanowires in a simulated space.

High dose ion implantation, where the final concentration exceeds 25 at. %, is a versatile method for controlled insertion of atoms into the surface thereby modifying its properties like, wear and corrosion resistance. However, considerable radiation damage and a very large number of interstitial atoms are produced. During high temperature implantation between 300 and 500 C, the interstitial diffusion and phase transformations are facilitated. In the present contribution, nitrogen implantation at ion energies between 10 and 30 MeV at fluxes larger than 14.8 cm.s^{-1} is investigated in molybdenum, titanium nitride, and molybdenum steel (as model for iron). The transition metals placed in the upper left part of periodic table, e.g. Ti, exhibit the highest stability of nitrides with a metal-nitrogen ratio of 1.1, with much lower formation enthalpies for later groups and periods (Fe and Mo). For stainless steel and Mo, this trend is confirmed in ion-implanted nitrogen. Nitriding of molybdenum steel leads to lattice expansion and nitrogen in solid solution with phase formation, whereas in only Mo2N was observed in the latter case. Albeit, a surprising result was obtained for Ti. At temperatures up to 500 C, the well-known TiN phase was observed in the implantation region and the surrounding diffusion layer. After a further increase of the implantation temperature up to 750 C, accompanied by a faster diffusion process, no TiN phase, but only a lattice expansion of the Ti was found with X-ray diffraction.

R2.2 Preparation and Characterization of GaSb Surfaces With Be-IAE for Antimonide Based Molecular Beam Epitaxy
Shinashikor Vangal1, B Kregel2, K Krishnamurthi2, B Zhu3, K Vu3, H Daphane4, D Blasi5 and W D Goodhue5, 1Photons Center, Dept. of Physics & Applied Physics, University of Massachusetts, Lowell, Massachusetts, 2Air Force Research Laboratory/SNHC, Hanscom AFB, Massachusetts.

In this paper, we demonstrate the use of Boron Ion Beam Assisted Etching (Be-IAE) as: 1) a method to remove surface and subsurface chemical mechanical polish (CMP) damage; 2) a method for creating micro- and nano-structure templates, and 3) a method for simultaneously stabilizing the etched surface with a relatively thin thermally desorbed oxide to overgrow the surface with molecular beam epitaxy. The Be-IAE technique is capable of etching GaSb at the rate of ~200nm/min while removing CMP induced damage irrespective of the quality of the initial surface. Both, (400) and (111) X-ray rocking curve data of etched samples show a significant decrease in the polish damage on GaSb wafers with significant CMP damage and no additional damage on wafers with high quality CMP finishes. Also, due to the high degree of anisotropy in the Be-IAE technique, it is capable of producing nano- and micro-structures in the substrates while simultaneously producing a thin desorbable oxide layer. X-ray photoelectron spectroscopy with a heavier stage shows that Be-IAE produces a mixed gallium and antimony oxide on (100) etched surfaces. The antimony oxides are desorbed between 100-300C while gallium oxides are completely desorbed at 535C, leaving a clean single-crystal GaSb surface for epitaxial growth. Upon our inspection, GaSb/AIGaSb/GaSb/Be-IAE/GaSb stacked the GaSb surfaces using molecular beam epitaxy. Thus, the Be-IAE technique is well suited as a surface preparation technique for damage removal, high fidelity patterning, producing a desorbable oxide layer, and epitaxial growth on selectively etched areas.

R2.3 Oxide films on Al (100) and Al (111) single crystals attacked by Energetic Atomic Oxygen Beam, Long Li and Judith C. Yang, Materials Science and Engineering, University of Pittsburgh, Pittsburgh, Pennsylvania.

Atomic Oxygen (AO) interacts with spacecraft materials in low earth orbit and greatly hastens their degradation and failure. For laboratory investigation, we exposed Al (100) and (111) single crystals at 220C under a unique hyperthermal atomic oxygen source, where the 5eV atomic oxygen are created by laser ablation of oxygen gas. A dense amorphous oxide layer of aluminum formed on the Al (100) surface with 50,000 AO shots. Plan-view and cross-section samples were characterized using JEM 2100FE-PEG analyses electron microscope (AEM). High-resolution cross-section transmission electron microscopy (HRTEM) shows the thin oxide film with thickness about 5 nm on the perfect crystal aluminum, revealing the presence of amorphous phase. HRTEM shows the reaction of Aluminum oxide surface and interface, suggesting AO facets from Al (100) toward Al (111). AO also reacts along the grain boundaries near the interface. The Al (111) single crystal covered with native alumina of 200 nm was simultaneously exposed with Al (100) sample. HRXTEM shows the dense amorphous oxide film formed at the interface area and the...
The thermal stability of liquid crystal alignment property between two kinds of thin films was investigated. Two layers of the thin films are hydrogenated amorphous carbon and amorphous carbon nitride thin films which are deposited on plasma enhanced chemical vapor deposition (PECVD). In order to generate liquid crystal alignment layer, we have exposed inclined ion beam after deposition of alignment layer. The novel alignment layers show the good thermal stabilities compared with conventional alignment layers such as polysilane and we can observe these results using the polarized optical microscopy (POM). Property of alignment layers are characterized by Raman, FT-IR and AFM.

The stationary plasma ion thruster (SPT) with the conic channel for better beam uniformity and outlet diameter 40 mm was investigated with the different working gases (O\textsubscript{2}, N\textsubscript{2}, Ar). The maximal ion current density \( j_{\text{i}} = 1.2 \text{ mA/cm}^{2} \) was obtained for O\textsubscript{2} at discharge voltage \( V_{d} = 340 \text{ V} \), discharge current \( I_{d} = 1 \text{ A} \) and flow rate \( q = 5.5 \text{ sccm} \). For all gases the dependences \( j_{\text{i}}(q) \) and \( V_{d}(q) \) with constant \( I_{d} = 1 \text{ A} \) were obtained. The ion energy distributions for all gases were obtained at different \( V_{d} \). In average the ion energy was approximately 2.7 keV, the discharge voltage \( V_{d} \) was 3000(800) V and ion beam is irradiated by N\textsubscript{2} at beam potential 300 eV in the ion dosage range \( 5 \times 10^{15} \text{ cm}^{-2} \) at room temperature. After ion bombardment, chemical bonding on the modified sapphire surface was investigated by x-ray photon electron spectroscopy. Below 1x10\textsuperscript{15}cm\textsuperscript{-2}, only non-bonded N\textsubscript{2} peak at the bonding energy 380.7 eV was found, but Al-N bonding was found up to 2x10\textsuperscript{17}cm\textsuperscript{-2} which was located at 300 eV. As the ion dosage was increased up to 1x10\textsuperscript{18}cm\textsuperscript{-2}, the occurrence of Al-N bonding was identified at the dose higher than 5x10\textsuperscript{17}cm\textsuperscript{-2} at 396.6 eV. From the high flux ion beam irradiation with low energy, the formation of nitride bonding on sapphire surface was confirmed at room temperature. And the evolution of the nitride bonding was discussed as the temperature is varied.

Ion implantation as a versatile and powerful tool for the fabrication of nanostructures has shown considerable promise in modifying the nanostructured mechanical, electrical and optical properties of materials. 64 keV Ni ion implantation was performed at room temperature up to a dose of 1 \times 10^{15} \text{ cm}^{-2}. The charge state, damage structure and UV-Vis absorption of implanted a-Al2O3 single crystals were studied by x-ray photoelectron spectroscopy (XPS), transmission electron microscopy (TEM) and optical spectroscopy, respectively. XPS analysis showed that implanted Ni ions are mainly in charge state of Ni\textsuperscript{2+} metallic), which may contribute to the sample's turning grey in color. Nanoparticles distributed from the surface to 30 nm in depth were observed in a cross-sectional high-angle annular dark-field (HAADF) TEM image. The size of nanoparticles ranges from 2 to 5 nm in diameter. After indexing the selected area diffraction (SAD) pattern, the nanoparticles were determined to be pure Ni. High-resolution transmission electron microscopy (HRTEM) image showed that the Ni-implanted area had been amorphized. A broad absorption band centered at 480 nm appeared in the optical absorption spectrum of implanted thin films. In contrast, the absorption band ranged from 240 to 280 nm, corresponding to F\textsuperscript{−} and F\textsuperscript{−}-centered, was observed in the absorption spectrum of electron beam irradiated samples at the same dose. Therefore, the absorption band centered at 480 nm is believed to be from the nanoparticles.

The effects of 8keV He ion bombardment on SiO\textsubscript{2}/PbMn exchange bias layers have been investigated in detail. Ion induced modifications in the ferromagnetic (FM) or antiferromagnetic (AFM) layer and at their interface have been separated by irradiating the samples between different deposition steps and thereby exploring the effects of irradiation to specific parts of the layer stack. In addition,
the relevance of the exchange coupling between the layers is demonstrated by irradiating samples at temperatures above the Neel temperature of the AFM layer. It is shown that the enhancement of the bias field which is observed at low ion doses is caused by structural modifications in the AFM layer. Yet, this enhancement is driven by the magnetic exchange force exerted by the FM on the AFM layer during irradiation. On the other hand, the suppression of the exchange bias effect at higher doses is caused by interface mixing at the FM/AFM interface as is shown by selective irradiation of this region.

R0.11

Abstract Withdrawn

R0.12

Dose and Isotope Effects in Low-Energy H/D Blistering of Silicon: Narrow Operational Window for Ion-Cutting at < 100 nm. Osamu Matsushita, Alexandre Giguère, Bernhard Hermann and Gay Ross. INHEMT, 0000 Quebec, Canada.

