SYMPOSIUM R

R: Radiation Effects and Ion Beam Processing of Materials

December 1 - 5, 2003

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* Invited paper

SESSION R1: Radiation Effects in Metals and Alloys
Chairs: L. Snead and H. Takahashi
Monday Morning, December 1, 2003
Room 306 (Hynes)

8:30 AM *R1.1
Microstructures of Irradiated and Mechanically Deformed Metals and Alloys: Fundamental Aspects. Steven J Zinkle, Nao Hashimoto, Yoshi Matsukawa, Roger E Stoller and Yuri N Osetsky; Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Pronounced microstructural changes are induced in pure metals and alloys by energetic particle irradiation. Fundamental theoretical and experimental investigations of these microstructural changes are indispensable for understanding the underlying physical processes. This presentation will review recent molecular dynamics and transmission electron microscopy results on irradiated metallic materials, with an emphasis on defect production in the displacement cascade and the fluence- and temperature-dependent accumulation of defect clusters. The presentation will include results on Fe, V, Cu, oxide dispersion strengthened Cu, austenitic stainless steel, V4%Cr4%Ti, and ferritic/martensitic steel. Intrinsic differences between the defect accumulation behavior of BCC and FCC metals will be highlighted. Results on the temperature-dependent vacancy cluster density will be analyzed to provide information on vacancy binding energies. Information on self-organization of planar defect clusters (dislocation loops and stacking fault tetrahedra), voids and He bubbles in irradiated metals will also be summarized. Finally, recent results on deformation behavior of irradiated, quenched, and deformed metals will be presented, with particular emphasis on flow localization mechanisms (e.g., dislocation channeling), and experimental and molecular dynamics studies of the detailed dislocation-defect cluster interaction.

9:00 AM R1.2
Computer Simulation of Irradiation Effects in Molybdenum. Richard Whiting Smith, Materials Technology, Bechtel Bettis Inc., West Mifflin, Pennsylvania.

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 hardening. If Mo-based alloys are to be made useful in nuclear applications, the embrittlement mechanisms have to 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 survival fractions 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 applied to the embrittlement 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 Han[1], Mikhail I Mendelev[1], David J Srolovitz[3,1] and Robeto Car[2,1]; [1]Princeton Materials Institute, Princeton University, Princeton, New Jersey; [2]Department of Chemistry, Princeton University, Princeton, New Jersey; [3]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 Fe to V at a few percent level drastically increases the rate at which V swells. In this study, we perform both first principles, 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 solute atoms. 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-interstitial motion is rapid in V at even 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 will be discussed.

9:30 AM R1.4
Atomistic Simulations of the Effects of Helium on Irradiation Damage in bcc Iron. Maria A. Okuniewski[1,2], Srinivasan G. Srivilliputhur[2], Stuart A. Maloy[2], Michael I. Baskes[2], Michael R. James[2] and James F. Stubbins[1]; [1]Nuclear, Plasma, and Radiological Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois; [2]Los 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, such as tensile and creep properties, and the addition of helium may exacerbate this damage. Molecular dynamics simulations are utilized to understand the atomistics of the processes occurring during irradiation in a Fe-He system, by varying the projectile energy. The modified embedded atom method potential, that explicitly includes angular forces which are essential to model the Fe-He system, is used. Attention is focused on the effects of irradiation on the evolution of defects, especially He interstitials, clusters, and bubbles of varying pressures. These results are compared to an irradiated Fe system without He.

9:45 AM R1.5
Helium Effects on EUROFER97 Martensitic Steel Irradiated by Dual-beam at 200°C and 250°C with 1000 He appm. Jinnan Yu, Nuclear Materials Division, China Institute of Atomic Energy, Beijing 102413, China.

The reduced activation martensitic (RAM) steel is presently the most realistic contender for application in fusion blankets near magnetically confined plasma. The serious issue is loss of fracture (associated with a DBTT shift) by irradiation at low temperature Tirr < 300°C. The history of low temperature operation maybe endanger the safety of FW and the blanket system, especially a blanket concept cooled by pressurized water. The dose dependence of impact properties of RAM steel at low irradiation temperature (< 300°C) seems to be in the low-dose range mainly an effect of helium generated by different levels of boron. The 10B isotope is burnt up with nearly the same characteristic time constant as DBTT increases towards saturation. The helium effects on DBTT at low-temperature irradiation below 300°C is proportional to He content. It is important to investigate helium effects by microstructural observation to address the helium action. EUROFER97 Martensitic steel specimens were irradiated by Dual-beam in HVTEM 1000 Multi-Beam High Voltage Electron Microscope with 1000 He appm at 200°C and 250°C. The energy of electron and helium beam is 1.00 MeV and 10 keV respectively. Electron beam is perpendicular to the specimen and the tilt angle of helium beam is 45° to the specimens. The specimen thickness was about 40 nm and the damage dose is 0.2 dpa. In-situ observation shows that bubbles with 2-3 nm in diameter were formed in irradiation temperatures 250°C and the dislocation density was increased, as well as observing the black-white spots. But it is difficult to find the bubbles in the specimen at irradiation temperature 200°C and the dislocation density was increased. The presented He bubbles or cavities effect on the crack initiation and transgranular crack propagation under high stress rate at high strain process or impact process, it is sensitive to the helium effect. On the other hand, at lower strain ranges the very small irradiation induced defects (e.g., dislocation loops, helium bubbles, defect clusters) as obstacles impede the dislocation and crack propagation, the tensile properties and creep are insensitive to helium effect.

10:30 AM *R1.6
Role of Irradiation in Stress Corrosion Cracking of Austenitic Alloys in High Temperature Water. Gary S Was, 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 environments. The degree of irradiation assisted stress corrosion cracking (IASCC) increases with dose, and the microstructure undergoes significant changes including the formation of dislocation loops, grain boundary segregation and hardening. Total dislocation loop line length correlates with increased hardening and with IASCC 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 IASCC. However, these various changes occur simultaneously and at comparable rates, complicating the attribution of IASCC to specific components of the microstructure. Each of the principal effects of irradiation has been considered as a potential cause of IASCC, but the multivariable nature of the problem obscures a definitive determination of the mechanism. Rather, the mechanism of IASCC 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 irradiated microstructure and RIS, and the interaction of localized deformation with the oxide film and the grain boundaries. Current understanding and proposed mechanisms of IASCC will be reviewed, and recent progress to identify additional factors or combinations of factors affecting IASCC will be presented

11:00 AM R1.7
The Irradiated Microstructure of Ferritic Steel T91 and 9Cr-ODS. Jian Gan[1], James I. Cole[1], Todd R. Allen[1], Shigeharu Ukai[2], Shuttha Shutthanandan[3] and Theva Thevuthasan[3]; [1]Nuclear Technology, Argonne National Lab-West, Idaho Falls, Idaho; [2]Japan Nuclear Cycle Development Institute, Ibaraki, Japan; [3]Pacific Northwest National Laboratory, Richland, Washington.

A ferritic steel T91 and an oxide dispersion strengthened alloy (9Cr-ODS) were irradiated with Ni ions at 500°C to doses of 5 and 50 dpa. Both alloys are iron-based with 9Cr. They have excellent high temperature strength in the application of non-radiation environment. However, the radiation effects on these two alloys are not well characterized. The microstructure was characterized using transmission electron microscopy. The effects of irradiation on network dislocation, dislocation loops, precipitates etc. will be reported in comparison with others' work. The stability of the Y_2O_3 oxides dispersion under irradiation will be addressed. Dose effect on the irradiated microstructure will be analyzed. This work was supported by the Department of Energy under NERI grant 2002-0110.

11:15 AM R1.8
Defect Diffusion in hcp Zirconium: A kinetic Monte Carlo approach. Cristina Arevalo[1], Maria J Caturla[2,3] and J Manuel Perlado[1]; [1]Instituto Fusion Nuclear, ETSII Universidad Politecnica de Madrid, Madrid, Spain; [2]Departamento de Fisica Aplicada, Universitat Alacant, Alicante, Spain; [3]Lawrence Livermore National Laboratory, Livermore, California.

α-Zirconium is currently used in nuclear reactor systems; in particular in fuel cladding and pressure tubes, and it is the first barrier between the radioactive material and the environment. Its integrity need 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 effect of radiation at operating temperatures on the mechanical properties of these materials. Present approaches to high-burnup fission fuel drive to the proposal of ZrNb alloy that is the final goal of our research; to start with that problem we need to clearly identify by multiscale modeling the physics in Zr irradiation. Irradiation damage produced in many fcc and bcc metals has been extensively investigated, but studies on hcp materials have been more limited. These studies however have been increasing in the last few years, in particular with the work of Bacon [1] and Pasianot [2] using molecular dynamics (MD). Currently important information on defect diffusion and clustering has been obtained from those MD simulations that let us think and propose a kinetic Monte Carlo model for defect diffusion in α-Zr. One of the challenges of hcp materials with respect to fcc or bcc is the anisotropy of point defect diffusion: vacancy diffusion is approximately isotropic but interstitial diffusion changes from the one-dimensional at low temperature (<300K) to two-dimensional in the basal plane and then three-dimensional at higher temperature. For this first attempt to study damage production and diffusion in α-Zr by using Object Kinetic MonteCarlo model we will limit our studies to low temperature (<300K) where the migration is mostly in one-dimension along a <11-20> direction. The parameters used in the simulations are those obtained from MD. We will focus on the case of electron irradiation where only point defects are formed and we can compare with experiments. The number of freely migrating defects will also be calculated using the displacement cascades obtained by Bacon et al with MD. [1] S. J. Wooding, D. J. Bacon, Phil. Mag. A 76 (1997) 1033 [2] R.C. Pasianot, A.M. Monti, G. Simonelli, E.J. Savino, J. Nucl. Mat. 276 (2000) 230

11:30 AM R1.9
Surface porosity development on metal substrates by helium implantation and annealing. R. Escobar Galindo[1], A. van Veen[1], H. Schut[1], J.H. Evans[2], A.V. Fedorov[1,4], P.Y. Hou[3] and J.Th. M. De Hosson[4]; [1]Defects in Materials, IRI, University of Delft, Delft, Netherlands; [2]Camrose Consultants, Abingdon, United Kingdom; [3]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California; [4]Materials 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 keV He^+ions up to doses of 3 and 5 x $10^{16}cm^{-2}$. In order to avoid the release of gas during annealing thin coatings were deposited on the substrates. Therefore W-C:H films with a thickness of 2 μm and an adhesive intermediate Chromium layer of 200 nm and multilayers of Ti and Al with a total thickness of 1.6 μm and a periodicity of approximately 20 nm were deposited by PVD on the copper substrates. Finally the samples were annealed afterwards in vacuum at temperatures from 773 to 1073 K for 30 minutes. After a post-deposition annealing, the implanted gas is collected as bubbles at the coating-metal interface. These bubbles are confined by the presence of the coating and developed into equilibrium bubbles with equilibrium pressure P$\sim$2 γ/R, with γ the surface energy and R the radius of the bubble. In the case of TiAl multilayers this leads to the formation of facetted structures in the substrate implanted with the highest dose. Low index facets develops. 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>873 K. In the case of W-C:H coated samples, after annealing to 973 K some blistering is observed but almost all the surface of the coating remains intact. Further annealing at 1073 K provokes blistering and flaking of the coating. Contrarily 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 aluminade sample coated with a thermally grown alumina layer 300 nm thick was implanted with helium ions at 120 keV with a fluence of $3x10^{16}cm^{-2}$. 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 one observed for the copper coated with TiAl multilayers. Similar procedures has been applied to titanium and aluminum deeply pre-implanted with helium at 140 keV. Samples were subsequently heated both by annealing in a vacuum oven 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.