Hydrogen implantation induced blistering has applications in the fabrication of silicon-on-insulator and other devices. Using low keV ions to produce such structures with sub-100 nm dimensions, we found puzzling results with implications for both silicon physics and device engineering. Si samples were implanted with 2 to 10 keV H or D ions at a dose of 5 x 10¹⁶ ions/cm². The samples were subsequently subjected to rapid thermal annealing under vacuum and thermal desorption spectroscopy was performed simultaneously. The resulting surface morphology was studied by atomic force microscopy. We discovered that: (1) In the absence of a threshold dose, the maximum dose for blistering; and (2) there is a giant isotope effect. At 1 and 2 keV respectively, the hydrogen blistering dose for "windows" were [1 – 2], (1.5 – 3), and [2 – 4] in units of 10¹⁶ H/cm², but was determined to be [4 – 8] x 10¹⁶ D/cm². Reflecting the high required doses, D blisters are more abundant than H blisters, reaching 80% surface coverage, and roughly twice as high, implying higher gas pressures and more efficient application. The absence of blisters at higher doses was associated with a sudden release of part of the gas by permeation through a porous layer. Future work includes infrared and RBS-spectroscopy to understand the giant isotope effect and measurement of the respective merits of H and D in ion-cutting and other applications.

R0.13

Structural and Magnetic Characterization of CoNi

Nano-particles Using X-ray Stabilized Zirconia Single Crystals. Sha Zhu, Qi Sun, Qiangyu Zhang, Xiaoyi Zu, Lamin Wagne and Rodney C. Ewing. 1Department of Nuclear Engineering, University of Michigan, Ann Arbor, Michigan; 2Science Key Laboratory for Materials Modification by Laser, Ion and Electron Beams, Dalian University of Technology, Dalian, China; 3Department of Applied Physics, University of Electronic Science and Technology of China, Chengdu, Sichuan, China.

Ion implantation has been used to synthesize magnetic CoNi nanoparticles at room temperature in the near surface of yttrium-stablized zirconia (YSZ) single crystals for potential applications in magnetic-optical devices. Transmission electron microscopy (TEM) and superconducting quantum interference device (SQUID) magnetometer, as well as vibrating sample magnetometer were utilized to characterize the structural and magnetic properties of the implanted nanoparticles. The TEM analysis showed that the nanoparticles of 3-10 nm in diameter formed in YSZ matrix during the process of ion implantation. Hysteresis loops were measured at both 300 K and 10 K, which showed a coercivity of 100 Oe or 250 Oe, respectively. Magnetization vs. temperature in zero-field-cooled (ZFC) and field-cooled (FC) fields was measured. No obvious superparamagnetism was detected below 300 K.

R0.14

Inorganic-Organic Nanocomposite Systems for Microelectronic Applications. Marie-Isabelle Brunot and Léonard Merle. 1STP CEMR CNRS 6038, University of Limoges, Limoges, France; 2ERCEM, Limoges, France.

In this review paper we will describe the specific characteristics of hybrid nanocomposites in the framework of microelectronic applications. We will particularly highlight the advantages of inorganic-organic nanocomposites as potential chemiresistive 100nm resolution electron beam lithography and ion beam lithography as well. Experimental results and Monte Carlo simulations will illustrate novel trends in nanotechnology like 3D microstructure engineering.

R0.15

Ge Nanocrystal Formed Directly by High-Dose-Ion-Implantation. Tiejian Lu, Yingjin Xue, Jie Liu, Lin Lin, Qingsun Zhang, and Jiaguo Yang. 1Department of Physics, Sichuan University, Chengdu, China; 2Key Lab for Radiation Physics and Technology of Ministry of Education, Sichuan University, Chengdu; 3Science and Academy of Physics and Technology of China; 4Analytic and Testing Center, Sichuan University, Chengdu, China; 5International Center for Material Physics, Chinese Academy of Sciences, Chengdu, China.

Ge nanocrystals (nc-Ge) embedded in SiO₂ films were prepared directly by high dose Ge ion implantation into SiO₂ films for the first time. In the experiments, the implanting energy of 40 keV, the dose from 5 x 10¹⁶ to 1 x 10¹⁷ ions/cm², temperatures from 250°C to 500°C were applied. Ge XRD and Raman were used to analyze the crystallization procedure. The results showed that nc-Ge can be fabricated without the subsequent annealing when the implanting dose is more than threshold dose 1 x 10¹⁷ ions/cm². With the implanting dose of Ge ions increasing, the ratio and size of nc-Ge in the film will enhance. As a comparison, the annealing behavior of the nc-Ge were studied. The formation mechanism of nc-Ge has also been discussed. The precipitation of nc-Ge without post-annealing is due to amorphous Ge clusters in SiO₂ films receiving part of the kinetic energy of incident Ge ions so that a part of atoms in these clusters move and assemble to form Ge clusters in SiO₂ films which are reached.

R0.16

Formation of High Quality β-FeSi₂ by Pre-Amorphism-Equivalent Atomic Mixing. Yuji Murakami, Atsushi Kenjo, Tsuho Sadoh, Yuji Yoshihiko and Masahito Miyoshi, 1Department of Electronics, Kyoto University, Paykura, Fukuhara, Japan; 2Department of Applied Science for Electronics and Materials, Kyoto University, Katsura, Fukuoka, Japan.

Semiconducting β-FeSi₂ is attractive for Si-based opto-electronic applications because of the direct band gap of 0.85 eV. For the device fabrication, a micro-patternning technique is required for selective etching of β-FeSi₂ on Si and SiO₂ is difficult. It is expected that irradiation with focused ion beams to Fe/Si structures will induce atomic mixing and enhance dissolution locally, which can be utilized for micro-fabrication. We previously found that amorphization of substrates as well as atomic mixing enhanced β-FeSi₂ formation. In the present study, effects of pre-amorphization of Si substrates by ion irradiation have been investigated. In the experiments, Si substrates were irradiated with 20eV Ar⁺ ions (dose: 2 x 10¹⁴ to 10¹⁵ ions/cm²) for pre-amorphization. For reference samples, some substrates were subsequently annealed at 800°C for 2h to recover damage [1]. Next, Fe films (thickness: 15nm) were deposited by using a facing target DC sputtering. The samples were annealed at 800°C in a vacuum. The formed β-FeSi₂ layers were characterized by using X-ray diffraction (XRD) and optical absorption measurements. The results of XRD showed that the initial formation rate (annealing time < 30 min) of β-FeSi₂ was the largest for the sample pre-amorphized with the highest dose (10¹⁵ ions/cm²). The amount of β-FeSi₂ saturated after 30 min. It is speculated that the enhancement of initial formation of β-FeSi₂ is due to the bond rearrangement induced during defect relaxation for the increase in the surface density of Si atoms to the growth front of β-FeSi₂ by enhanced diffusion of Si atoms. Optical measurements revealed the direct band gap of 0.87 eV for pre-amorphized samples. These results demonstrate that pre-amorphization enhanced the crystallization and crystal quality of β-FeSi₂ [1]. Y. Murakami, H. Yamauchi, A. Kenjo, T. Sadoh, and M. Miyoshi, Solid State Phenomena 78 – 79 (2001) 341.

R0.17


We discuss activation of impurity atoms doped in polycrystalline silicon films using the ion doping method. 50 mm-thick amorphous silicon films formed on glass substrates were first crystallized by 28-nm-pulsed XeCl excimer laser irradiation with a laser energy density of 360 mJ/cm². 1.0 x 10¹⁷ cm⁻² phosphorus atoms were implanted into laser crystallized silicon films by the ion doping method at an accelerating energy of 10 keV. Samples were then treated at 250°C with 13.56 MHz RF oxygen plasma at 50W and 1.3 Torr for 1 h. Samples were also heated at 250°C in the air for 3h. The electrical conductivity was 1.6 x 10¹⁵ S/cm for samples as implanted into the polycrystalline silicon films. Most of phosphorus atoms were not activated. On the other hand, the electrical conductivity markedly increased to 7.3 S/cm after the oxygen plasma treatment at 250°C for 1h. The electrical conductivity also increased 1.7 x 10¹⁵ S/cm after heat treatment at 250°C in the air for 3h. Here, the effective role of activation of phosphorus atoms and carrier generation in polycrystalline silicon films. The crystalline volume ratio was also increased.
investigated using measurements of the optical reflectivity spectra. The crystalline volume ratio was low of 0.2 for the as implanted state, while the volume of silicon crystal is 0.84. Serious disordered states were caused by phosphorus implantation. The crystalline volume ratio increased to 0.38 after the oxygen plasma treatment and 0.34 after heat treatment in air. Both of the heat treatments elucidated the disordered states and crystalline states, but there were still residual disordered states after the heat treatments. We discuss the mechanism of the high carrier generation rate in the case of oxygen plasma treatment.

R1.18 Electron Irradiation Effects on Poly-Si Thin Films Used for Solar Cells. Young-Soo Zheng, Qing Liu, Jing Li,
Ying Xu4 and Yuwen Zhao4. 1Department of Physics, Sichuan University, Chengdu, China; 2Key Laboratory for Radiation Physics and Technology of Education Ministry of China, Sichuan University, Chengdu, China; 3Solar Energy Research Institute, Yunnan Normal University, Kunming, China; 4Beijing Solar Energy Research Institute, Beijing, China.

The poly-Si thin films used for solar cells were prepared on ceramic silicon substrate by Rapid Thermal Chemical Vapor Deposition (RTCVD). And were irradiated by electron beams with energy of 1MeV and fluence of 1×10¹⁷/cm² to 1×10²⁰/cm². Before and after irradiation, the electrical properties of these films and their solar cells were measured. It is shown that after irradiated with lower electron fluence, the resistivity of poly-Si thin films decreased, the main result from the effect of ionization; after irradiated with high electron fluence, the resistivity of poly-Si films sharply increased, which is the result from the effect of displacement. And the surface degradation shows approximately linear relation with the electron fluence. The results for parameters of poly-Si such as short-circuit current (Isc), open-circuit voltage ( Voc) transfer efficiency η also show the effects of electron fluence. All of these were discussed in detail.

R1.19 Magnetic Properties in Fe-Ni Invar alloys Irradiated with High-Energy Ions. Fujimasa Oke1,2, Ken Sato1, Y. Chiba3, N. Ishikawa3, T. Kumbar2 and A. Iwase2. 1Department of Physics, Okayama University, Okayama, Japan; 2Department of Materials Science, Japan Atomic Energy Institute, Tokai, Ibaraki, Japan; 3Atomic Physics Laboratory, The Institute of Physical and Chemical Research, Wako, Saitama, Japan; 4Research Institute for Advanced Science and Technology, Osaka Prefecture University, Sakai, Osaka, Japan.

Anomalous large shift of the Curie temperature of the order of 100 K has been recently observed in Fe-Ni Invar alloys irradiated with high-energy heavy ions. This large effect can be attributed to the large positive magneto-volume effect essentially originated in the itinerant electron ferromagnetism in Fe-Ni Invar alloys. To investigate the mechanism of the large modification of the ferromagnetism in the structure of the modified portion, measurements of the beam energy dependence of AC-susceptibility temperature curves have been made. It was found that the amount of the shift of the Curie temperature did not change by increasing the beam energy. On the contrary, the intensity of the susceptibility of the modified portion increased with the beam energy. The high beam energy excitation is considered to be responsible for the large modification of the ferromagnetism in Fe-Ni Invar alloys.


Different from bulk silicon crystal, nano-sized Si crystalline embedded in silicon dioxide (SiO₂) as an efficient photoluminescence (PL) center. In nano-crystalline Si, excitonic electron-hole pair is considered to be attributed to radiation recombination. But the defects surrounding crystalline no-Si suppress radiative recombination efficiency, which work non-radiative decay paths. Hydrogenation is usually utilized in order to en-capitalize the dangling bonds in the SiO₂ interface, that dramatically enhances luminescence yield. Unfortunately because hydrogen has a relatively higher mobility than other elements in a matrix, subsequent thermal process may reduce the enhancement effect by hydrogenation. Thus instead of easily moving hydrogen, phosphorus was introduced by implantation. Samples were prepared by 400 keV Si implantation with dose of 1×10¹⁷/cm² and 1×10²⁰/cm², followed by implantation with dose of 3×10¹⁵ P/cm². They were annealed at 1100°C for 2 hours in the Ar environment in the temperature range between 500°C and 1100°C. The PL measurements were performed with 488 nm Ar laser and GaAs PM tube at a power density of 250 mW. Although phosphorus doping doesn’t enhance PL intensity so much as hydrogenation, it uniformly enhances PL yield along the emission wavelength. Experimental data such as an enhancement effect of PL yield, decay time characteristics and thermal stability of the phosphorus implanted and phosphorus terminated nano-crystalline Si are shown, and the possible mechanism will be discussed.

R2.21 Thermal Stability of Thin Films of Ion Beam Deposited C₇N₅, David C Ingram1, Asghar Kuyuni1, William C Lanter1 and Charles A DeJongh2,3. 1Physics and Astronomy, Ohio University, Athens, Ohio; 2Innovative Scientific Solutions, Corp, Bexevscreek Ohio, USA; 3AFRL/PRPE, Air Force Research Laboratory, Wright-Patterson AFB, Ohio.

A dual ion beam deposition system has been used to deposit thin films of C₇N₅ from a carbon target. A 1 keV nitrogen ion beam from a 3 cm Kaufman source is used to sputter carbon from a graphite target and a second nitrogen ion beam of 50 eV, from an RF ion source, is used to bombard the growing film with nitrogen ions. By varying operating parameters of the ion source used to bombard the growing films it is possible to reduce the amount of hydrogen in these films from the residual gas in the chamber, 3×10⁻¹⁰ torr, to one the order of one atomic percent and to boost the nitrogen content to over thirty percent. These films have been then subjected to isochronal annealing up to 1000°C to determine the stability of the films as compared to those with much higher concentrations of hydrogen. C₇N₅ is a material that is difficult to fabricate without the inclusion of large amounts of hydrogen. This has the tendency make the material sensitive to property changes as it is heated over 200°C. Hydrogen is lost from the films and the optical, electrical and mechanical properties of the film change. Comparison with the losses of hydrogen is the loss of nitrogen. In the films with lower amounts of hydrogen it is found that the loss of nitrogen, and hydrogen, is delayed until higher temperatures are reached, 600°C. Further work is proceeding on determining any changes to the properties of the films before significant loss of nitrogen occurs.

R2.22 Trapping of Argon in Unbalanced Magnetron Sputter Deposited Films of C₇N₅Hₓ, Asghar Kuyuni and David C Ingram; Edwards Accelerator Laboratory, Ohio University, Athens, Ohio.

Unbalanced magnetron sputtering deposition of C₇N₅Hₓ films has been performed with various levels of negative substrate bias and with different flow rates of nitrogen and hydrogen. Argon was used as a sputtering gas and formed the majority of the gas in the plasma. The elemental concentrations of the films were measured in samples deposited on glassy carbon with a 2.2 MeV beam of He ions used to perform simultaneous Rutherford Backscattering Spectroscopy (RBS) and Elastic Recoil Spectroscopy (ERS). Argon was found to be trapped in the non-hydrogenated films to a level of up to 4.6 at %. The concentration of argon increased for the films deposited under higher negative bias, indicating that the argon is implanted into the films. With the introduction of hydrogen, argon trapping was first reduced and later completely eliminated, even at higher bias conditions, suggesting that the softness of the films brought on by hydrogenation also caused the films to be unable to trap argon during growth showing that argon stability is dependent on burial below a surface of particular structural properties.

R2.23 Nanowire formation in metal oxides by ion implantation and thermal annealing. A. Tom et al. Van Deusen, A. M. van Hurs, H. Schut1, B.J. Kooi2 and J.Th.M. de Hessen2,3, TH, Delft University of Technology, Delft, Netherlands; 2 Materials Science Centre, University of Groningen, Groningen, Netherlands.

Cavities can be created rather easily in metal oxide ceramics by the vacancies produced during stopping of the energetic ions. Post-implantation thermal annealing promotes the nucleation and growth of the clusters. In the depth zone where the implanted ions are strongly precipitated, the implantation depth profile is complex. A general overview is given on investigations on cavity formation in MgO, MgAl₂O₄, Al₂O₃ and ZrO₂ by light ion implantation (He, H₂), and in MgO by implantation with metallic ions, e.g. Cu, Zn, Ag, Au or by protons. In all cases cavities are formed by heave beam implantation followed by thermal annealing. However, the cavities are observed only at the implantation depth of the ions. First, bubbles are formed at this depth, but after coalescence...
as elevated temperature the bubbles cease the gas by permeation to the surface. In Al2O3 a different behavior is observed: bubbles grow larger but only up to a very high temperature. Thereafter the bubbles shrink by helium and vacancy dissolution. Metal ion implantation causes a zone of cavities between the surface and the implantation zone. During annealing the cavity zone develops in a different manner. The implantation of ultra-light helium (He, 0.1 keV), and helium (He, 0.1 keV, is), (i.e., high-resolution electron microscopy and transmission electron microscopy (HRTEM)) of implanted samples shows the occurrence of the implanted material and the substrate. No nucleation and evolution of the bubbles and cavities will be discussed in terms of recombination, clustering, dissociation and mobility of the defects and defect complexes in the investigated metal oxides.

**RO 24**


Formation and nucleation of "ridge" like structures synthesized using MeV Au2+ implantation in SrTiO3 single crystals was investigated using Rutherford backscattering spectrometry (RBS) along with channeling, scanning electron microscopy (SEM), energy dispersive x-ray emission (EDX) and high-resolution transmission electron microscopy (HRTEM). Approximately 500 Au+24 implantation was performed with normal to the surface at 300 K and 973 K in SrTiO3 (100) substrates. Measurements of the samples were conducted directly after implantation and following ex-situ annealing at 1475 K in air for 10 hours. Subsequent annealings of the sample implanted at 300 K show that the gold is uniformly distributed to a depth of 400 nm from the surface. However, the gold depth profile obtained from the sample implanted at 973 K shows a narrower Gaussian like profile probably due to Au diffusion and microregions. The Au implanted sample at 300 K show that the surface of the implanted region underwent substantial rearrangement and formed "ridge" like structures, which are parallel to the (100) planes. These "ridge" like structures are formed throughout the implanted region with an average height of 1 to 2 microns. The external annealing at 1475 K in air for 10 hours doesn’t make any significant changes in the "ridge" like structures. In contrast, the SEM micrographs from the sample implanted at 973 K show no evidence of surface rearrangement and the surface appears to be very flat. Channeling measurements performed on the annealed samples show some shadowing of Au atoms and thermal recovery of damage generated in the substrate during implantation.

**RO 25**

Incorporation of supersaturated Fe centers in n-InP by high-energy ion implantation: effect on the microstructural and electrical properties. Tiziana Cacca, Andrea Giaparot1, Beatrice Fraboni2 and Francesco Pricolo1,2,3,4,5. Dept. of Physics, INFN-University of Padova, Padova, Italy; 1Dept. of Physics, INFN-University of Padova, Bologna and Pavia, Italy; 2School of Physics and Astronomy, INFN-University of Catania, Catania, Italy.