11:45 AM R1.10
In Situ TEM Study of Irradiation-induced Transformation in TiNi Shape Memory Alloys. Xiaotao Zu[1], F.R. Wan[2], S. Zhu[3], Z.G. Wang[1] and L.M. Wang[3]; [1]Department of Applied Physics, University of Electronic Science and Technology of China, chengdu, China; [2]Department of Materials Physics, University of Science and Technology of Beijing, beijing, China; [3]Department 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 becoming an important topics. Some irradiation-induced diffusion-dependent phase transformations, such as amorphization, have been reported before. In the present work, the behavior of diffusion-independent phase transformation in TiNi SMA was studied by 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 show that the microstructure of samples is R phase in the room temperature. Electron irradiations were carried out using several different transmission electron microscopes (TEM) with accelerate voltage of 200 kV, 300 kV, 400 kV and 1000 kV. Also the accelerate voltage in the same TEM was changed to investigate the critical voltage for the effect of irradiation on phase transformation. It was found that a phase transformation occurred under electron irradiation at above 320 kV, but never appeared at 300 kV or lower accelerate voltage. Such phase transformation took place in a few seconds of irradiation and was independent of atom diffusion. The mechanism of Electron-irradiation-induced the martensitic transformation is due to displacements of atoms from their lattice sites produced by the entered electrons. The critical displacement energy of the TiNi SMAs is less than 17eV calculated by the results.

SESSION R2: Radiation Effects in Ceramics, Glasses and Polymers I
Chairs: Y. Watanabe and L.M. Wang
Monday Afternoon, December 1, 2003
Room 306 (Hynes)

1:30 PM *R2.1
Radiation Effects In Nuclear Waste Forms: A Review.
R. C. Ewing, Department of Nuclear Engineering & 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 is to predict the response of materials 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 as more recent results from actinide-doping experiments. This presentation will review the state-of-knowledge 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.

2:00 PM *R2.2
Channeling Study Of The Damage Induced In Ion-Irradiated Ceramic Oxides. Lionel Thome 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 forms for radiotoxic element disposal and the development of inert fuel matrices for actinide burning. Among the materials of potential use to that purpose, a particular attention was recently focused on crystalline single-phased ceramic oxides. The evaluation of nuclear waste matrices relies on numerous conditions 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 item, which has been the object of extensive investigations 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 with the channeling technique of the damage induced in ceramic oxide single crystals. 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.

2:30 PM R2.3
Radiation Effects on Hollandite Ceramics Developed for Radioactive Cesium Immobilization. Virginie Aubin[1], Adeline Dannoux[1], Daniel Caurant[1], Didier Gourier[1], Noel Baffier[1], Thierry Advocat[2] and Jean-Marc Costantini[3]; [1]LCAES, CNRS, ENSCP, Paris, France; [2]DEN/DIEC/SCDV Marcoule, CEA, Bagnols-sur-Ceze, France; [3]DEN/DMN/SRMA Saclay, CEA, Gif sur Yvette, France.

Progress on separating the long-lived fission products from the high level radioactive liquid waste (HLW) has led to the development of specific host matrices, notably for the immobilization of cesium. Hollandite (nominally $BaAl_2Ti_6O_{16}$), one of the main phases constituting Synroc - an assemblage of ceramics designed for the conditioning of unseparated HLW - receives renewed interest as specific Cs-host wasteform. The radioactive cesium isotopes consist of short-lived ^{134}Cs and ^{137}Cs of high activities and ^{135}Cs of long lifetime (half-life of 10^6 years). All decay according to $Cs^+ \rightarrow Ba^{2+} + e^-$ (0.51 MeV) + γ (0.6 MeV). Therefore, Cs-host forms must be both heat and (β,γ)-radiation resistant. Nevertheless, the amount of works reported on the stability of single phase hollandite under external $\beta\gamma$ radiation, simulating the decay of Cs, is very limited. This is the purpose of this study. Several materials having the $Ba_xCs_yC_{2x+y}Ti_{8-2x-y}O_{16}$ (C= Al^{3+}, Cr^{3+}, Ga^{3+}, Fe^{3+}, Mg^{2+}, Sc^{3+}) composition type ($1.16 \leq x \leq 1.28$; $0 \leq y \leq 0.28$) synthetized by oxide route were essentially irradiated by 1 and 2.5 MeV electrons with different doses to simulate the β particles of cesium. γ and X-ray 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 $Ba_{1.16}Al_{2.32}Ti_{5.68}O_{16}$ sample generated defects of the same nature (oxygen centers and Ti^{3+} ions) but in different proportions varying with electron energy and dose. The annealings 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. Yanwen Zhang[1], Vaithiyalingam Shutthanandan[1], Ramaswami Devanathan[1], Suntharampillai Thevuthasan[1], William J Weber[1], Jonathan Andreasen[2], Geetha Balakrishnan[3] and Don M Paul[3]; [1]Fundamental Science Directorate, Pacific Northwest National Laboratory, Richland, Washington; [2]Physics Department, Northwestern University, Evanston, Illinois; [3]Department of Physics, University of Warwick, Coventry, United Kingdom.

Damage evolution and thermal recovery of Au^{2+} irradiated samarium titanate pyrochlore ($Sm_2Ti_2O_7$) single crystals were studied by Rutherford backscattering spectroscopy and nuclear reaction analysis using $^{16}O(d,p)^{17}O$ and $^{18}O(p,\alpha)^{15}N$. The damage accumulation follows a nonlinear dependence on dose that is well described by a disorder accumulation model, which indicates a predominant role of defect-stimulated amorphization processes. The critical dose for amorphization at 170 and 300 K is $\sim$0.14 dpa, and a higher dose of $\sim$ 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 $Sm_2Ti_2O_7$ and current 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 an ^{18}O environment reveals a damage recovery stage at $\sim$ 850 K that coincides with a significant increase in ^{18}O exchange due to oxygen 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
Kinetic of Alkali Ion-Exchange of Irradiated Glasses. Michael I. Ojovan, Engineering Materials, University of Sheffield, Sheffield, United Kingdom.

Alkali 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. Ojovan 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 structural barrier model of McGrail et al [J. Non-Cryst. Solids, 296, 10-26 (2001)] to incorporate radiation-induced changes in the kinetic of alkali-exchange. Rates of alkali ion-exchange have been calculated depending on irradiation dose D (Gy) and dose rates P(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 are changes in the activation energies. Sodium ion-exchange energy barriers have been revealed for glasses Na2O- SiO2-Al2O3 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 radiation fields. Radiation-induced changes are most pronounced at relative 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-heat-generating nuclear waste, and high-level waste after its cooling to ambient temperature. Numerical estimations show that changes in alkali ion-exchange kinetic are notable already at D far below damaging doses of waste forms.

3:30 PM *R2.6
Radiation-induced defects in nonradioactive natural minerals: mineralogical and environmental significance. Georges Calas, Thierry Allard, Etienne Balan and Guillaume Morin; Mineralogy, University of Paris, PARIS, France.

Short-lived radionuclides, formed by radioactive decay of natural U and Th, generate a background radioactivity, which will influence the mineral structure. The radiation-induced defects observed in 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 alkali- and alkaline earth halides, natural fluorites do not exhibit native F-centers. Positive holes may be trapped on rare earths (Sm3+). However, most defects consist in an association between the point defect and an impurity located nearby, such as theY-associated F-center. Finally, Ca colloids may be formed under severe irradiation conditions. Other minerals, as 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 significant point defects in kaolinite. The high specific surface area makes clay minerals sensitive to the geochemical radiation background and provides a record of the past occurrence of radionuclides in geosystems. Point defects in kaolinite are hole-centers associated to oxygen atoms linked to Si- and Al-sites. 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 migrations of radioelements in natural analogues may be used in the safety assessment of radioactive waste disposals.

4:00 PM R2.7
Coupling Between Order Parameter and Compositional Fluctuations in the Irradiation Induced Monoclinic Tetragonal to Tetragonal Phase Transition in Pure Zirconia.
David Simeone, [1]Essonne, CEA, Gif sur YVette, France; [2]CEA/DMN/SRMA/LMS, 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 mechanisms 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 1300 K prevents the use of pure monoclinic zirconia stable 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 modelling the effects of radiation damage on the structural instabilities within the unified approach 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 primary order parameter (M point phonon).

4:15 PM R2.8
Structure of Cu Ions in (Cu + Halogen or Chalcogen)-Ion Implanted Silica Glass. Kohei Fukumi, Akiyoshi Chayahara, Hiroyuki Kageyama, Naoyuki Kitamura, Kohei Kadono, Atsushi Kinomura, Yoshiaki Mokuno, Yuji Horino and Junji Nishii; Kansai Center, National Institute of Advanced Industrial Science and Technology, Ikeda, Osaka, Japan.

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 atoms in the ion-implanted glasses was investigated by XAFS. It was found that Cu atoms were coordinated with oxygen atoms in the as-implanted glasses. Heat-treatment at 600 degree C caused the formation of Cu-X 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 atoms form Cu-X 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-X bonds were formed in silica glass prior to the formation of crystalline compounds.

4:30 PM R2.9
Damage Mechanisms of Ion Implanted Bulk (0001) ZnO Single Crystals. Bunmi Adekore[1], Igor Usov[2], Bijay Patnaik[2], Nalin Parikh[2] and Robert F. Davis[1]; [1]Materials Science and Engineering, North Carolina State Univ, Raleigh, North Carolina; [2]Physics and Astronomy, University of North Carolina, Chapel Hill, North Carolina.

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/ω) x-ray diffraction and Rutherford backscattering (RBS). The former revealed the presence of implantation-induced strain through the broadening of the isometric and asymmetric (2θ -ω) reflections. However, RBS indicated that the damage introduced during implantation of these ions was insufficient to transform the crystalline 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 R2.10
Space Environment Effect on Fluorinated Polymers.
Mircea Chipara[1], David L Edwards[2], Bao Hoang[3], Jeffrey Zaleski[4] and Barbara Przewoski[1]; [1]Indiana University Cyclotron Facility, Bloomington, Indiana; [2]Environmental Effects Group, Marshall Space Flight Center, Huntsville, Alabama; [3]Space System Loral, Palo Alto, California; [4]Chemistry 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 most fluorinated polymers is good, the competition between the radiation induced degradation and the oxidative degradation leads to a rapid deterioration of fluorine based polymers. Accordingly, the space applications of such polymers have to be considered with caution, as ionizing radiations trigger the degradation of fluorinated polymers, opening the route for their fast autoaccelerated oxidation. The effects are expected to be stronger Low Earth Orbits where a 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 (polytetrafluorethylene and polyvinyl fluoride) and composites based on fluorinated polymers (graphite-polytetrafluorethylene and Tedlar), and to quantify the time and temperature evolution of these 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 KGy and 100 KGy. Additional mechanical and electrical tests on these samples are analyzed. It was observed that the irradiated spectra present immediately after irradiation an incompletely resolved hyperfine structure due to the delocalization of the uncoupled 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, affecting adversely their mechanical properties and ultimately 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 limitations imposed to the space applications of fluorinated polymers is presented.

SESSION R3: Poster Session: Radiation Effects: Experimental Observation
Chairs: H. Takahashi and L. M. Wang
Monday Evening, December 1, 2003
8:00 PM
Exhibition Hall D (Hynes)

R3.1
Diffraction Contrast Image Analysis on the Defects of the GaAs Crystals Caused by ECR Cleaning Process.
Shang-Cong Cheng[1] and Mike Ouyang[2]; [1]Characterization Science & Services, Corning Inc., Corning, New York; [2]Thin Film and Surface, Corning Inc., Corning, New York.

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, anode voltage and the etching time. By TEM diffraction 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 Nitrogen Ion Beam on Carbon Nitride Thin Films. Shinichiro Aizawa, Yuka Nasu, Nobuaki Kitazawa, Masami Aono and Yoshihisa Watanabe; Materials Science & Engineering, National Defense Academy, Yokosuka, Japan.

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 as-deposited films show a densely distributed columnar structure and the films change to be a sparsely distributed cone-like structure after irradiation. This suggests 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 invasion into films is more prominent after irradiation by low-energy nitrogen ions such as 0.2 keV than 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 Multiwall Carbon Nanotubes Under the Influence of Ion Bombardment. Mariya M. Brzhezinskaya[1], Evgeniy M. Baitinger[1] and Shnitov V. Vladimir[2]; [1]Physics, Cheliabinsk State Pedagogical University, Cheliabinsk, Russian

Federation; [2]Ioffe Physical-Technical Institute Russian Academy of Science, St.Petersburg, Russian Federation.

Recently carbon nanotubes reported to be used in nanolithography [1]. Therefore the problem of influence external factors to CNT properties is very important. The influence of ion irradiation on the spectra of π-plasmon excitations is of great interest since they are very sensitive to the extent of damage produced by ion bombardment. Here we present the results concerning irradiation of the MWNT samples with the flux of 1 keV argon (Ar^+) ions and obtained by using electron energy loss (EEL) spectroscopy. The experiments were carried out at the Ioffe Physical-Technical Institute using high vacuum electron spectrometer with original multichannel energy analyzer [2]. The MWNT powder consisted of nanotubes with $8 \div 16$ nm in diameter and about 10 mm in length. To study how ion bombardment changes the electron structure of MWNT layers, the samples were periodically irradiated with the specified flux Ar^+ ions, and after each irradiation the EEL and CKVV Auger spectra of MWNT sample were measured. We established how the energy of π-plasmon depends on the dose of ion irradiation. The rate of π-plasmon energy decreasing is specified by exponential factor k_E, which, in turn, depends on the Ar+ ions energy. At the 1 keV energy of Ar^+ ions the best fitting value of k_E amounts 0.074 $cm^2/\mu C$. Thus, at the value of Ar^+ ions flux used in our experiment (0,75 $\mu C/cm^2 s$) the total amorphization of the MWNT sample surface required $\sim$300 seconds. Ar^+ ion irradiation of MWNTs inevitably generates in their graphite-like walls a great number of various defects destroying, thereby, the walls uniformity. A broadening of π-plasmon peak as well as a decrease of its energy just evidences increase of short-range disorder in the atomic structure of MWNTs, and, therefore, can serves as indicator of the quality of the carbon nanotubes. This work was supported by Russian Ministry of Education, grant # PD02-1.2-170. 1. A. Okazaki, S. Akita, Y. Nakayama, Physica B 323 (2002) 151. 2. Yu.S. Gordeev, V.M. Mikoushkin, V.V. Shnitov. Molecul. Mater. 11 (1998) 81.

R3.4
Gamma-Ray Detectors Based on A1B5C6 Semiconductors.
Galina Khlyap, [1]General Physics, State Pedagogical University, Drogobych, Ukraine; [2]General Physics, State Pedagogical University, Drogobych, Ukraine.

Composite semiconductors A1B5C6 due to their unique structural and electrophysical properties are seemed to be attractive materials for design of gamma-ray deterectors operating at the room temperature under external electric field. There are no literature data cocerning the problem. The abstract reports first experimental data on electric field-induced effects observed in metal-semiconductor structures based on Ag3AsS3 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-homojunctions; at the same time, three different tunneling modes were observed. The experimenttal 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.
Yasuhiro Chimi[1], Norito Ishikawa[1] and Akihiro Iwase[2]; [1]Department of Materials Science, Japan Atomic Energy Research Institute, Tokai Research Establishment, Tokai-mura, Naka-gun, Ibaraki-ken, Japan; [2]Research 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 $\AA$ thick) are irradiated below $\sim$10 K with several kinds of energetic (100-200-MeV) heavy ions. The resistivity of the specimen is measured $in-situ$ at $\sim$7 K during irradiation. After irradiation, annealing behavior of the resistivity is observed up to $\sim$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 $\sim$6 K, high-density electronic excitation due to energetic heavy-ion 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.

R3.6
Luminescence Properties of Rare-Earth Activated Oxide Phosphors.
Alexadr F. Rakov[1,2], Mukhsin Kh Ashurov[1,2] and Ahatkul A Islamov[1,2]; [1]Research Laboratory, Phonon Scientific Industrial Association, Tashkent, Uzbekistan; [2]Radiation Physics Division, Institute for Nuclaer Physics, Tashkent, Uzbekistan.

The conception of crystal structure as a system of precise order of atoms or ions is an idealistic 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 behaviors. The present work is dedicated to study the influence of intrinsic structure defects on optical and luminescence properties of rare earth (RE) activated garnet (YAG) and orthoaluminate (YAP) crystals. Dosage fast neutron-irradiation was accomplished to regulate the Frenkel defects' concentration. Due to the original design of the gamma-ray source, the radiation field was practically homogeneous so that the whole sample body was excited evenly by high-energy photons. The main results are as follows. Self-trapping of intrinsic electronic excitations is a fundamental event 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 thermalization process, non-complete RE luminescence quenching occurs even at low temperatures. Fast neutron bombardment causes a deep coloration of the samples, and several additional wide absorption bands appear in the whole spectral range of 200-1000nm. Activator GSL intensity decreases with the fast neutron fluence although this decrease is subsequently lager than that which was expected due to emission reabsorbing (passive losses) estimated by taking into account the optical density volume at the corresponding wavelength. Both anion and cation Frenkel defects (displacement defects) are responsible for damaging the mechanism of the energy transfer to activator luminescence centers (active losses). 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.

R3.7
Abstract Withdrawn

R3.8
The Origin of Radiation Resistance of Magnesium Aluminate Spinel.
Vasyl T. Gritsyna[1], Yurij G. Kazarinov[1], Volodymyr A. Kobyakov[1] and Kurt E. Sickafus[2]; [1]Department of Physics and Technology, Kharkiv National University, Kharkiv, Ukraine; [2]Los Alamos National Laboratory, Los Alamos, New Mexico.

Magnesium aluminate spinel attracts the general attention as inert matrices to be used in nuclear reactors and waste forms for radioactive materials because it fulfills different criteria such as high thermal conductivity, a small neutron capture cross section, and high stability under neutron irradiation [1]. The existence of cationic disorder in spinel leads to formation of antisite defects: Al3+ ion in tetrahedral positions and Mg2+ in octahedral sites. In present study we have investigated the origin of high radiation tolerance of this material to displacive irradiation. By using optical methods of measurement it was revealed that kinetics of accumulation of optical absorption centers under different types of irradiation and decay after termination of irradiation, the processes of radio-, photo- and thermoluminescence in spinel are consistent with model, which includes the existence of spatially correlated antisite defects forming dipole complexes "positively charged alumina ions in tetrahedra-negatively charged magnesium ion in octahedra", which serve as centers for annihilation of radiation Frenkel pairs [2]. High concentration of structure vacancies in spinel lattice promote the high mobility of both components of Frenkel pairs to the same dipole centers increasing the probability of annihilation of radiation created defects and preventing the formation of defect clusters, dislocation loops or amorphization spinel crystal. In conclusion there will be discussed the main structural features of other oxides which they should posses as possible radiation resistant ceramic materials. [1]. V. T. Gritsyna, I. V. Afanasyev-Charkin, V. A. Kobyakov and K. E. Sickafus. Neutron irradiation effects in magnesium aluminate spinel doped with transition metals. J. Nucl. Mater. 283/287 (2000) 927-931. [2]. V. T. Gritsyna, Yu. G. Kazarinov, V. A. Kobyakov and K. E. Sickafus. Defects and radiation induced electronic processes in magnesium aluminate spinel on different compositions. Radiat. Eff. and Defects in Solids 157 (2002) 659-663. This research was made possible in part by Award No. UE2-2226 of the U.S. Civilian Research and Development Foundation for the Independent States of the Former Soviet Union (CRDF).

R3.9
The Shallow Traps and Luminescence Properties of Lead Tungstate Crystals.
Alexandr F. Rakov[1,2], Mukhsin Kh. Ashurov[1,2], Eldar M. Gasanov[1,2], Igor R. Rustamov[1,2] and Shukruloh Kh. Ismoilov[1,2]; [1]Research Laboratory, Phonon Scientific Industrial Association, Tashkent, Uzbekistan; [2]Radiation Physics Division, Institute for Nuclear Physics UzAS, Tashkent, Uzbekistan.

In recent years a great attention has been paid to investigations of scintillating and optical properties of Lead Tungstate (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 1300nm were detected after the crystals had been UV-irradiated at 9K in the spectral range shorter than PWO crystals' fundamental 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 up to 50K causes a change in the IR absorption band in shape and replacing of peak position from 1300 to 1150nm. This seems to be due to release the carries from shallowest traps, which are responsible for the longest wavelength band at 1300nm. The experiments on photo-stimulated color centers' transformation have shown this band is negative by nature and might be ascribed to electron-like center (self)- trapped in regular site. The wide luminescent band in the blue-green spectral range can be observed under UV-excitation in the range of zone-zone transitions of PWO crystal. Luminescence temperature dependencies measured at 420 and 520nm 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 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. Jia Ye and Pascal Bellon; Materials Science and Engineering, Univ. of Illinois 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 relocation range and the size of the cascades. We showed that, when the atomic relocation 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 A3B alloy that forms an L12 ordered phase at equilibrium. A dynamical phase diagram is built that yields the stable steady state as 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 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 account for 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. Enrique, P. Bellon, 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. wang[1], Xiaotao Zu[1], s. zhu[2], j.h. wu[1] and l.m. wang[2]; [1]Department of Applied Physics, University of Electronic Science and Technology of China, chengdu, sichuan, China; [2]Department of Nuclear Engineering and Radiological Sciences, University of Michigan, Ann Arbor, Michigan.

Ti-50.6at%Ni, Ti-43at%Ni-7zt%Cu and Cu-21.5wt%Zn-5.85wt%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 produced by electron irradiation migrate to the stressed borders of the Ti3Ni4 precipitates modifying the local atomic configuration, and relaxing 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 matensitic phase and decrease of the elastic energy between the matensitic variants, thus cause the shift of austenite transformation start/finish temperature (As/Af) to higher temperature. The decreasing of ordering degree induced by 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 elastic stress fields around the Ti3Ni4 in TiNi alloy, the interface energy between parent and matensitic phase and the elastic energy between the matensitic variants in TiNiCu alloy and the ordering degree in CuZnAl alloy have significant effects on the transformation characteristics.

R3.13
Effect of Dose Rates on End-of-Range Defects Induced by Sb Implantation. Yi-Sheng Lai[1,2], J. S. Chen[1], Y. S. Ho[2], H. L. Sun[2] and K. B. Huang[2]; [1]Materials Science and Engineering, National Cheng Kung University, Tainan, Taiwan; [2]Diffusion, Taiwan Semiconductor Manufacturing Company, Tainan, Taiwan.

Extended defects formed by antimony 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 technology. Given the dose of 1×10^{14} 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 crystalline Si (c-Si). The EOR defects are located near the lower bound of the transition region. Since high-mass Sb ions used for ultra shallow implantation usually exhibit a low amorphization threshold density. The irradiated region, such as depth of amorphous/transition layers, vacancy/interstitial distribution and interface morphology are affected by dose rates. Therefore, in this work, 70-keV Sb ion irradiation with various dose rates are conducted to induce the amorphization/crystallization structure, which was examined by cross-setional TEM, ultraviolet-visible spectroscopic ellipsometry, and therma-wave. The location, density and size of EOR defects related to the amorphization/crystallization structure will be addressed.

R3.14
Mossbauer Studies of 50 MeVLi^{3+} Ion Irradiated $Mg_{0.9}Mn_{0.1}In_xFe_{2-x}O_4$Ferrites. M. Singh[1], Ravi Sharma Kumar[2] and Anjana Dogra Kumari[3]; [1]Physics, H.P.University, Shimla, India; [2]Material Science, Nuclear Science Centre, New Delhi; [3]Physics, Himachal Pradesh University, Shimla.

A series of samples of $Mg_{0.9}Mn_{0.1}In_xFe_{2-x}O_4$ for X=0.0,0.3,0.5 were prepared by conventional solid state technique. The spinel structure of these ferrites were confirmed by X -Ray Diffraction technique.The samples were irradiated with 50 MeV Li^{3+} ions with fluence 5×10^{13} ions/cm^2.The Mossbauer studies were performed on un-irradiated as well as irradiated samples.Mossbauer study for un-irradiated samples show insignificant variation of isomer shifts at 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^{3+} ions. The Quadrupole splitting of un-irradiated samples are negligibly small, shows the presence of Cubic symmetry at both the sites. On irradiation appreciable changes were observed in Quadrupole splittings. Huperfine field of un-irradiated and irradiated samples decreases with the substitution of In^{3+} ions. However,decrease in hyperfine field after irradiation is slow as compare to un-irradiated samples.