Fe is one of the most important transition metal impurities in InP-based materials. This is due to its deep acceptor character which is widely employed to compensate n-type dopants and to produce bulk or epitaxial semi-insulating InP. Moreover, it has interesting optical properties related to luminescent emission in the mid-IR region of the electromagnetic spectrum. In order to display these properties, high concentrations of Fe atoms have to be introduced in substitutional (In) sites in the InP lattice. Recently we demonstrated that high densities of electrically and optically active Fe centers can be incorporated in InP by high temperature ion implantation and proper post-implantation annealing treatments; by this method both solubility limitations and damage-related undesired redistribution phenomena can be overcome and avoided. Creating a supersaturation of substitutional Fe atoms in InP by optical excitation is not feasible. The aim of the present work is to investigate the effect of the implantation process and the subsequent annealing treatments on the Fe-related physical properties of the implanted InP crystal. The main goal is to understand the mechanisms leading to the final location of the Fe atoms and to correlate the structural information (with regard both to the local environment of the Fe atoms in the InP lattice and to the interaction with the substrate) with the Fe-related electrical and optical properties. For this study several characterization techniques were employed providing complementary information. The damage behavior and the local structure of Fe were studied by RBS and PIXE-channeling. Moreover, in order to obtain an overall picture of the implantation process, the samples were also characterized with other structural techniques, as high resolution X-ray diffraction, transmission electron microscopy and X-ray absorption spectroscopy. Current voltage and DKTS-PICTS measurements instead were employed to investigate the electrical properties. The results show that a high concentration of Fe atoms can be incorporated in the InP matrix after the high temperature implantation; post-implantation annealing treatments at increasing temperatures favor an escape process of Fe from substitutional sites towards low symmetry sites; this process seems to be mediated by the implant-induced interstitial kinetics. Nonetheless, in spite of the substitutional Fe density reduction, the damage recovery induced by the annealing eventually leads to the formation of a semi-insulating layer whose properties are controlled by the residual active Fe centers. Moreover, the correlation between the structural and electrical results suggests that the Fe-escap process is controllable either by the substrate donor concentration. The possible extension of this study to ternary alloys, like e.g. InGaP and InGaAs, will be also considered.

**RO 26**

Electron Stimulated Oxygen Desorption Study of Materials for Low Temperature Solid Oxide Fuel Cells (SOFCs). Haydn Chan1,2, Yanfeng Chen1,2, Thomas Orchido1,2, Jun Dong2,3, and Michael E. Tung1,2. 1School of Materials Science & Engineering, Georgia Institute of Technology, Atlanta, Georgia; 2School of Material Science & Engineering, Georgia Institute of Technology, Atlanta, Georgia.

The realization of cost-effective low-temperature (below 650 degree Celsius) solid oxide fuel cells (SOFCs) depends strongly on the advancement of bifunctional materials with high catalytic activities for fuel cell reactions at relatively low temperatures. As the current search for new materials is heavily based on empirical approaches, a fundamental understanding at the electronic structure level of the factors contributing to the most desirable properties of the materials would make the development of new materials more effective. In solid oxide cathodes or electrodes, the contribution to the ionic conductivity is mainly from the mobility of oxygen vacancies. Therefore, probing the electronic states (including defect states) related to the oxygen desorption and diffusion using electron stimulated desorption (ESD) of oxygen (ions and neutrals) from the SOFC materials should provide information that could be correlated with the mobility of oxygen vacancies. Our current research is focusing on measuring the thresholds of O₂ desorption with low energy electron (2-10 eV) excitation from the SOFC materials. The results will be presented.

**RO 27**

The effect of ion implantation temperature on the blistering and exfoliation in hydrogen implanted Si. Jung-Kun Lee1,2, Sheng Huang2, Lisong Liu2, and Michael Nastasi1,2. 1Materials Science and Technology, Los Alamos National Laboratory, Los Alamos, New Mexico; 2ECE department, University of California, San Diego, San Diego, California.

We have examined the role of implantation temperature on the nature of the blistering and exfoliation phenomenon in H implanted Si, which leads to the transformation of the ion-implanted damage and the hydrogen concentration in the as-implanted and Si films were analyzed with Rutherford back scattering (RBS) in channeling mode and the elastic recoil detection (ERD), respectively. Comprised with the 140 O-s implantation, the room temperature implantation resulted in a deeper and narrower damage distribution, which leads to different thicknesses and surface morphologies of transferred Si films. With the aid of infrared spectroscopy (IR) study, the different blistering and exfoliation behaviors for two conditions were found to be correlated with an enhanced interaction between implanted H and displaced Si in room temperature implanted Si. The implantation of these observations on the fundamental physics underlying the blistering and exfoliation phenomena in hydrogen implanted Si will be discussed. Also, the electrical characteristics and its correlation with ion-solid interactions will be presented.

**RO 28**


Carbon nanotubes have unique properties arising from their molecular structure and shape. In order to harness them for applications, it is essential to create interconnected mesoscale architectures in organized configurations. Here, we demonstrate the use of 10-30 keV focused ion
beams to weld, slice and dope multilayered carbon nanotubes (MWN'Ts) at preselected locations. Ga ions beams with spot-sizes ranging from 0.5 to 2 μm were accelerated at preselected sites on a highly-oriented MWN'Ts array on silicon, and MWN'Ts dispersed on electron-transparent grids. Scanning and transmission electron microscopy (SEM and TEM) characterization indicate that nanotubes doped with 10 – 100 ions/cm² of 30 keV Ga⁺ ions show no observable structural changes. Increasing the dose to ~10² – 10³ ions/cm² results in the thinning of large diameter MWN'Ts and slicing of smaller diameter tubes, and the welding of overlapping nanotubes.

High-resolution TEM and electron diffraction reveal that the irradiated areas the MWN'Ts shells collapse into the hollow, transforming the nanotubes into amorphous nanorods. This is consistent with increasing disorder and amorphization regions showing a higher degree of disorder due increased dangling bond density. Similar results were obtained for 30 keV ions at smaller ion doses of 10⁹ – 10¹⁰ ions/cm², indicating that both ion dose and energy are factors that determine structural changes. Spatially resolved energy dispersive X-ray spectrometry (EDX) shows that the irradiated sections of the MWN'Ts contain Ga, some of it in the form of Ga nanoclusters as indicated by TEM. Thus, in addition to welding and slicing the nanotubes, the high density of 30 keV Ga⁺ ions for creating compositionally modulated nanotube structures, or engineer high defect densities to enable safe site-selective attachment of other nanomaterials via further chemical treatments. These features make the ions beam method an attractive alternative for fabricating interconnected architectures of nanostructures.

**R9.20**

**High-speed Machining with Cluster Ion Beams.**[1][2][3]

Joji Matsumoto, 1 Quantum Science and Engineering Center, Tokyo University, Tokyo, Japan; 2Collaborative Research Center for Nano-scale Machining with Advanced Quantum Beam Technology, Tokyo, Japan; 3Collaborative Research Center for Cluster Ion Beam Process Technology, Tokyo, Japan.

A cluster is an aggregate of a few to several thousands atoms. When many atoms clustering as a cluster ion bombarded a local area, high-density energy deposition and multiple-collision processes are realized. Because of the interactions, cluster ion beam processes can produce not only damage but also low-damage sputtering and ion beam processes, especially when the extreme high-energy ion beam can be realized using reactive cluster ion beams. High current SF₆ gas cluster ion beams were generated using recent high current cluster ion beam techniques. The cluster size distribution was measured using Time-of-Flight (TOF) method and the mean size of clusters was about 500 molecules. Si substrates were irradiated with SF₆ cluster ions at an acceleration energy of 5 – 45 keV. Sputtering yield with SF₆ cluster ion was increased with acceleration energy and was about 2100 atoms/ion at 45 keV. The sputtering yield was about 1000 ions higher than that of Ar monomer ions and was higher than that of Ar cluster ions. It was found that the high-speed sputtering occurred with SF₆ cluster ion irradiation. These results indicate that high-speed machining can be done with reactive cluster ions at high energy. In the future, high-efficiency machining by the Ministry of Economy, Trade and Industry (METI) and New Energy and Industrial Technology Development Organization (NEDO).

**R9.30**

**Properties of Ordered Nanoporous Alumina as a Template for Pattern Transfer by MeV Ion Irradiation.**[4][5][6][7][8]

Goran Porsnert, 1 Anders Johansson, 1 Mohamed Abidi, 1 and Anders Hallgren, 1 Ångström Laboratory, Uppsala University, Uppsala, Sweden; 2Department of Microelectronics & IT, Royal Institute of Technology, Stockholm, Sweden.