R3.15
Modification of lattice structure and magnetic properties of Fe-Rh alloys by using energetic particle irradiation. Masafumi Fukuzumi[1], Ryoichi Taniguchi[1], Fuminobu Hori[1], Seiji Komatsu[2], Yasuhiro Chimi[3], Tadashi Kambara[4], Fumihisa Ono[2] and Akihiro Iwase[1]; [1]Materials Science and Engineering, Osaka Prefecture University, Sakai, Japan; [2]Okayama University, Okayama, Japan; [3]Japan Atomic Energy Research Institute, Ibaraki, Japan; [4]The 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 temperature. It is well known that the magnetic transitions are very sensitive to composition, heat treatment, magnetic field and external pressure. Resent 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-50at.%Rh alloys with 1 MeV/u - 10 MeV/u heavy ions (Ta, 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 TIH_2PO_4. Se-Hun Kim, Kyu Won Lee and Cheol Eui Lee; Physics, Korea University, Seoul, South Korea.

We have investigated the proton beam irradiation effect on TIH_2PO_4 (TDP) showing an antiferroelectric phase transition and a ferroelastic phase transition. The samples were irradiated by 0.5-1 MeV proton beams and studied by means of ^{1}H 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.

R3.17
UVO and Electrion Beam Radiation Effects on Carbon nanotube/polymer Composite Thin Films. Ebrahim Najafi and Kwanwoo Shin; Materials Science and Engineering, Kwangju Institute of Science and Technology, Gwangju, South Korea.

Carbon nanotubes are one of the preferred fillers for polymer composites due to their exceptional electrical and mechanical properties. In this work, we would like to 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 beams, the surface modification and stripping effects on their CNT/PMMA 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 of the composite materials. The results are then correlated with systemic 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. M102KS010001-02K1901-01810).

R3.18
The evolution of chemical states of MgO surface at the initial stage of aging in ac-PDP. Yeonjin Yi[1], Sangwan Cho[1], Myungkeun Noh[2], Myeon Chang Sung[1], Chung-Nam Whang[1], Kwangho Jeong[1] and Hyun-joon Shin[3]; [1]Institute of physics and applied physics, Yonsei university, SEOUL, South Korea; [2]Yonsei Center for Nanotechnology, Yonsei university, SEOUL, South Korea; [3]Pohang accelerator labolatory 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 spectromicroscopy and corresponding photoemission spectra study. Spectromicroscopy 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, MgCO3, Mg(OH)2, and Mg1+ states. As the panel operation continued, the rapid disappearance of Mg(OH)2 and Mg1+ phase and the sharp increments of MgCO3 phase were observed. Our experimental approach successfully releases 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. Lam[1], C. C. Ling[1], H. M. Weng[2], Deng Sheng Hang[3], C. D. Beling[1] and S. Fung[1]; [1]Physics, The University of Hong Kong, Hong Kong, Hong Kong; [2]Physics, University of Science and Technology of China, Hefei, China; [3]Physics, 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. V_{Si} and divacancy type defects were identified and their annealing behaviors were investigated. Implicationis on the microstructures of the deep level defects E_{1}/E_{2} and Z_{1}/Z_{2} will also be discussed. ACKNOWLEDGEMENT This project is supported by the RGC, HKSAR (project no.: 7085/01P).

R3.20
Lattice location of As in MeV irradiated Si:As investigated by atomistic simulation of Rutherford backscattering-channeling spectra. Alessandra Satta[1,3], Eros Albertazzi[1], Simone Balboni[1,2], Marco Bianconi[1], Luciano Colombo[3] and Giorgio Lulli[1]; [1]IMM, CNR, Sezione di Bologna, Bologna, Italy; [2]CeSIA - Settori Reti e Comunicazioni, Universita' di Bologna, Bologna, Italy; [3]INFM-Dipartimento di Fisica, Universita' 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 atomistic 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.

R3.21
Radiation Induced Nanoparticles in an Iron Phosphate Glass. Kai Sun, Tianhua Ding, LuMin Wang and Rod Ewing; University of Michigan, Ann Arbor, Michigan.

An iron phosphate glass with a composition of 45mol% Fe2O3 and 55mol% P2O5 was irradiated under electron and ion beams. High-resolution electron microscopy (HREM) 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 naoparticles 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., ion irradiation resulted in the formation of bcc-Fe nanoparticles in the glass. On the contrary, after a small dose electron beam (200 keV) 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 nanocrystalline particles 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 Lu[1,2,4], Libin Lin[1,2], Xiaotao Zu[1,2], Sha Zhu[3] and Lumin Wang[3]; [1]Department of Physics, Sichuan University, Chengdu, China; [2]Key Lab for Radiation Physics and Technology of Ministry of Education of China, Sichuan University, Chengdu; [3]Department of Nuclear Engineering and Radiological Sciences, University of Michigan, Ann Arbor, Michigan; [4]International Center for Material Physics, Chinese Academy of Sciences, Shenyang.

Rutile (TiO_2) single crystals with (110) and (100) orientation were irradiated by high-fluence reactor neutrons with the high fluence of $1\times10^{23}m^{-2}$, by protons with the energy of 4.9-18MeV, and with the fluence from 1×10^{15} to 1.9×10^{22} m^{-2}, respectively. UV-VIS-IR, LRS and HRTEM 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 are different for different plane. Both high-fluence neutron irradiation and proton irradiation induce the variations of the frequencies and strength of vibration modes of different orientated samples. Moreover, new vibration modes are shown in irradiated sample. It looks like high-fluence irradiation induce recrystallization phenomenon, which is demonstrated by

HRTEM 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 Poust[1], Benjamin Heying[2] and Mark Goorsky[1]; [1]University of California, Los Angeles, Los Angeles, Illinois; [2]Northrop Grumman, Redondo Beach, California.

The exfoliation of thin GaN layers from 600 nm GaN layers grown on sapphire substrates was achieved using H_2^+ implantation and subsequent annealing. We demonstrate that the extent of exfoliation depends on the crystallinity of the GaN layer. Extended defects are not uniformly distributed over the wafer, so certain areas showed much 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,[1] whereas blistering was reported for lower implant temperatures (20 °C) but only at somewhat higher doses ($\geq 5\times10^{17}$ 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 $Al_{0.25}Ga_{0.75}N$ cap layer. With an implantation energy of 60 keV (to provide a projected range depth of about 200 nm), hydrogen doses as low as 2.5×10^{16} 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 and Nomarski microscopy. We observed blistering for all implant doses. For example, blistering was observed for a much lower implant dose (2.5×10^{16} 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 measured in the GaN layers after implantation for even the low doses. After blistering, the strain was reduced. However, for samples that did not show blistering (e.g. dose of 2.5×10^{16} 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 periphery 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) Tong, Q.Y., et al., J. Electron. Mater. 29 2000 pp.928-932. 2) Kucheyev SO, et al., J. Appl. Physics, 91, 2002, pp.3928-30.

R3.24

The development of low energy neutral beam scattering systems combined with time-of-flight impact collision ion scattering spectrometer. Kenji Umezawa[1], Shigemitsu Nakanishi[1], Walter M Gibson[2] and Shigo Okaura[1]; [1]Dept. of Materials Sciences, Osaka Prefecture University, Sakai, Osaka, Japan; [2]Physics, The University at Albany, SUNY, Albany, New York.

We have been developing the low energy ion beam scattering sysytems combined with time-of-flight ion scattering spectrometer for the analysis of insulator surfaces besides metal, semiconductor surfaces. Insulator surface structural analysis has difficulty in measurements because of charge up using convenient electron or ion beams. Structural analyses of insulator surfaces are very attractive in the fundamental research as well as technological fields. In our scheme, charged ion beams, He+, Ne+ are onverted 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 systems are quite useful for the measurements of defect, surface strcture of ion beam synthesized insulator materials. [1] T. Suzuki, R. Souda, Surf. Sci. 442 (1999) 283.

R3.25

Proton Beam Irradiation Effects on Magnetic Nanocomposites. Mircea Chipara[1], David Hui[2], Jeffrey Zaleski[3], Septimiu Balascuta[1] and Diandra Leslie Pelecky[4]; [1]Indiana University Cyclotron Facility, Bloomington, Indiana; [2]Department of Mechanical Engineering, University of New Orleans, New Orleans, Louisiana; [3]Chemistry Department, Indiana University, Bloomington, Indiana; [4]Physics 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 the analysis of X Ray diffraction lines, the average diameter of magnetic nanoparticles was estimated to be about 20±4 nm. 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 SIS and BaFe-SIS films exhibit a cylinder like nano-morphology. The nanocomposites were irradiated with proton beams accelerated up to 205 MeV, at various fluences up to $2x10^{14}$ protons/cm^2. 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 magnetization at saturation and coercive field was investigated. The temperature dependence of the average magnetocrystalline anisotropy has bee estimated from the dependence of the magnetization on the applied magnetic field, for large external magnetic fields. The transparency of nanocomposite magnetic films as measured by UV-VIS spectrometry 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 no 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 weak). 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 Polyakov[1], Alexandr Rukovishnikov[2], Victor Ralchenko[3] and Igor Vlasov[4]; [1]Microelectronics, Institute of Radio Engineering & Electronics RAS, Moscow, Russian Federation; [2]Microelectronics, Institute of Radio Engineering & Electronics RAS, Moscow, Russian Federation; [3]General Physics Institute, Moscow, Russian Federation; [4]General 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-based Deep Level Transient Spectroscopy (Q-DLTS) was applied to determine the density, activation energy Ea, and capture cross-section of native 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 atabilization of boron atoms 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 01-02-16046 and Grant INTAS-01-2173.

R3.27

MAS NMR Study on the Structural Changes of Zeolite-NaY under Neutron Irradiation. Jian Chen, Lu-Min Wang, Binxi 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 and original zeolite samples. It is found that the 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 solid-state 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. This suggests zeolite with higher Si/Al ratio is more resistant to neutron irradiation damage. It is also found that [AlO6] formed at higher dose level, which means that mild dealumination occurred during neutron irradiation. The contract of the frame work under neutron irradiation by the decrease of both 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-Irradaition Effects upon the Optical Behavior of Transparent $MgAl_2O_4$ Ceramics. Libin Lin[1,2], Jie He[1,2], Tiecheng Lu[1,2] and Peng Wang[1,2]; [1]Department of Physics, Sichuan University, Chengdu, China; [2]Key Lab for Radiation Phys. & Technol of Education Ministry of China, Sichuan niversity, Chengdu.

The transparent ceramics samples of $MgAl_2O_4$ were irradiated by proton beams with energy of 7.5-18MeV and flux from $1\times10^{11}/cm^2$ to $2\times10^{14}/cm^2$. After irradiation, the samples were annealed at different temperatures from 250 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 237nm of F color center and absorption band at 370nm of V color center after irradiation with the flux of $1.53\times10^{14}/cm^2$ and energy of 18MeV. After annealing, V centers and partial of F centers can be eliminated. In order to explain these processes, positron lifetime spectrum is measured. It is shown that while more defects disappeared after annealed, some F centers were accumulated during the annealing.

R3.29

Ion Beam Irradiation Effects on Polymers. Mircea Chipara, Indiana 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 ionisation processes that finally result in scissions reactions. The products of these reactions (ions, radicals and radical- ions associated to macromolecular chains, low molecular mass compounds and fragments, or volatile residues) are able, under certain conditions, to recombine. If these recombination processes involves dominantly fragments of macromolecular chains resulted from the previous scission step, the increase of the molecular mass is observed and assigned to overall chemical processes defined as cross linking reactions. The fine balance between cross linking and scission reactions modifies both the molecular mass distributions and the average molecular mass of the bombarded 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 huge 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 U 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 polyethyleneterephtalate and polycarbonate films the local heating is relatively modest and that a big fraction of the latent track is not heated above the melting temperature, that the free radicals are coupled by extreme exchange interactions in clusters along the incident particle track, that the exchange interactions are anisotropic, and that the anomalies associated with the onset of segmental motions above the glass transition temperatures are affecting the free radical concentration 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 modifications in polymers is presented. 1. M. Chipara, J. Reyes-Romero, Electron spin resonance investigations on polycarbonate irradiated with U ions, Nucl. Instrum. and Meths. B, 185,1-4, 77-82, 2001. 2. O. Puglisi, M. Chipara, W. Enge, G. Compagnini, J. Reyes Romero, U. Bacmeister, M. D. Chipara, Spectroscopic investigations on ion beam irradiated polycarbonate, Nucl. Instrum. and Meths. B, 166-167 (1-4), 944-948, 2000. 3. M. Chipara, ESR investigations on ion beam irradiated polymers, Nucl. Instrum. and Meths. B, 131, 85-90,1997.