Ordered nanoporous alumina [1] has recently been considered as a template for pattern transfer by ion beam irradiation. Porous alumina of thickness 500 nm has already been used as a mask for low energy heavy ion implantation [2]. However, in order to apply this material as a template, high production of ordered pores with high aspect ratio, light ions with MeV energies with larger penetration depth as well as the irradiation area needed due to the small opening size for ions passing through the pores. Typical size of pores in the alumina foils was 50 nm, and foil thicknesses were around 2 μm. Polysilicon with metacoeating was the sacrificial layer selected. The resulting incident beam is the basic tool for the following experiments. The accommodation of 10⁹ ions/cm² at 30 keV can be achieved. The study carried out the transmission electron microscopy (TEM) and high-resolution transmission electron microscopy (HRTEM) of the sample. Energy dispersive X-ray spectrometry (EDX) was used to identify Ga⁺ ions from Ga ion implantation. Energy spectra were analyzed for different target orientations with respect to the primary beam as in a traditional channeling experiment. The beam's diameter was 5 m and the ratio of 400 m was used for small-spot TEM analysis. The sample was examined using a high-resolution transmission electron microscope (HRTEM) at an accelerating voltage of 100 keV. The Ga⁺ ions were implanted at a dose of 3 – 4 x 10¹⁵ ions/cm², which corresponds to a Ga⁺ density of 3 – 4 x 10¹⁵ ions/cm². The Ga⁺ implantation resulted in a significant change in the electrical properties of the sample, such as a decrease in the mobility of the implanted regions. The Ga⁺ ions were implanted at a dose of 3 – 4 x 10¹⁵ ions/cm², which corresponds to a Ga⁺ density of 3 – 4 x 10¹⁵ ions/cm². The Ga⁺ implantation resulted in a significant change in the electrical properties of the sample, such as a decrease in the mobility of the implanted regions. The Ga⁺ ions were implanted at a dose of 3 – 4 x 10¹⁵ ions/cm², which corresponds to a Ga⁺ density of 3 – 4 x 10¹⁵ ions/cm². The Ga⁺ implantation resulted in a significant change in the electrical properties of the sample, such as a decrease in the mobility of the implanted regions. The Ga⁺ ions were implanted at a dose of 3 – 4 x 10¹⁵ ions/cm², which corresponds to a Ga⁺ density of 3 – 4 x 10¹⁵ ions/cm². The Ga⁺ implantation resulted in a significant change in the electrical properties of the sample, such as a decrease in the mobility of the implanted regions.
material as well as the deposited material. All FIB processes are typically associated with ion implantation and microstructural changes due to ion beam damage. This work uses advanced characterization techniques to quantify these effects the focused ion beam has on the substrate. The depth of the amorphization of the substrate surface has been evaluated by transmission electron microscopy [TEM] of cross-sectional samples. The effect of the acceleration voltage on the interface layer could be imagined. The chemical composition of the interface was obtained by a depth profile with secondary ion mass spectroscopy [SIMS]. This observation reveals that the crystalline states present in the multilayers of the doping profiles. The morphological effects of locally confined implantation have been determined by atomic force microscopy (AFM) on the irradiated surface. The modification of material properties and chemical characters by deliberate local implantation of Ga has been applied for local doping of n-Si. Experimental data on the resistivity of Ga-implanted regions was obtained by 4-point probe measurements. The focused ion beam exposure during deposition was found to be effective in microstructuring of n-Si by occurring in solids during energetic ion irradiation. This work offers a comprehensive outline of most recent experimental observations of ion irradiation effects in different semiconductor materials.

R9.34

When surfaces are sputtered with inert or reactive ions in an off-normal incident geometry, corrugated patterns often form. Previous experiments on amorphous silicon dioxide surfaces showed that the morphology [wavelength, amplitude] of these corrugations depended on the ion energy. The present work has examined the surface morphology due to the transfer of energy by the bombarding ions and 2) the curvature-dependent sputter yield. We report here investigations of the dependence of the corrugation wavelength on ion energy for sputtering of hydrogenated amorphous silicon carbide films. For ion energies between 500 eV and 1 keV, the wavelengths range from 25 to 50 nm for sputter energies from 5 to 50 eV for the glass. The wavelength varies with ion energy as a power law with a correlation coefficient of 0.5. By sequentially sputtering the display glass using a range of incident angles and ion energies, the surface pattern develops a two-dimensional periodic character.

R9.35
Low Energy Ion Channeling and Implications in CuAl (100), A. K. N. Reddy, B. S. et al., and P. G. P. A. M. Institute, Theoretical Dept., Irvine, CA, 1; Arista Institute of Electronic, The University of Tashkent, Tashkent, Uzbekistan.

Low energy ion irradiation of crystals opens the new perspectives in the field of ion beam treatment of solids, in particular for modification of physical-chemical properties of crystals by ion implantation. In the present work the peculiarities of ion channeling and implantation processes at low energy implantation of CuAl (100), Cu (100) and Au (100) have been investigated by computer simulation in the binary collision approximation. The trajectories of incident ions, their ranges and energy losses as well as the depth profiles of implanted particles have been calculated for different kinds of bombardment ions. It was observed that in comparison with Cu (100) in the case of CuAl (100) the range of projectiles decreases, the relative contribution of elastic energy losses increase due to presence of Al atoms which lead to increasing the amplitude of trajectory oscillations of channelled particles. The angular and energy distributions of ions passing through thin (<500 Å) single crystals have been calculated and studied in detail. The angular distributions of such ions in the neighborhood of the liquid argon have been investigated in dependence on geometry and structure of the channel. In the case of CuAl (100) the half-width and range of angular distributions are wider and the number of channelled particles are significantly more than ones obtained for case of pure Cu (100) crystal. In the case of CuAl (100) the energy losses of passing particles are more that results to shifting the main peak to low energy part of spectrum. The calculated depth profiles show that the shape of these profiles are essential not only in well known cases of pure CuAl (100), but also the depth of particles is shifted to move deeper layers in the case of Cu (100).

R9.36
Fast Neutral Ar Penetration during Gas Cluster Ion Beam Irradiation to Magnetic Thin Films, Shigeru Katakura, 1 Yoko Kuma, 1 Hiroshi Seki, 1, Shinya Sasaki, 1, Kenji Harusawa, 1, Takanori Aoki, 1, and Jiro Matsuo, 1 Scoggin Technology Research Center, Hitachi, Ltd., Yokohama, Japan, 2 Collaborative Research Center of Nanoscale Machining with Advanced Quantum Beam Technology, Kyoto, Japan, 3 Quantum Science and Engineering Center, Kyoto University, Kyoto, Japan.

Gas cluster ion beam technology can provide ultra-smoothing processes for various materials with very low damage. Properties of magnetic materials are extremely sensitive to their components and structures. Therefore, fast monomer ions and neutral have to be suppressed. Suppression of fast neutrals is important, since monomer ions can cause permanent microstructural changes in the target. Fast neutral Ar penetration during gas cluster ion beam (GCIB) irradiation to NiFe thin films has been investigated by secondary ion mass spectroscopy (SIMS). Neutral clusters were generated by adiabatic expansion of Ar gas with pressure of 6000 Torr through a nozzle into vacuum and were ionized by electron impact with bombardment energy of 300 eV. The ionized clusters were accelerated by electric field and transported to a target. Cluster ions with the neutral voltage range from 800 to 2000 V and their properties were estimated to be 50 nm thick NiFe films deposited on Si wafers by Ar sputtering. Depth profiles of penetrating Ar were obtained through SIMS measurement with O ions beam used as a primary ion beam. It was found that the density of penetrated Ar by GCIB irradiation with the acceleration voltage of 20 kV reached a maximum at 16 nm and that it decreased gradually with increasing the depth. The depth at the density maximum decreased with the acceleration voltage of GCIB and was independent to ion dose. It was also realized that Ar penetration into the NiFe thin film also occurred during neutral Ar beam irradiation. The neutral beam was obtained by elimination of all charged particles from GCIB by deflecting field applied horizontally to the beam. This result suggested that Ar penetration resulted from GCIB irradiation was attributed to fast Ar neutrals included in GCIB. The fast Ar neutrals were produced by charge transfer collision of monomer ions with atoms in the atmosphere. The monomer ions were neutralized by electron impact together with cluster ions. Consequently, Ar penetration should be suppressed by decreasing the pressure of the space along with GCIB, since the probability of charge transfer collision decreases with the pressure. This explanation was confirmed by the depth profile of Ar beam obtained by SIMS.

R9.37
Heavy Ion bombardment of electroformed Ni-Co alloys for stress release / mechanical properties enhancement, Ilia C. Muntele, Sergey Sarksiev, Claudia I. Muntele and Daruysh Ilia, Physics, Alabama ACM University, Normal, Alabama.

Electroformed Ni-Co alloys have a structure strongly dependent on the deposition parameters and the bath composition. Internal stress, which is also affected by the growth conditions, affects in its turn the structure by introducing pores and cracks. The samples described in this work were obtained from a nickel sulfamate bath operated at 45 °C under various current densities. The current densities were chosen such that the stress in the plating bath to be at its minimum under established bath composition. The grain size, as well as the amount of atomic and molecular species adsorbed at the grain boundary, is of great relevance for the mechanical properties of the electroformed material. The energy deposited by heavy ions bombarding the surface of the sample produces a local melting, reducing the amount of hydrogen and sulphur/sulphur complexes incorporated during the electroforming process at the grain boundaries. Atomic Force Microscopy [AFM] was used for characterization of the surface and cross-section of samples obtained under three different current densities. For hydrogen profiling, nuclear reaction analysis was used.

R9.38
High rate etching of GaAs and GaP by gas cluster ion beams, Masahiro Nagano, 1 Susumu Yamanada, 1 Shirane Akiti, 1 Shingo Housumi, 1, Noriaki Toyoda, 2, and Isao Yamanada, 2, Electrical Physics, Central Research Institute of Electric Power Industry, Tokyo, Japan, 3 Laboratory of Advanced Science & Technology for Industry, Himeji Institute of Technology, Higashi, Japan.

Many types of nano-structure devices have been developed and many varieties of etching, deposition and lithography processes are used for nano-structure fabrication recently. Recently, gas cluster ion beam (GCIB) techniques have been proposed as new processing methods. The cluster consists of several thousands of atoms, so it impacts a surface with equivalent low energy and high density, which realizes high-rate etching without causing significant damages. In this study, etching of GaAs and GaP with GCIB were studied as a function of ion dose and etching time, and their sputtering yields. Cluster beams were formed by supersonic expansion of high pressure gas (1x10^16 Pa) through a nozzle. The average Ar cluster size was 4000 atoms/cluster in these etching experiments. Both the sputtering depths of GaAs and GaP were increased monotonically with increasing the ion fluence. 1x10^16 to 1x10^17 ion/cm^2 at acceleration energy of 20 kV. The GaP
We have demonstrated a position controlled GaN nano structures with a combination of surface treatments and nucleation sites control assisted by low energy focused ion beam (LE-FIB). GaN and related compounds have been focused as promising materials for future optical devices and nano structured GaN has also a great potential to realize an innovative optical devices. However, ordered nanostructures of GaN or position controlled GaN micro crystals must be demonstrated for their practical applications. The critical issues are nucleation site control and selective growth from the sites. The LE-FIB system possesses the ability to modify the surface selectively by ion sputtering (nucleation site control) and can deposit materials via ion-induced deposition (selective growth). The combination of these procedures can be used to fabricate the position controlled GaN three-dimensional nanostructures. As-terminated Si(100) or SiN deposited Si surfaces were used as the substrates. At first, Ga ions in the range of 100 eV - 10 keV were irradiated onto the surface to create the nucleation sites. Subsequently, Ga molecules were evaporated to a pressure of ~5 x 10^-8 Pa at 550°C which produced ~50 nm thick Ga film on the pre-irradiated surfaces. After sputtering, the film thicknesses were measured by ellipsometry to be ~50 nm. The GaN microcrystals were then grown by molecular beam epitaxy (MBE) on the nuclei. The GaN microcrystals were then characterized by low angle X-ray diffraction (XRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM).

In situ characterization of defects in GaN microcrystals is crucial for understanding the material properties and device performance. The use of advanced characterization techniques, such as electron energy loss spectroscopy (EELS) and atom probe tomography (APT), allows for the identification of nanoscale defects and composition variations within the GaN films. These techniques provide valuable insights into the quality and performance of GaN-based devices.

9:00 AM R10.2
In Situ Study of Modifications in Glasses. Nan Jiang, Physics, Arizona State University, Tempe, Arizona.

Irradiation effects in glasses promise an efficient approach to modify the electronic and optical properties of glasses. Various mechanisms have been introduced to interpret irradiation effects in glasses, such as ion migration, phase decomposition, gas bubble formation and even crystalization in different glasses. However, the understanding of irradiation mechanisms in glasses on the atomic level is limited and is highly desirable in order to predict modification by electron beam. Here, we discuss the irradiation effects in silicate glasses on the atomic scale based on in situ electron energy loss spectroscopy (EELS) observations of several silicate glasses. In short, we found that, in glass network modifiers, along with the non-bridging oxygen (NBO), are very sensitive to electron irradiation. This probably arises from the highly localized DOS on the NBO - cation bonds. There is a tendency to eliminate NBOs in the region under irradiation. Phase separation into cation rich and poor regions is thus an unavoidable trend for silicate glasses. During the reconstruction under irradiation, some of the NBOs are converted into bridging oxygen, while some form O2 molecules or clusters. These two processes are in competition, and depend on the irradiation rate and glass composition. At higher rates of irradiation, larger amounts of O2 are formed. Once the NBOs are all consumed, O2 may eventually disappear into vacuum. The released cations may either fill the vacancies outside the irradiated region left by Si and form cation rich region or capture free electrons created by electron irradiation and become neutralized atoms. Therefore the precipitation of metallic particles is also an expected product of irradiation. This is also dependent on the amount of NBOs. This work is supported by NSF Grant DMR0245792.

9:15 AM R10.3
The atomic structure and interstitial or vacancy nature of individual parameterized defects are determined by quantitative measurements and computer simulations of electron spin resonance spectra. Irradiation-produced defects in gold, tantalum, and silicon are studied to establish the methods. Experimentally, diffuse scattering by isolated single dislocation loops is measured by energy filtered TEM in the high resolution microscrope, A CS measured from Bragg scattering at weak excited diffraction peaks. Computer simulations of kinematical elastic electron scattering from defect structures, modeled by both analytical and molecular dynamic methods, are compared with experimental results. Comparison with previous x-ray scattering simulations are also made. Often, the pattern of diffuse scattering within a single reciprocal lattice plane, when compared with these simulations, reveals the defect geometry and interstitial or vacancy nature of defects. The sensitivity of this method to the diffusion conditions, dynamical scattering, and degrees of electron beam coherence and convergence are discussed. This work is supported in part by the U.S. Department of Energy, Office of Basic Energy Sciences under contracts W-31-109-ENG-38 (ANL) and DEFG02-91ER45428 (UIUC).

9:30 AM R10.4 High-Resolution Spectrochemical Analysis of Columnar Defects formed in Bi2Sr2CaCu2Ox by Swift Heavy Ion Irradiation. Michiaki Terawaki1, Fumiharu Kano1, Takahisa Mitamura1, Tatsushi Kambara2, Yukiko Saeki2 and Yuichi Kohara3, 1Laboratory of Advanced Materials Science and Technology, AIST, Tsukuba, Ibaraki, Japan, 2Institute of Applied Physics, National University of Singapore, Singapore, 3Micro-structure Analysis Research Center, Osaka University, Osaka, Japan.

Single crystal of high temperature superconductor Bi2Sr2CaCu2Ox was irradiated with 3.5GeV Xe ions at room temperature up to 1.0×1011 ions/cm2. Significant enhancement of magnetization by the irradiation was confirmed. The irradiated specimens were studied by using a high resolution transmission electron microscope with field immersion gun (FEG-TEM), and also, with an energy dispersive x-ray analyzer. Columnar defects with diameter of about 6 nm were observed along the incident ion tracks. Nano-scale high resolution x-ray spectrochemial analysis across the columnar defects revealed enrichment of Cu and depletion of Sr and Ca in the columnar defects center, suggesting that the defects were formed due to a Coulomb explosion induced by the Xe ion irradiation.

9:45 AM R10.5 Stability and Structure of Thin Cu Films on Mo and Ta Investigated by X-ray and Optical Techniques. Yuming Meng1, Borys Vanyukov1, Ivan J Seigiel1 and Barend J Thijssen2, 1Laboratory of Materials Science, Delft University of Technology, Delft, Zuid Holland, Netherlands.

Thermal helium desorption spectroscopy (THDS) of ion-implanted helium is a powerful technique for quantitative analysis of small concentrations of defects in surface layers. We have found that THDS can also be fruitfully used for the study of morphology changes in nanostructured film/substrate systems. In this work we present results for thin Cu films (0.5-20 nm) deposited on Au on Mo and Ta substrates by electron beam evaporation. These systems were selected to serve as model systems for investigating Fe films on Fe substrates and to improve our understanding of the structure and stability of Cu seed films, such as those used in IC interconnect metallization where Ta is the diffusion barrier. As a first step after film deposition, low-energy implanted helium (75 eV) becomes trapped in the defects present in the Cu film at the interface. Information about the Cu film/substrate interface. Subsequently, on heating the samples, helium release is seen not only by desorption but also as a result of different morphological transformations of the Cu film. One is evaporation (close to the Cu melting temperature of 1354 K). The other is 3D island formation, taking place at lower temperatures. This could be identified by a combination of pre-implantation annealing and medium-energy helium desorption. For example, a 10 nm Cu film is opaque for 1000 eV helium, while after annealing the desorption spectrum looks similar to that of a bare Mo substrate, showing that the film has become ion-transparent over much of its area. The kinetics of this island formation process, which shows up as a broad peak in the He desorption spectrum, strongly depends on film thickness, is investigated. The differences between the Mo and Ta substrates and the influence of film thickness are discussed.

10:45 AM R10.6 Recovery Effect of Electron Induced Damage in 4H-SiC Schottky Diodes. Anna Daniela Cavallini1, Antonio Castaldini2, Lorenzo Bigatti2, Filippo Nava2, Pier Giorgio Paschi2 and Paolo Vanni2, 1INFN and Dipartimento di Fisica, Università di Bologna, Bologna, Italy, 2INFN and Dipartimento di Fisica, Università di Modena e Reggio Emilia, Modena, Italy, 3Istituto ISOF, CNR, Bologna, Italy.

Deep level transient spectroscopy (DLS) and capacitance-voltage (C-V) characteristics were used to investigate the effects of electron irradiation on the defects associated electronic levels in Schottky diodes on 4H-SiC carbide epitaxial grown by chemically vapor deposition. DLS and C-V investigations have been performed before and after irradiation with 8.6MeV electrons at different doses. Four traps with an enthalpy equal to (Ec -0.23 eV), (Ec -0.39 eV), Ec -0.60 eV and (Ec -0.75 eV) were detected and their concentration was monitored as a function of the irradiation dose. Their thermal stability, a key point to determine their structure on the basis of recent theoretical and experimental results, was carefully investigated since it was earlier observed that during DLS analyses up to 500 K a slight but significant recovery of a few levels generated by the irradiation occurs. This effect was previously observed in literature for the level at (Ec -0.7kV) after thermal treatment at 500 C, but the present results indicate that it involves more than a single level and is also effective at lower temperature. DLS analyses were, then, performed from room temperature to liquid nitrogen temperature and vice versa up to 500 K. The annealing kinetics is here reported and a few conclusions on the structure of the defects involved in the recovery are drawn. The correlation with the diode charge collection efficiency is also reported.

10:30 AM R10.7 Gas Cluster Ion Beam Processing of GaSb and InSb Surfaces. Kiran Krishnamurthy1, S Vangala1, L P Allen2, C Santefeuem3, D Bliss2, D Dzuba2, M Ocampo3, X Liu4, J Whitten3, C Song5 and W D Goodhue6, 1Photonics Center, Dept. of Physics and Applied Physics, University of Massachusetts, Lowell, Massachusetts, 2Epion Corporation, Billerica, Massachusetts, 3Air Force Research Laboratory/SNH, Hanscom AFB, Massachusetts, 4Center for Advanced Materials, University of Massachusetts, Lowell, Massachusetts.