R3.30

Influence of ionizing radiation on montmorillonite. Stephanie Sorieul[1], Thierry Allard[1], Bruno Boizot[2], Georges Calas[1], Lumin Wang[3] and Rodney C. Ewing[3]; [1]Mineralogy, University of Paris, PARIS, France; [2]Laboratoire des Solides Irradies, Ecole Polytechnique, Palaiseau, France; [3]Nuclear 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 wastes repositories (HLNWR). In order to predict the long-term performance of the bentonite, various physical and 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 radiations. The present study focuses on radiation damage in montmorillonite considered as a simplified model of bentonite. Two clays have been selected, one from Liaoning (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 radiations effects, irradiations with electron and Helium ions have been performed, using a large dose range consistent with HLNWR, up to 3.5 109 Gy. Radiation effects have been determined by combining X-ray diffraction, Fourier Transform Infrared spectroscopy, Electron Paramagnetic Resonance (EPR) and Mossbauer 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 annealing experiments. The response of Na+-exchanged montmorillonite is different in terms of nature and production of point defects, indicating a role of layer composition and structural precursors. The second effect concerns a modification of the oxidation state of structural Fe, as detected by EPR and Mossbauer 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 has also a consequence in the influence of the water content on the redox effects; each saturated montmorillonite presents a specific response to irradiation with and without thermal treatments. Results will be compared for a- and b-irradiations and with data on of 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 SiO_2: Compositional and Structural Modifications. Giovanni Mattei[1], Valentina Bello[1], Giovanna De Marchi[1], Chiara Maurizio[1], Paolo Mazzoldi[1], Cinzia Sada[1] and Giancarlo Battaglin[2]; [1]Dept. of Physics, University of Padova, Padova, Italy; [2]Dept. of Physical Chemistry, University of Venice, Venice, Italy.

Composite materials made by monoelemental or metal alloy nanoclusters embedded in SiO_2-based matrices exhibit peculiar nonlinear optical properties which are function of the cluster size and composition. Sequential ion implantation in glass has demonstrated to be a very effective technique to obtain such composite materials. In this work we report on the use of ion beam irradiation to induce transformation (either compositional or structural) on metallic nanoclusters in SiO_2. An elemental selective 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_xAg_{1-x} cluster. For a proper comparison, all the irradiations were performed keeping constant the energy density and the power density released to the samples, while varying the nuclear (S_n) vs. electronic (S_e) 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 oxygen with copper promotes Cu_2O formation, therefore extracting Cu from the alloy. Effect of ion irradiation on other systems (like In nanoclusters in SiO_2) 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],

S. Ashok[1], C.L. Liu[2], E. Ntsoenzok[2], M.F. Barthe[2], P. Desgardin[2] and M.O. Ruault[3]; [1]Engineering Science and Mechancs, The Pennsylvania State University, University Park, Pennsylvania; [2]CERI/CNRS, Orleans, France; [3]CSNSM/CNRS-University Paris XI, Orsay, France.

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 lifetime control, and compliant substrates for lattice-mismatched heteroepitaxy. 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, few of them deal with 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 electron cyclotron resonance (ECR) high-density hydrogen plasma treatment. Epitaxial Si (111) samples were first implanted with 1.55 MeV He at a dose of 5 E 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 ($\sim$ 210 nm) around the He projected range ($\sim$5.6 m). 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 cavities decreases. Such effects can be interpreted in terms of the vacancy-type defects introduced by to 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 hydrogenation-induced vacancies in He cavity generation.

R3.33
Density Fluctuations In α-Decay Self-Irradiated Zircon. Susana Rios and Ekhard K. H. Salje; Department of Earth Sciences, University of Cambridge, Cambridge, United Kingdom.

Minerals containing uranium and thorium undergo amorphization over geologic periods of time, providing us with fundamental data to assess the extrapolated behaviour of nuclear waste forms experiencing self-irradiation during long periods of time. α-decay induced amorphization in natural zircon, $ZrSiO_4$, 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-recoil cascades. As found in molecular dynamic simulations (MD), these contain densified regions populated with SiO_n polymers, and a core of depleted matter. While the prediction of polymerization agrees with ^{29}Si-NMR results, no direct experimental evidence exists so far concerning the existence of depleted regions or nano-size voids. Even in the case where such density fluctuations are produced after the release of the recoil nucleus, these might anneal 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. Small-angle x-ray scattering 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 observed. Its intensity increased as the 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 orientated, having a characteristic diameter $\sim$ 6 $\AA$, in good agreement with nano-size voids 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)

R4.1
Molecular dynamics simulation of point defect accumulation in 3C-SiC. Ram Devanathan, Fei Gao and William J Weber; Fundamental Science Directorate, Pacific Northwest National Laboratory, Richland, Washington.

Defect accumulation in 3C-SiC has been simulated by molecular dynamics using a Brenner-type potential connected smoothly to the Ziegler-Biersack-Littmark potential. This combination was chosen as 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. Displacement damage in 3C-SiC, which is known to consist of point defects, vacancy and interstitial clusters and anti-site defects, was modelled by exchanging Si and C atoms at random or by introducing random Frenkel pairs of Si or C. The simulation cell was allowed to relax with the NPT ensemble and defect accumulation was analyzed. The results provide insights into the relative importance of Frenkel pairs and anti-site defects in the radiation-induced amorphization of SiC.

R4.2
Atomistic simulations of defect production in SiO2 by neutron irradiation. Fernando Mota[1], Maria Jose Caturla[2,3], Esteban Dominguez[1], Alison Kubota[3] and Jose Manuel Perlado[1]; [1]Instituto Fusion Nuclear(DENIM), Madrid, Spain; [2]Fisica Aplicada, Universidad de Alicante, Alicante, Spain; [3]Lawrence Livermore National Laboratory, Livermore, California.

Silica is one of the candidate materials for final focusing mirrors in inertial fusion reactors. These materials could be exposed to high energy and intensity neutron fluxes during operation. Radiation damage results in point defects that can lead to obscuration; that is, degradation of the optical properties of these materials. Since currently a neutron source of such high energy does not exist we need to use predictive computational methods to understand the effects of the irradiation. We have applied molecular dynamics simulations to study the effect of high-energy recoils in fused silica. Firstly, the threshold displacement energies of Si and O atoms have been calculated using molecular dynamics with the parallel code MDCASK. This study was done simulating recoil energies in steps of 10 eV starting at 50 eV until we find atoms are displaced to stable positions. We have used two different simulation boxes containing 1536 and 12288 atoms. Both 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 will 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 quantified. In particular, we will focus on oxygen deficient centers generated during irradiation since they will be able to convert 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 Mattoni and Luciano Colombo; INFM and Department of Physics, University of Cagliari, Monserrato (CA), Italy.

Boron-doped pre-amorphized silicon recrystallizes upon solid-phase epitaxy (SPE) so to incorporate boron atoms as substitutional defects, i.e. electrically active p-type dopants. It is however well known that it exists a solubility limit for boron incorporation in substitutional sites. This feature is the key limiting factor for the realization of ultrashallow p+/n junctions with very high active carrier concentration. Recent large-scale molecular dynamics simulations [Mattoni et al., Europhys. Lett., vol.62, p.862 (2002)] have attributed the existence of such solubility limit to the formation of mixed boron/self-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 nanometer-sized BICs dissolution is about 3.2eV. In this work we present a thorough computational investigation on BICs formation and dissolution, as 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 atomic scale mechanisms driving to the formation of BICs during SPE. In particular, we pointed out the transition from boron-rich BICs (as observed just after SPE) to self-interstitial-rich BICs, driving such complexes to more stable configuration. Finally, we investigate several possible reactions ruling the dissolution of BICs by emission of interstitial defects. The theorerical prediction for BICs binding energy is about 3eV, 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 Zhou[1], S L Dudarev[2], M L Jenkins[1], A P Sutton[1,3] and M A Kirk[4]; [1]Materials, University of Oxford, Oxford, Oxfordshire, United Kingdom; [2]UKAEA, Culham Science Centre, Abingdon, Oxfordshire, United Kingdom; [3]Laboratory of Computational Engineering, Helsinki University of Technology, Helsinki, Finland; [4]Materials Science Division, Argonne National Laboratory, Argonne, Illinois.

Nanometer-sized dislocation loops in crystals are usually investigated by using diffraction contrast images produced by conventional transmission 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 the simulation of 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.

R4.5
Percolation of Electron Tunneling between Si Nanocrystals Synthesized in Thin SiO_2 Films by Ion Implantation. Torsten Mueller and Karl-Heinz Heinig; Institute of Ion Beam Physics and Materials Research, Research Center Rossendorf, Dresden, Germany.

The controlled fabrication of a narrow layer of Si nanocrystals (NCs) in thin SiO_2 films for multi-dot non-volatile memories (NC memory) is still a considerable materials issue, which will be addressed in this contribution. The synthesis of NCs by Si^+ implantation of SiO_2 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 charge can spread over neighboring NCs by direct e^- tunneling, i.e. due to electrical in-plane percolation paths. 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^+ implanted SiO_2 is simulated using a kinetic lattice Monte Carlo code [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 narrow layer at high density but are sufficiently electrically isolated. The work was supported by the EU trough the growth project no. G5RD/2000/00320. [1] T. Mueller, K.-H. Heinig, W. Moeller, *Appl.Phys.Lett.* 81 (2002) 3049.

R4.6
Structural Stability of Ion Bombarded Thin Films. Alessio Lamperti and Paolo Maria Ossi; INFM - Dipartimento di Ingegneria Nucleare, Politecnico di Milano, Milano, Italy.

We discuss the segregation-charge 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. This is due to the preferential migration one of film constituents to the interface, which becomes enriched in it. Local charge transfer reactions (CTR), each involving a pair of dissimilar atoms of the initial compound, mimic system relaxation via formation of dimers of an effective compound. The energy cost to produce one such dimer, the difference of formation enthalpy between each effective compound and the corresponding initial compound and the local deformation associated to a CTR are calculated. We analyse a meaningful set of metallic and non-metallic 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 amorphised or retaining a crystalline structure upon ion bombardment, irrespective of their chemical nature.

R4.7
Molecular Dynamics Study of Surface Morphological Evolution By Cluster Impacts. Takaaki Aoki[1,2,3] and Jiro Matsuo[1]; [1]Quamtum Science and Engineering Center, Kyoto University, Kyoto, Japan; [2]Collaborative Research Center for Cluster Ion Beam Process Technology, Kyoto, Japan; [3]Collaborative 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 impacts onto the solid target, 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 Ar_{2000} 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 flat surface. In this presentation, 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.

R4.8
Modeling of Plastic Deformation of Irradiated Metals. Masato Hiratani and Vasily V Bulatov; CMS/MSTD, Lawrence Livermore National Laboratory, Livermore, California.

Development of nanoscale defects in metals induced under high-energy environments significantly affects the mechanical behavior at macroscopic length 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 tetrahedras, perfect loops, <100>{100} type loops, and <111>{111} type loops. Simulation results indicate typical 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-FG03-01ER54629).

SESSION R5: Radiation Effects in Ceramics, Glasses and Polymers II
Chairs: D. Simeone and S. Thevuthasan
Tuesday Morning, December 2, 2003
Room 306 (Hynes)

8:30 AM *R5.1
Experimental and Computational Studies of Ion-Solid Interactions in Silicon Carbide. William J Weber, Fei Gao, Ram Devanathan, Weilin Jiang and Yanwen Zhang; Fundamental Science Directorate, Pacific Northwest National Laboratory, Richland, Washington.