Gas Cluster Ion Beam (GCIB) processing has recently emerged as a novel surface smoothing technique to improve the surface morphology of chemical-mechanical polished (CMP) GaSb (100) and InSb (111) wafers. This technique is capable of removing CMP induced damage and subsurface damage and smoothing the surface, while simultaneously producing a thin oxide layer that can describe for epigrid growth. Implementing recipes with specific gas mixtures, cluster energy sequences, and cluster dose produce oxide layers of controllable thicknesses and elemental compositions, thereby producing an engineered oxide. Using high quality CMP GaSb wafers, we have successfully demonstrated surface smoothing by reducing the average roughness from 2.8 to 1.7 from a dual energy, dual gas GCB sequence incorporating CF4/O2 at 10 kV followed by O2 at 5 kV. In the first time, we report a GCIB grown oxide layer, deposited on gallium and antimony oxides, that fully desorbed at 560°C in our molecular beam epitaxy (MBE) system. Upon desorption, GaSb/AlGaSb epilayers were successfully implemented on the GCIB processed surfaces. Using InSb, we successfully demonstrate smoothing by reducing the average roughness from 2.5 to 1.6 using oxygen gas clusters in a triple energy GCIB process with energies 20 kV, 10 kV, and 5 kV. In order to demonstrate the ability of GCIB to smooth InSb surfaces, sharp 850 nm high tips formed on the (111) plane were successfully flattened by SF6/O2 gas clusters in a triple energy GCIB process with energies 30 kV, 10 kV, and 5 kV which reduced the tip heights to less than 100 nm, indicating an improvement by a factor of eight. GCIB is a powerful process capable of producing ultra-smooth, damage free GaSb and InSb substrates with an engineered oxide for epigrid growth. These important criteria for rendering "epi-ready" substrates.

10:45 AM R10.8 Experimental study of cluster size effect with size-selected cluster ion beam irradiation system. Noritaka Togoda, Shingo Hoshiumi and Isao Yamaoka, LASI, Institute of Technology, Kaminori, Hyogo, Japan.

It has been shown by molecular dynamics simulations that cluster size is important for electronic structure calculation. Though the total acceleration or energy per atom are the same, the damage formation in solid materials are different depending on the impinging cluster ions. There were cluster ion beam systems that could select cluster size. However, the ion currents were very small or operated in a pulsed mode. Therefore it is difficult to perform experiments that require high dose by size-selected cluster ion beams. Recently, we have developed a high current cluster ion beam system with size selection functions at the first time. This system equipped a
permanent magnet with a magnetic flux density of 1.2 T. There is a sliding detector and sample holder on a guiding rail perpendicular to the incident X-ray beam axis. When the sample was positioned at a certain point on the rail depending on the momentum of the cluster ions, the desired size of cluster ion can be irradiated continuously with affordable ion current density. In this study, preliminary results of mass spectra of cluster size effects for damage formations and sputtering phenomena are discussed. *Supported by New Energy and Industry technology Development Organization / Ministry of Economy Trade and Industry, Japan.

11:00 AM R10.9
N-wells Voltage Contrast Imaging with a Focused Ion Beam
Erwan Le Roy and Mark Thompson, NPItest, San Jose, California.

It has been discovered that a focused ion beam can be used to image n-wells through oxide on the backside of thinned ICs without electrical biasing. Charging and discharging phenomena lead to the observation of ion-beam assisted etching of the n-well structure in the oxide area. A method to use the I/BM image signal to reveal surface area of the n-well and conductive contact between the n-well and p-substrate is presented. Simulated cross-sectional view of an oxide structure is given to illustrate the shape and distribution of the etched area. By varying the beam energy, the depth of the etched area and the contrast of the image can be varied. The ion dose required to achieve stable and consistent changes in the image signal can also be controlled. The method has the advantage of not requiring electrical biasing of the IC or any accompanying power supply, and it can be used to characterize structures that would be inaccessible to electrical biasing.

11:45 AM R10.12
One-step nanofabrication of diffractive structure via focused ion beam scanning on glass
Fu Yenong, Singapore-SMT Alliance, Nanyang Technological University, Singapore, Singapore.

A diffractive structure was obtained by directly scanning on a glass substrate in an area of 2x20 micron2 by use of focused ion beam (FIB) with energy of 30 keV and beam current of 1 nA. It is a pattern transfer free process. Ripples with regular shape and period were observed on glass after FIB scanning. The ripples could be used as diffractive grating. Wavelength and amplitude of the ripples was characterized by use of atomic force microscopy (AFM), ranging from 1.2 to 2.3 micron, and 30 to 256 nm, respectively. The ripples have potential application in optics as blaze grating for the working wavelength in the range from visible light to ultraviolet (UV). However, physical properties of the glass may be damaged to a certain extent due to more or less Ga4+ implantation during the scanning with energy of 30 keV. Considering this, the phase variation, refractive index, and transmission were investigated in this paper. To further study the implanted Ga4+, the implantation depth was calculated by TRIM software, which is commonly used for ion beam analysis. The compound percentage of the implanted Ga4+ was measured using electron dispersion X-ray spectrometer (EDX).

SESSION R11: Modification of Physical Properties
Chairs: C. Arevelo and H. van Swygenhoven
Thursday, December 4, 2003
Room 306 (Hyatt)

1:30 PM R11.1
Ion Beam Processing for Silicon-Based Light Emission
Wolfgang Skorina1, Juming Sun1, Thomas Hohage1,2,1 NTU, 2NTU, Munich, Germany.

In this talk an overview will be presented on the synthesis of silicon-based light emitters with ion implantation techniques. After a short view to the field we will concentrate on two activities performed at the PZK during the last years, [i] blueviolet (400 nm) light emitters based on metaloxide-silicon (MOS) capacitors, and [ii] infrared (~1 micron) light emitters based on p-n junctions formed by B+ implantation in n-doped Si. Both approaches use ion beam processing as a key doping technique of advanced semiconductor technologies. For the first time we have employed implants of group IV ions (C, Si, Ge, Sn) into thermally grown silicon dioxide layers followed by an appropriate annealing step. These MOS structures exhibit electroluminescence with a power efficiency of 0.5%, corresponding to an external quantum efficiency of 10%. This preparation method leads to the formation of semiconductor nanoclusters in the oxide matrix; the luminescence itself is related to defects. Compared to other oxide production techniques such as sputtering or evaporation it is shown that such high electroluminescence values are only achieved by means of ion beam processing, i.e. the combination of nanocluster synthesis and beam-induced energy deposition. For the second time we investigate the electroluminescence from implanted silicon ion dipoles as a function of the implantation dose. Low temperature electroluminescence measurements in combination with microstructural analysis reveal the relevance of local boron.
saturate in combination with strain effects for efficient elektrochromic switching which, of course, is only possible by ion implantation. A model developed the carrier and exciton dynamics in the diodes underlines the importance of the defects introduced.

2.00 PM R11.2
Characterization and Room-Temperature Ferromagnetic Properties of Co- and Fe-Implanted TiO₂ Films, C.F. Chow1,2,3, K.H. Cheng4,5, J.R. Wang6, Y.W. Liu5, K.W. Lo5, L. Lin7,8, Y. Gao9, Q. Li10,11, N. Ke12, W.Y. Chung11,12, and S.P. Wong11,12,13, Chinese University of Hong Kong, Shatin, Hong Kong; 2Physics, Chinese University of Hong Kong, Shatin, Hong Kong; 3Materials Science & Technology Research Center, Chinese University of Hong Kong, Shatin, Hong Kong.

In this work, TiO₂ thin films were prepared by RF sputtering onto thermally grown oxide layers on Si substrates. Cobalt or iron implantation was performed using a metal vapor vacuum arc (MEVVA) ion source at an extraction voltage of 65 kV to doses ranging from 4×10¹⁴ cm⁻² to 1×10¹⁴ cm⁻². Annealing was performed in vacuum at 600°C for 2h. The cobalt and iron composition and distribution in the implanted TiO₂ were studied using Rutherford backscattering spectrometry. The microstructures were studied using transmission electron microscopy and x-ray diffraction microscopy. The optical properties were studied using spectroscopic ellipsometry in the wavelength range from 350 to 700 nm. The magnetic properties were measured by vibrating sample magnetometry. We observed clear room-temperature ferromagnetic properties for all the as-implanted and annealed samples prepared under the above conditions. The measured Mₜ values for the Co- and Fe-implanted samples ranged from 0.5 to 1.7 μB/Co atom and from 0.5 to 1.6 μB/Fe atom, respectively, both exhibiting an excitatory dependence on the implantation dose. The coercivity values ranged from 100 Oe to 400 Oe for the GP-implanted samples, and from 500 Oe to 900 Oe for the Fe-implanted samples, depending on the Co and Fe dose and the annealing conditions. The correlation between the optical properties, the magnetic properties and their structures will be discussed. This work is supported in part by the Research Grants Council of Hong Kong SAR (Ref. number: CUHK-421/08E and CUHK-4221/08E).

2.15 PM R11.3
Microstructures and Electron Field Emission Properties of Ion Beam Synthesized and Modified SiC Thin Layers, S.P. Wong1,2,3, W.M. Tsong1,4, J.-L. Y. S. Tsang1,2, Y.W. Liu1,2, Y.W. Cheung1,4, N. Ke2,5, and J.K.N. Lindner2,3, Electronic Engineering, Chinese University of Hong Kong, Shatin, Hong Kong; 4Institute for Physics, University of Augsburg, Augsburg, Germany; 5Materials Science & Technology Research Center, Chinese University of Hong Kong, Shatin, Hong Kong.