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. Atomic-level simulations are used to determine stable defect configurations, defect production, cascade-overlap effects, and defect migration energies and pathways. These studies show that energetic C and Si collision cascades, with energies up to 50 keV, 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 stimulates cluster growth and produces long-range structural disorder. For energetic Au cascades, nanoscale amorphous clusters are produced directly within about 25% of the Au cascades, along with point defects and smaller clusters. Structural image simulations of the subcascade structures produced by energetic Si and Au recoils are consistent with experimental high-resolution transmission electron microscopy images. The disordering behavior and volume change obtained experimentally and from molecular dynamics simulations are in good agreement, thus providing atomic-level interpretation of experimentally observed features. Multi-axial channeling 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 stable configurations, as well as close-pair 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 from 150 to 870 K, and these stages 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 Yasuda and Chiken Kinoshita; Applied Quantum Physics and Nuclear Engineering, Kyushu University, Fukuoka, Japan.

Atomic disordering of $MgO{\cdot}Al_2O_3$ was examined on specimens irradiated with 1 MeV Ne^+ (4.5×10^{20} ions/m^2), 500 keV He^+ (2.0×10^{21} ions/m^2) at 870 K, and 200 MeV Xe^{14+} ions (5.0×10^{15} ions/m^2) at an ambient temperature. High Angular Resolution Electron Channeling X-ray Spectroscopy (HARECXS) of analytical electron microscopy was utilized for the quantitative analysis of atomic configurations. 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 Al^{3+} ions on octahedral (VI) sites and Mg^{2+} ions on tetrahedral (IV) sites. Displacement 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 ascribed to a higher ionizing rate under He irradiation, since recovery or reordering is more promoted with ionization-enhanced migration of displaced ions. Ion tracks with structural disorder were observed in plan-view of a specimen irradiated with 200 MeV Xe ions. HARECXS X-ray profiles also indicate that the disordering has taken place in some degree even at an extremely small amount of knocked-on displacements (less than 10^{-4} 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[1] and Lev Ginzbursky[2]; [1]PMCL, Motorola, Tempe, Arizona; [2]L.G. Tech-Link, Chandler, Arizona.

Radiation is known to cause point defects formation in different materials. In the case of cubic SiC single crystal radiation flux on the order of 2*10$\hat{2}$0 neutrons/cm$\hat{2}$ at 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 (100-300 microns), wide temperature range (100-1400 C), "no-lead" 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 diffraction measurements, crystal 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, IMM Bologna, CNR, Bologna, Italy.

Silicon Carbide (SiC) is a wide band gap semiconductor regarded with great interest for power electronic applications for space ambient too thank to the good tolerance 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 fluencies. 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 epitaxial SiC Schottky diode. The diode was not biased. The pulse charge amplitude (PHA) per He+ ion was recorded versus the beam spot position over the diode area and versus time. He+ fluencies were studied in the range 1-500 ions/beam-spot, i.e. in the range 10E7-10E10 ion/cm2. A statistics of about 1000 events per fluency value was constructed. The average values of these PHA distributions were almost constant from 1 ion/spot up to 10 ions/spot while they monotonically decreased with increasing fluency 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 regions, was evaluated 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 computed by the algebra described in ref (1). The effect of the ion damage was located at plane in the diode neutral region placed at the depth corresponding to the ion projected range. The charge recombination velocity at this plane was assumed different from that of the surrounding. So doing, the trend of the PHA values versus the He+ ion fluency 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., Nul. Instr. and Meth. Phys. Res. B136-138 (1998) 1340-1344

10:00 AM R5.5
Irradiation-Induced Recovery Of Disorder In Gallium Nitride And Silicon Carbide. Weilin Jiang[1], William J. Weber[1], Yanwen Zhang[1], Lumin Wang[2] and Kai Sun[2]; [1]Fundamental Science Directorate, Pacific Northwest National Laboratory, Richland, Washington; [2]Department of Nuclear Engineering and Radiological Sciences, The University of Michigan, Ann Arbor, Michigan.

Both gallium nitride (GaN) and silicon carbide (SiC) are wide bandgap semiconductor materials that have great potential for a wide range of electronic and optoelectronic applications, and SiC also has significant potential for use in future nuclear power applications. 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. Studies have indicated 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. In the case of GaN, alternative methods of damage recovery that do not involve high-temperature conditions 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 epitaxial 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 the same temperature. 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 temperature for thermal recovery. The dependence of recovery fraction on the preexisting damage level and ion fluence for irradiation will be presented. Results for SiC indicated evidence for irradiation-induced recovery on both the Si and C sublattices near room temperature. Epitaxial recrystallization in SiC under thermal and ion-irradiation conditions will also be compared and discussed.

10:30 AM *R5.6
Radiation Damage Tolerance In Complex Oxides.
Kurt Edward Sickafus[1], Robin W Grimes[2], Mark R Levy[2], James A Valdez[1], Ming Tang[3] and Ping Lu[3]; [1]Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, New Mexico; [2]Department of Materials, Imperial College, London, United Kingdom; [3]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 irradiations 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 fluorite, pyrochlore, bixbyite and perovskite-structured oxide ceramics to test the predictions from computer models. Our computer simulations reveal that atomic disorder energies in 3-3 ABO_3 perovskite compounds are considerably larger than in $A_2B_2O_7$ fluorite-structured compounds, as well as some $A_2B_2O_7$ pyrochlore compounds. Also, disordering in perovskites is considerably less favorable than in the sesquioxide bixbyite-structured compounds. These results may help to explain our observations of poor radiation damage behavior in 3-3 perovskites such as $LaAlO_3$ and $YAlO_3$, compared to most fluorite-structured oxides as well as bixbyite-structured sesquioxides such as Dy_2O_3 and Er_2O_3. This

presentation will examine theoretical predictions of radiation damage behavior and the results of experimental tests using ions.

11:00 AM R5.7
Thermal and Hydrothermal Stability of High Density Polyethylene and Ultra-High Molecular Weight Polyethylene Crosslinked by Gamma Irradiation for Application In Burnable Posion Rod Assemblies In Presurized Water Reactors. Jinho Kim[1], Ronald H Baney[1], James S Tulenko[2] and Kenneth S Allen[2]; [1]Material Science and Engineering, University of Florida, Gainesville, Florida; [2]Nuclear and Radiological Engineering, University of Florida, Gainesville, Florida.

The focus of this study is the development of hydrogen containing polymeric burnable poison material. 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). Boron-10 which has a high neutron absorption cross section has been used for a burnable poison in separate lattice pin or plate form of B_4C/ Al_2O_3 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 5w% 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^{o}C and 3,000 psi), 3) They must have good thermal stability to withstand the operating temperature (above 350^{o}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 autoclave test. High-density polyethylene (above 300Mrads) and ultra-high molecular weight polyethylene (above 100Mards) crosslinked by high gamma irradiation dosage were shown to have acceptable hydrothermal stability under 350^{o}C and 3,000 psi of autoclave condition. All Samples were prepared by exposing to the gamma irradiation in a ^{60}Co source to obtain a range of dosages between 70 and 700 Mrads. The samples both after and before autoclave 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 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 Schuermann, Joern Erichsen, Vladimir Zaporojtchenko and Franz Faupel; 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 subjecting the material to a variety of surface modification techniques, one of which is low-energy ion-beam treatment, which allows 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 fluencies from 5 x 10E12 to 10E16 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 noble metal cluster embedding method [1]) confirmed the cross-linking on the surface. The Tg rose with increasing ion fluencies. The ΔTg increased up to 20 K for the polymer treated with Ar ion fluence of 5 x 10E13 cm-2. At this fluence the cross-linking density increased up to $\sim$ 20%. It is known that metals of low reactivity such as Cu or Au do not wet untreated surfaces, 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 $\sim$ 1 nm and a density of $\sim$ 10E13 cm-2. The ion bombardment created a defined concentration of defects that acted as a new adsorption sites on PS, leading to the enhancement in the condensation coefficient and the cluster density with increasing ion fluence. [1] V. Zaporojtchenko, T. Strunskus, J. Erichsen, F.Faupel, Macromolecules, 34(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, Daejon, 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 consist of long carbon-based molecular chains 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 samples. We found that each of the polymeric powder particles can be completely transformed into diamond crystals under irradiation of a high-fluence electron beam. Single-crystalline diamonds with the sizes ranging from several ten nanometers up to several micrometers were produced from the polymer 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 studing of unusal carbon phases.

11:45 AM R5.10
γ-Ray Irradiation Practical Conditions for Low Molecular Weight Chitosan Material Production. Rangrong Yoksan[1], Mitsuru Akashi[3], Mikiji Miyata[3], Biramontri Siriratana[2] and Suwabun Chirachanchai[1]; [1]The Petroleum and Petrochemical College, Chulalongkorn University, Bangkok, Bangkok, Thailand; [2]Office of Atomic Energy for Peace, Ministry of Science and Technology, Bangkok, Bangkok, Thailand; [3]Graduate 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 intra-molecular 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 [1]. 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/or oligochitosan 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 [2], the practical conditions have never been proposed. The utilization of irradiation should be acceptable only if the structural clarification 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 dose for lowering molecular weight at the level that the chitosan 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 time 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. Gao and K.-H. Heinig
Tuesday Afternoon, December 2, 2003
Room 306 (Hynes)

1:30 PM *R6.1
Topological Identification of Defects and Amorphous Regions In Irradiation-Disordering Crystalline Structures. Linn W. Hobbs[1,2], Clark L. Allred[1,3] and Xianglong Yuan[1]; [1]Department of Materials Science & Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts; [2]Department of Nuclear Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts; [3]Charles Stark Drapper Laboratory, Cambridge, Massachusetts.

Computer simulations of defect formation in irradiation cascades in crystalline structures typically require identifying defects or—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 cluster, 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 (referenced 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 crystalline arrangement) are recognized by comparing their local 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 SiC structures. The evolution of disorder can thus be followed through a complete range of interim and final disordered arrangements. Examples discussed are drawn from collision-cascade MD simulations in Si and SiC structures; however, it is relatively straightforward to extend this method to other simple crystalline structures, disordering 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.

2:00 PM *R6.2
Atomistic 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. We discuss how atomistic simulations 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 polymerization, 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 percolative behaviour of diffusion. We also discuss the mechanisms 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 stimulating new experiments.

2:30 PM R6.3
Abstract Withdrawn

2:45 PM R6.4
Molecular Dynamics Simulation of Displacement Cascades in Zircon. Ram Devanathan[1], L Rene Corrales[1], Constantin Meis[2], Alain Chartier[2] and William J Weber[1]; [1]Fundamental Science Directorate, Pacific Northwest National Laboratory, Richland, Washington; [2]CEA Saclay, Gif-Sur-Yvette, 91191, France.

Displacement cascades in zircon, spanning a range of primary knock-on atom (PKA) energies from 250 eV to 10 keV, have been simulated at 300 K. The interactions were modeled using the Coulombic 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 PKA 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 Hobler; 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 types 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
Atomic-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 of not only 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, in-cascade damage recombination in single cascades, and athermal recombination 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. I will present our simulation results and related experiments which show that irradiation can be used to weld 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.

4:00 PM R6.7
Comparative Study of Defect Properties in GaN: Ab Initio and Empirical-Potential Calculations. Fei Gao, Eric J Bylaska, Anter A El-Azab and William J Weber; MS K8-93, Pacific Northwest National Laboratory, Richland, Washington.