It was reported several years ago that good electron field emission (FE) properties with a very low turn on field of about 15 V/μm could be obtained from ion beam synthesized (IBS) SiC/Si heteroepitaxy [1]. More recently, by correlating the FE properties with the surface morphology and local surface conductivity, it was demonstrated that there were two distinct electronic field enhancement mechanisms for electron FE from SiC/Si heteroepitaxy [2] required by these understandings, modification of the IBS SiC layers by metal implantation was performed aiming at improving the FE properties. The SiC layers were synthesized by implanting carbon ions into Si wafers using a metal vapor vacuum arc (MEVVA) ion source at various energies and doses. Modification of the SiC layers was performed by tungsten implantation also by the MEVVA source. Characterization of the implanted samples was performed using atomic force microscopy (AFM), conducting AFM, Fourier transform infrared absorption spectroscopy, x-ray diffraction, x-ray photoelectron spectroscopy, and transmission electron microscopy. Excellent field emission properties with an ultra-low turn-on field of 0.35 V/μm have been achieved in some of these samples exhibiting a nanocomposite structure prepared under appropriate implantation and annealing conditions. The details of the FE properties, the structures, and their dependence on the processing conditions will be presented and the field emission mechanisms will be discussed. This work is supported in part by the Research Grants Council of Hong Kong SAR (Ref. CUHK2420/08E) and by the Germany-Hong Kong Joint Research Scheme of RGC, Hong Kong SAR and DAAD, Germany (10/0012, Project 722, 1999-2000 (1998). [2] W.M. Tsang et al., Appl. Phys. Lett. 81, 3942 (2002).

2.30 PM R11.4
Changes in Microstructure and Tribological Behavior of Thin-Film Bimetallic Layers Irradiated by Pulsed Ion Beams, Timothy J Renk1, Paul P Provencio1, Somari V Prasad2, and Michael O Thompson1, 1Sandia National Laboratories, Albuquerque, New Mexico; 2Cornell University, Ithaca, New York.

The objective of our study was to produce wear-resistant surfaces by exposing 1 μm thick bimetallic layers of transition metal coatings to intense pulsed ion beams. The ~200ms ion pulse produces fast melt and cool cycles, leading to grain refinement and formation of metastable alphas. Ta niton alloy substrates, with and without sputter-deposited metal coatings, were treated using nitrogen and other ion beams, producing cooling rates of up to 10⁶K/sec. The fluences used produced a melted layer several microns thick, with all ion beam produced at the highest doses. The microstructure and tribological samples were studied by electron diffraction (SAD) and both bright field and dark field cross-sectional TEM (XTEM).

Conventional changes were measured by non-contact interferometric displacement spectroscopy (EDS). Both miscible (Hf/Ti) and nearly immiscible (Pt/Ti) systems have been studied. The resulting microstructure is significantly different in the two cases. Both bimetallic layers are subjected to tribological testing, to study the relation between the microstructures and frictional behavior. In both cases, improvements in friction and wear behavior are observed, compared to both untreated and untreated Ti alloy. In addition, changes in the Ti substrate occur (martensite conversion, enhanced dislocation density) well below the melt zone, up to 100 microns deep, which may contribute to improved mechanical properties. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Co., under US DOE. Contract DE-AC04-94AL85000.

2.45 PM R11.5
The Effects of Proton Irradiation on the Structural and Optical Change of VO₂ Thin Film. Lichao Li1,2, Jianyong Jiang3,4, Hongzhong Lu1,2, Department of Physics, Sichuan University, Chengdu, China; 2Key Laboratory for Radiation Physics and Technology of Education Ministry of China, Sichuan University, Chengdu, China.

VO₂ thin films with special phase-transition properties prepared by vacuum evaporation combined with vacuum deposition were irradiated by proton beam with fluence of 1×10¹⁴ cm⁻²-1×10¹⁵ cm⁻² and energy of 7.0 MeV. After irradiation, the samples were annealed at different temperatures. Before and after irradiation, both phase transition and crystalline structures are characterized by X-ray diffraction and X-ray photoelectron spectroscopy. UV-VIS transmission and Raman spectroscopy. The results indicate that after irradiation, VO₂ thin films can also be transferred from the phase of amorphous to rutile, but the phase-transition temperature and the width of phase-transition hysteresis changed as well as the valence of ion and the crystalline structure changed. The results of Raman spectroscopy measurement show the transformation of OH clusters induced by protons.

3:30 PM R11.6
Tailoring Magnetic Properties by Light Ion Irradiation, Jurgen Passendorfer, Fachbereich Physik, University of Kaiserslautern, Kaiserslautern, Germany.

Nanostructured thin films are of crucial importance for magnetic storage technology. Ion irradiation based techniques exploit the potential to produce improved storage media, since it becomes possible to tailor the magnetic properties on a nanometer scale without a modification of the surface topography. The achievable out-of-plane density will thereby be pushed further to the limits. Also for position sensing devices simplified fabrication processes are currently tested which rely on ion irradiation. Further research shows that ion and the crystalline structure changed. The results of Raman spectroscopy measurement show the transformation of OH clusters induced by protons.

3:30 PM R11.6
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4:00 PM R11.7
Optimizing the Fracture Toughness of Brittle Materials by Ion Implantation, J Gregory Swallen1, Michael Biske2, Thomas E Fertig3, Chin J Wettlaufer4, Joseph R Tesmer2, Xingfang Zhang3, and Michael Nix5, 1MSI-L, Los Alamos National
Elaboration of a combined experimental and molecular dynamics study on the formation and growth of small and medium-sized crystals of the cellulose polymer, leading to the formation of clusters of disordered matrix. The presence of these clusters is crucial for the formation of the crystalline structure of the cellulose polymer. The results of this study have been presented in the Materials Science of Crystallinity Research Symposium, sponsored by the Office of Basic Energy Sciences, USA. The work was supported under Contract No. W-31-109-Eng-38 by the University of California, Lawrence Livermore National Laboratory.

In conclusion, the experimental and molecular dynamics study on the formation and growth of small and medium-sized crystals of the cellulose polymer has provided valuable insights into the formation of clusters of disordered matrix. The presence of these clusters is crucial for the formation of the crystalline structure of the cellulose polymer. The results of this study have been presented in the Materials Science of Crystallinity Research Symposium, sponsored by the Office of Basic Energy Sciences, USA. The work was supported under Contract No. W-31-109-Eng-38 by the University of California, Lawrence Livermore National Laboratory.

Pattern Formation in Ar-sputtered InP and Sample Rotation. Gih Sheng Lim, Jiasheng Pan and Jin Wei Chai, Institute of Materials Research & Engineering, Singapore, Singapore.

We study the formation and self-organization of cones appearing during Ar+ bombardment of InP surface with ion beams having varying beam energies and sample rotation speeds. Our results obtained from the AFM imaging and XPS analysis of the sputtered surfaces show that cone density increases with beam current and energy. Formation of cones has been significantly suppressed by the introduction of sample rotation during Ar+ bombardment. We attribute the formation of cones to the preferential sputtering of P atoms from InP and accumulation of In atoms on the surface.

Beam Assisted Deposition. James K. Hirdon, WMRD-MS, Army Research Laboratory, APG, Maryland.

The beneficial roles energetic ions play in thin film vacuum processes have long been recognized by the coating community. Early work on ion plating [D. Mattox, Sandia, 1963] showed the importance of ion bombardment on coating properties when present during vapor deposition processes. The optical coating community was among the first to adopt the process in the form of concurrent ion, directed ion beam bombardment of physical vapor deposition [electron beam] coatings for producing dense, adherent, robust optical coatings. The international R&D ion beam community has also been actively pursuing the study of ion beam assisted deposition (IBAD) for both studying the mechanisms of ion/solid interactions during thin film growth as well for developing coating protocols for specific application areas, including tribological coatings, anti-corrosion coatings, optical coatings, and electronic/magnetic films. This presentation will review selected areas of this maturing field and will attempt to assess promising future R&D and application areas.


Gold nanoclusters in silicon are prepared using electron beam evaporation of gold and silicon with or without Ar bombardment followed by post deposition annealing. X-ray diffraction, x-ray reflectivity, and transmission electron microscopy are used to characterize the gold cluster orientation, size, and spatial distribution. The effects of ion bombardment on the cluster formation and evolution are investigated.


Crucial to nanostructure efforts is the ability to make reliable and well-characterized contacts to specific nanostructures in order to determine their electronic and optical properties. We have used a commercial dual beam FIB/SEM system to deposit conductive platinum (Pt) nanowires on oxidized silicon substrates as potential nanoscale interconnects. Decomposition or pyrolysis of a nanoparticle gas by a focused ion or electron beam resulted in localized metal deposition. The resistivity of the nanowires was easily tuned by varying parameters such as beam energy and current. However, the deposition rate was not entirely restricted to the beam raster area, with some surrounding metal decoration. The spread function of the deposition was quantified by energy dispersive spectrometry (EDS) as well as by time-of-flight secondary ion mass spectrometry (TOF-SIMS). The electrical impact of the spread was quantified by measuring the leakage current between closely spaced nanowires. The origins of the metallic spread and strategies to mitigate its impact will be discussed. Optimal deposition conditions were identified for obtaining low resistivity wires with minimal spread-induced leakage current. This work will enable the use of FIB/SEM based direct write nanolithography for the fabrication of planar interconnects between building blocks such as semiconducting nanowires and nanotubes.
produced and subsequently decelerated in an electrostatic lens to
well-defined energies between 0 and 200 eV. Prior to deposition, the
substrates were cleaned with a two-step silicon flux method to achieve
the Si(111) 7x7 reconstruction. After deposition the samples were
transported through vacuum to an in situ scanning tunneling
microscope. For low coverage (~ 0.3 ML) we observe that the
periodicity of the 7x7 structure gradually degrades with increasing
deposition energy. These early stages of the layer formation are
expected to influence the growth of thicker films. For higher coverage
(~2 ML) we investigated the influence of the deposition energy on the
surface morphology. Depositions with LEED show a higher cluster
density and a lower surface roughness compared to MBE depositions.
The influence of the film thickness and deposition energy on the
surface roughness will be discussed. We found an optimal ion energy
of ~25 eV for growing films with minimal roughness. Ab initio
calculations were used to examine the preferred site for 0.5 ML and 2
ML of Co on an unreconstructed Si(111) substrate, from which
information on the binding energies of different Co-locations and on
the initial silicide formation can be obtained. This information will be
linked with the experimental observations.