Gallium nitride (GaN), together with other wide bandgap 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<0001> split interstitial. All N interstitials, starting from any possible sites, eventually transfer into the N-N<11-20> split interstitial, forming N2 molecules. This defect is predicted to be the most favorable interstitial in GaN. In the case of Ga interstitials, the most favorable configuration is the Ga octahedral interstitial. However, it is found that the Ga-Ga<11-20> split interstitial can bridge the gap between nonbonded Ga atoms along the <11-20> direction, which leads to the formation of Ga atomic wires in GaN, 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 Samaras[1], Peter M Derlet[1], Helena Van Swygenhoven[1] and Max Victoria[2]; [1]Paul Scherrer Institute, PSI-Villigen, Switzerland; [2]CRPP-Fusion 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 it's polycrystalline counterpart, with the nc rapidly saturating in terms of dose. This contribution discusses the role of the grain boundary during cascade evolution within nc-Ni. Large-scale molecular dynamics of cascade production of the primary damage

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 5keV to 30keV have been investigated. The simulations show that GBs acts as a strong sink for self interstitial atoms/clusters (SIAs) via two possible mechanisms: replacement collision sequences and 1D/3D motion. In these processes, parameters characterizing the GB structure such as misfit areas, excess free volume, GB dislocations and internal stresses are qualifying the sink efficiency for interstitials. The GBs initially play the role of a defector plate, and when the SIA cluster arrives within a few atomic distances from the GB, it starts seeing the detailed atomic structure and chooses an annihilation area in the GB with a dilatative pressure and where there is enough free volume. This results in the observation of large clusters (up to seven SIAs) that move 1D/3D, something that has not been observed in single crystals. Furthermore, the nanosized GBs 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. Xiaokang Shi, Min Yu, Ru Huang, Xing Zhang and Yangyuan 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 notably influence the range profiles and cause dose effect, so they dramatically affect the precision of the simulators. In addition, the damage build-up due to cascade collisions is amply necessary for further annealing simulations. To reduce the statistical noise, Beardmore 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 of cascade collisions becomes very difficult. 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 as-implantation damage's 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 Table1. REACE also makes it possible to simulate middle energy implantation using MD technique and build up the damage distribution simultaneously. All in all, based on MD technique REACE can efficiently not only simulate cascade collisions and damage build-up but also reduce the statistical noise. Besides, due to the simultaneous simulations of both dopant profiles and damage build-up, REACE can also be used to simulate the multi-ion implantation, which has a very critical requirement on damage distribution.

SESSION R7: Ion Beam Processing of Semiconductors and Devices
Chairs: D. Ila and R. Nipoti
Wednesday Morning, December 3, 2003
Room 306 (Hynes)

8:30 AM *R7.1
Application of High Energy Ion Beam on the Control of Boron Diffusion in Silicon. Wei-Kan Chu, Lin Shao and Jiarui Liu; Dept of Physics and Texas Center for Superconductivity & Advanced Materials, University of Houston, Houston, Texas.

The microelectronics community is facing an unprecedented challenge when the device size shrinks, where junction depth reduces down to a few 10-nm scale. To make such a junction based on ion implantation and solid state diffusion becomes extremely challenging. This is due to the fact that 1) fast anomalous diffusion of B in Si makes fabrication of ultra-shallow junctions difficult to accomplish under a reasonable thermal budget, and 2) with a finite B solid solubility in Si, the sheet resistance is too high for the next generation device even if a shallow junction is formed. Recently, we developed a new approach called point defect engineering (PDE). This approach, inspired by a non-equilibrium thermodynamic concept uses high-energy Si ion bombardment into Si to create a vacancy-rich region near the surface. The excessive vacancies retard boron diffusion to below normal rates, improves activation and modify the boron depth profile favorably for use in the next-generation CMOS devices. In this talk, I will present an excellent example on how to use high energy ion beam to control physical properties such as solid state diffusion. I will describe the anomaly and control of Boron diffusion in Silicon.

9:00 AM R7.2
A new way of probing structural differences between relaxed and unrelaxed ion-amorphized silicon: nanoindentation. Jodie E Bradby[1], James S Williams[1], Bianca Haberl[1] and Michael V Swain[2]; [1]Electronic Materials Engineering, The Australian National University, Canberra, Australian Capital Territory, Australia; [2]Mechanical and Mechatronic Engineering, The University of Sydney, Sydney, New South Wales, Australia.

Self ion-implantation was used to generate continuous amorphous Si (a-Si) surface layers up to a micron in thickness. After implantation, the samples were annealed at 450°C (below the crystallization temperature) to induce so-called 'structural relaxation' in the amorphous layers. The annealed (relaxed) and unannealed (unrelaxed) amorphous films were essentially identical when analyzed by Rutherford backscattering spectroscopy, channeling and cross-section transmission electron microscopy (XTEM). The mechanical properties of both the relaxed and unrelaxed a-Si layers were then investigated using spherical indentation. Analysis of the mechanically deformed regions were carried out using XTEM and Raman microspectroscopy. Results from this study show that the deformation behavior of a-Si depends dramatically on the thermal history of the sample. Unrelaxed a-Si was found to deform by plastic flow of the amorphous phase without any evidence for phase transformation. In contrast, relaxed a-Si appears to undergo a series of phase transformations during indentation, similar to that previously observed in crystalline silicon. That is on loading, a transformation to the metallic Si-II structure can be detected, and on unloading, the high-pressure phases Si-III/Si-XII are formed. In light of the dramatically different mechanical behavior of the unrelaxed and relaxed a-Si, various models of structural differences between these states of a-Si, such as the presence of defects, bond angle distortions and the existence of paracrystals in unrelaxed a-Si, are examined.

9:15 AM R7.3
The Role of Ge in Cluster Formation in B, BF2, and BF3 Implanted Si Wafers After Ge Pre-amorphization. Mehmet Alper Sahiner[1], Charles W. Magee[1], Edwin A. Arevalo[2], Daniel F. Downey[2] and Joseph C. Woicik[3]; [1]Evans East, East Windsor, New Jersey; [2]Varian Semiconductor Equipment Associates, Gloucester, Massachusetts; [3]National Institute of Standards and Technology, Gaithersburg, Maryland.

Cluster formation in high dose B, BF2, or BF3 implanted Si wafers is an important problem in silicon doping, since it is one of the leading causes of the electrical deactivation of the dopant. In this study, we used Ge pre-amorphized, ultra low energy B, BF2, and BF3 implanted Si wafers in order to probe these clusters from a local structural point of view. Ge K-edge x-ray absorption spectroscopy (XAFS) is a powerful tool in obtaining local structural information around the Ge atom. The effects of different implant species with various implant doses and annealing conditions on the cluster formation will be presented using Ge K-edge multi-shell XAFS analysis. We will present the concentration profiles obtained from secondary ion mass spectroscopy (SIMS) for B and Ge and correlate the concentration profiles to the structural information obtained from XAFS analysis. Using the calculated XAFS standards for B, F, and Ge doped Si crystals, the contribution of the B and F to the Ge K-edge XAFS, and the results on the local structure of the clusters will be discussed.

9:30 AM R7.4
Hydrogen implant induced lattice damage of semiconductor layers for exfoliation. Sumiko Hayashi[1], David Bruno[1], Rajinder Sandhu[1,2], Michael Wojtowicz[2] and Mark Goorsky[1]; [1]University of California, Los Angeles, Los Angeles, Illinois; [2]Northrop Grumman, 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 second substrate. 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. In this study, we compare the lattice damage introduced to silicon layers and InP layers by hydrogen ion implantation (at a dose of $\approx 5\times10^{16}$ cm^{-2} and energy ranging from 70 to 200 keV). In both cases, the hydrogen is implanted at -20 °C. Wafer bonding is initiated at low temperatures (150 °C) after an

oxygen plasma surface activation step. Next, exfoliation through blistering ($T \geq 250$ °C) leads to the transfer of large area silicon or InP films. The silicon is transferred to SiO_2/Si substrates and the InP layers are transferred to SiN / InP and SiN / GaAs substrates. For comparison, unimplanted companion structures were also wafer bonded. Transmission electron microscopy (TEM), triple axis x-ray reciprocal space mapping (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 exfoliation steps. The surface roughness, as determined using AFM, is approximately the implant straggle depth. The TEM images show no signs of crystalline damage to the transferred layer and the crystalline 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 ($\approx 0.1°$) between the layer and substrate. These results confirm that silicon is an ideal candidate for layer transfer. The InP transferred layer shows different behavior. An unimplanted InP wafer that was wafer bonded 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 straggle. The damage introduction into 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 exfoliation 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 differences in the implant-induced defects that are produced and the differences in the mechanical properties of the two materials.

9:45 AM R7.5
Formation of SiO2/SiC/Si Heterostructure in Si by C+ Implantation and Annealing in Controlled Atmospheres.
Kai Sun, Sha Zhu and LuMin Wang; University of Michigan, Ann Arbor, Michigan.

SiO2/SiC/Si multilayer structure on a Si substrate was synthesized by high-dose C+ implantation and subsequent annealing in controlled atmospheres. The implantation was performed using a metal vapor vacuum arc (MEVVA) ion source to a fluence of 1x10 17 ions/cm2 and an extraction voltage of 50 kV. The annealing was conducted firstly at 1000 K for 2h in 4%H2/Ar then 2h in air atmosphere, respectively. High-resolution electron microscopy (HREM) and electron diffraction studies indicated that the as-implanted material has a three layer structure, a defected surface crystalline layer (200 nm), an amorphirized layer (600 nm) and then the crystalline Si substrate. After annealing in 4%H2/Ar, the amorphirized layer was crystallized consisting of SiC nanoparticles. Further annealing in air oxidized the surface crystalline layer resulting in amorphous SiO2 (probably containing some C). Energy-filtered transmission electron microscopy (EFTEM) was used for characterizing C, Si and O element distribution. Atomic-resolved electron energy-loss spectroscopy (EELS) together with high-angle annular dark-field (HAADF) imaging was used for the study of the interface structures and chemistry of the material.

10:15 AM *R7.6
Defect Evolution and Dopant Motion During Millisecond Annealing of Ion Implanted Silicon.
Kevin Jones, Materials Science and Engineering, University of Florida, Gainesville, Florida.

Recently systems have been developed that enable millisecond to microsecond high temperature annealing of ion implanted silicon. The two most common methods being explored involve either flash lamp systems or scanned lasers. Flash uses a convention bank of RTA lamps to heat the wafer to an intermediate temperature (600-900C) followed by a inert gas lamp flash to raise the temperature to >1100C for a few milliseconds or less. The alternative is to use a scanning laser to heat the wafer from room temperature to near the melting point for a few microseconds. For a number of reasons including reduced random channeling and better activation, there is much interest in using a pre-amorphizing implant prior to dopant implantation for these annealing processes. When pre-amorphization is used for flash annealing there can be dopant motion during the recrystallization of the amorphous layer. Impurities such as fluorine can greatly influence this motion. In addition the majority of the dopant activation occurs during the solid phase epitaxial recrystallization (SPER) of the amorphous layer not during the high temperature flash. Thus understanding dopant activation during SPER becomes critical. Junction leakage from the end of range damage can be significant after SPER. Upon High temperature processing these defects are observed to coarsen. In the case of flash annealing, the evolution of this damage is greatly influenced by the low temperature processing prior to the high temperature step. The effect of ramp rate and intermediate temperature on the defect evolution during flash will be reviewed. For laser annealing there is also a coarsening of the defects despite the extremly short time frame of the anneal. In summary as the high temperature annealing processes become shorter, the effects of the low temperature processing dominate the dopant diffusion, activation and defect evolution.

10:45 AM R7.7
Fabrication of Nanotips and Microbeams in Antimonide Based Semiconductor Material using Bromine Ion Beam Assisted Etching.
Brian Krejca[1], Shivashankar R. Vangala[1], Rathna S. Kolluru[1], Maria C. Ospina[2], Changmo Sung[2] and William D. Goodhue[1]; [1]Photonics Center, University of Massachusetts Lowell, Lowell, Massachusetts; [2]Center for Advanced Materials, University of Massachusetts Lowell, Lowell, Massachusetts.

Antimonide-based compound semiconductors have emerged as the materials of choice for fabricating high-speed low-power electronics and electro optics for applications requiring miniaturization and portability. In this work Br-IBAE is shown to be an anisotropic antimonide etching technique that is capable of generating novel structures as well as performing standard etching tasks. When etching less than optimally chemical-mechanical polished (111) InSb wafers, sharp-tipped cone structures with tip radii of the order of less than 60 nm are produced. These structures may be ideally suited for the development of field-emission devices, where small tip radii are required for useful emission currents. The anisotropic nature of the IBAE technique allows one to etch channels in the surface at angles up to 70 degrees from perpendicular, making the fabrication of microbeams feasible. Using an angled sample holder, the first etch undercuts the masked beams from one side. The sample is then removed and realigned so as to undercut the beams from the other side. The triangular shaped microbeams are left suspended from either one or both ends. Using a combination of atomic force microscopy and mechanical engineering beam analysis techniques, the elastic parameters of the material can be measured. The microbeams can be aligned along various directions on the surface to investigate anisotropic characteristics. This is particularly important for determining the mechanical characteristics of materials that can only be grown in thin epitaxial layers, such as quaternary antimonide-based compound semiconductors.

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

The evolution of surface morphology during ion beam erosion of Si(111) at glancing ion incidence (60° from normal, 500 eV Ar+, 0.75 mA/cm^2 collimated beam current) was studied over a temperature range of 600 − 800 Celsius. 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 sputter 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 730 Celsius), both parallel and perpendicular growth modes contribute to the surface morphological evolution, which leads to the formation of bumps ("dots") 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 Fink[1], Alexnader Petrov[1], Wolfgang Fahrner[2], Kurt Hoppe[3], Alexander Berdinsky[4] and Amita Chandra[5]; [1]SF4, Hahn-Meitner-Institute, Berlin, Germany; [2]University Hagen, Hagen, Germany; [3]Technical Highschool South Westfalia, Hagen, Germany; [4]Novosibirsk State Technical University, Novosibirsk, Russian Federation; [5]Panjab 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 nano-and microelectronic devices. We present as examples miniaturized transformers, condensors, 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 SiON on Si. They stand in between classical FETs, tunnel diodes, varistors, and sensors. Some 30 circuits have been designed and tested successfully with these new elemetns. They are simpler in design than classical electronics, suitable for high frequency applications, and presumably radiation-hard.

11:30 AM R7.10
Microstructure and He bubble effects on Al-Cu thin film interconnects. Cristiano Camacho[1], Paulo F.P. Fichtner[2], Fernando Claudio Zawislak[1] and Gerson Feldmann[3]; [1]Instituto de Fisica, Universidade Federal do Rio Grande do Sul, Porto Alegre, RS, Brazil; [2]Departamento de Metalurgia, Universidade Federal do Rio Grande do Sul, Porto Alegre, RS, Brazil; [3]Departamento de Fisica e Matematica, UNIJUI, IJUI, RS, Brazil.

The effects of film morphology (mosaic- or bamboo-like 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 device interconnects are investigated using Rutherford backscattering spectrometry, elastic recoil detection analysis and transmission electron microscopy. The grain size of the as deposited Al bamboo-like samples and mosaic samples are of 65 and 25 nm. After annealing (773 K, 2h) 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 annealings at temperatures from 473 to 580 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 theta and theta-prime Al-Cu precipitates in the Al matrix. It is also shown that mosaic-like grain structures allow the control of grain size distribution within the 25 to 1500 nm size range, thus providing an additional microstructure engineering tool to improve device reliability against electromigration failures.

11:45 AM R7.11
Dynamic Annealing in Group-III Nitrides under Ion Irradiation. Sergei O. Kucheyev[1], J. S. Williams[2], C. Jagadish[2] and J. Zou[3]; [1]Lawrence Livermore National Laboratory, Livermore, California; [2]RSPhysSE, Australian National University, Canberra, Australian Capital Territory, Australia; [3]Division 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 attractive processing tool. 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 range of intriguing behavior involving extreme property changes under ion bombardment. Here, we present a systematic study of the damage buildup behavior in wurtzite $In_xGa_{1-x}N$ (with $x \leq 0.2$) and $Al_xGa_{1-x}N$ (with $x \leq 0.6$) films monitored by a combination of Rutherford backscattering/channeling (RBS/C) spectrometry and cross-sectional transmission electron microscopy (XTEM). Results show that an increase in In concentration strongly suppresses dynamic annealing 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 annealing 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. Fromknecht 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 Kishimoto[1], Hanna Boldyryeva[2,1], Naoki Umeda[3,1], Oleg A. Plaksin[4,1] and Yoshihiko Takeda[1]; [1]Nanomaterials Laboratory, National Institute for Materials Science, Tsukuba, Ibaraki, Japan; [2]KMF, Charles University, Prague, Czech Republic; [3]Inst.of Materials Science, University of Tsukuba, Tsukuba, Japan; [4]SSC RF, A. I. Leypunsky Inst. of Phys. and Power Eng., Obninsk, Russian Federation.

Nano-sized metal precipitates embedded in dielectrics are candidates for optical nonlinear materials with ultrafast response (∼pico-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 electronic energy, is effective to promote the metal precipitation via radiation-induced diffusion of implanted atoms. Since the precipitation process, more or less, is accompanied by post-collision atomic migration, understanding the kinetic behaviors is prerequisite to use the ion-irradiation method for metal nanoparticle formation. In this paper, we study mechanisms of nanoparticle precipitation in insulators and polymers. Negative Cu ions of 60 keV, which alleviate surface charging for insulating substrates, irradiated SiO_2, $MgO{\cdot}2.4(Al_2O_3)$, $LiNbO_3$, and polymers of PMMA, polycarbonate and polyethylene up to $3{\times}10^{17}$ ions/cm^2. In-situ and ex-situ optical measurements were conducted to evaluate dynamic processes and resultant SPR, respectively. Nonlinear transient response at SPR energy was also measured. Nanoparticle morphology was studied by cross-sectional TEM. An SPR peak around 2 eV appeared, more or less, at doses $\geq$ several at% at the higher dose rate. The ion-beam energy assisted spontaneous metal precipitation and the morphology significantly depended on insulator species and dose rate. The metastable nature of SiO_2 and radiation resistance of $MgO{\cdot}2.4(Al_2O_3)$ gave rise to characteristic morphologies. Nonlinear response of pico-sec was confirmed for the insulators, and especially $LiNbO_3$ showed a sub-picosec 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 also in polymers, electronic energy deposition 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 Binary Metal Systems. X.Y. Li, R.F. Zhang and Baixin Liu; Dept. Mat. Sci. & Eng., Tsinghua University, Beijing, China.

We developed a new scheme namely ion beam manipulation, i.e. interface-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 about 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 Pd and Ru first transformed into a single crystalline fcc phase, and then turned into a well grown ordered structure, which, however, showed an apparent tendency to transform back to the same fcc phase upon over-irradiation [3]. For the Ag-Co case, an ordered layered structure was observed and identified to consist of two overlapping fcc lattices, corresponding to a new magnetic state of Co atom with an average magnetic moment of 2.84 μ_B, which was about twice the equilibrium value and probably the largest one ever observed [2]. The experimental observations as well as a brief discussion concerning the associated mechanism were presented in this paper. References 1. B. X. Liu, W. S. Lai and Q. Zhang, Mater. Sci. and Eng.: Reports 29, 1-48 (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 Au-nanocrystals in TiO2 and SrTiO3 by Ion Implantation in restricted volumes. Rainer Fromknecht[1], Gerhard Linker[1], Kai Sun[2], Sha Zhu[2], Lumin Wang[2], Marijn van Huis[3], A. van Veen[3], Jing Wang[4], Juergen Niemeyer[4], Thomas Weimann[4], Tieshan Wang[5] and Frank Eichhorn[5]; [1]Forschungszentrum Karlsruhe, Institut fuer Festkoerperphysik, Karlsruhe, Germany; [2]University of Michigan, Dept. of Nucl. Eng. and Rad. Science, Michigan, Michigan; [3]University of Delft for Technology, Interfacultare Reactor Institute, Delft, Netherlands; [4]Physikalisch-Technische Bundesanstalt, Quantenelektronik, Braunschweig, Germany; [5]Forschungszentrum Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany.

Au-ions were implanted into TiO2- and SrTiO3-single crystals with doses ranging from 1x1015Au+/cm2 to 6x1016Au+/cm2 at RT and the samples subsequently were thermally annealed at temperatures of 550K to 1550K. The Au-atoms precipitate to nanocrystals already during implantation at RT with an average particle size of 1.5nm.

HRTEM investigations revealed that the Au-nanocrystals, embedded in amorphous TiO2- and SrTiO3 regions, have a broad size and range distribution varying from large sizes in the near surface region to smaller sizes at larger depths. In the annealing process a reorientation of the Au-nanocrystals 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 at 1000K the particle size of the textured 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 holes of 120μm diameter resulted in an almost equidistant arrangement of the Au-nanocrystals with a narrow size distribution of 2-6nm in TiO2 and 3-5nm in SrTiO3 in the near surface region. Au-ion implantation through an e-beam resist mask (50nm x 50nm squares), with doses ranging from 1x1015Au+/cm2 to 4x1015Au+/cm2 at RT and annealed at 1000K, lead to a periodic structure of the Au-nanocrystals with a narrow size distribution was achieved in a crystalline TiO2-matrix.

2:45 PM R8.4
A multi-step process to manipulate the size distribution of nanoparticles formed by ion implantation. Vidya Ramaswamy[1], Tony E. Haynes[2], Warren J. MoberlyChan[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 synthesis technique. Precipitates of uniform size can be obtained, in principle, by an understanding and manipulation of the kinetics of nucleation, growth, and ripening, and of the associated irradiation effects. 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 isolate 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 SiO_2 Layers Sandwiched between c-Si/poly-Si.
Karl-Heinz Heinig[1], Bernd Schmidt[1], Torsten Mueller[1], Lars Roentzsch[1], Karl-Heinz Stegemann[2], Michele Perego[3] and Marco Fanciulli[3]; [1]Inst. Ion Beam Physics & Materials Research, Research Center Rossendorf, Dresden, Germany; [2]ZMD AG, Dresden, Germany; [3]Laboratorio MDM-INFM, Agrate, Italy.

Si nanoclusters (NCs) are fabricated in very thin (~10 nm) buried SiO_2 layers by ion beam mixing and subsequent phase separation. This method might have considerable technological advantages compared to Si NC synthesis in very thin SiO_2 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-dot nonvolatile memories. In this contribution we present both 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^{15} 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 ToF-SIMS and XTEM. 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 performened. Here, results of step (i) are taken 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 Si/SiO_2 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. G5RD/2000/00320. [1] B. Schmidt, D. Grambole, and F. Herrmann, Nucl.Instr.&Methods B191(2002) and K.-H. Heinig et al., E-MRS2003 Meeting, Symp.E [2] T. Mueller, K.-H. Heinig, and W. Moeller, Appl. Phys. Lett. 81 (2002) 3049.

3:30 PM *R8.6
Nanostructural Fluctuations in Radiation-Amorphized Alloys.
Seiichi Watanabe[1], Heishichirou Takahashi[2] and Nghi Q Lam[3]; [1]Materials Science and Engineering, Hokkaido University, Sapporo, 060-8628, Japan; [2]CARET, Hokkaido University, Sapporo, 060-8628, Japan; [3]Materials Science Division, ANL, Argonne, IL60439, 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 in situ observations inside a high-resolution high-voltage electron microscope and image analyses of molecular-dynamics-simulated atom configurations. Nanometer-sized clusters were found to appear and disappear in the irradiated region. The random formation and annihilation of such nanoclusters are believed to be responsible for nanostructural fluctuations which appear to be related to transitions among manifold inherent structural ordering (MISO) states, involving multirelaxation processes. Temporal 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-Lorentzian picture, the resultant power law describes the distribution of multirelaxation times or cluster lifetimes. In addition, a unified relation for the autocorrelation functions for such fluctuation phenomena has been derived. The 'self-organized-criticality' behavior of the irradiated NiTi system will be discussed.

4:00 PM R8.7
Comparison of Kinetic MC Simulations and EFSTEM Observations of Phase Separation in Si^+ Implanted Thin SiO_2 Films. Torsten Mueller[1], Karl-Heinz Heinig[1], Caroline Bonafos[2], Hubert Coffin[2], Gerard Ben Assayag[2], Sylvie Schramm[2], Gerald Zanchi[2], Alain Claverie[2], Marcel Tence[3] and Christian Colliex[3]; [1]Institute of Ion Beam Physics and Materials Research, Research Center Rossendorf, Dresden, Germany; [2]CNRS/CEMS, Toulouse, France; [3]Laboratoire de Physique des Solids, Universite Paris-Sud, Orsay, France.

Studies on the ion beam synthesis of narrow Si nanocrystal (NC) layers in thin SiO_2 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, former work shows that the characterization of the Si NCs embedded in SiO_2 by conventional Transmission Electron Microscopy (TEM) is difficult. It requires careful con-siderations and special imaging conditions [1] due to the weak contrast between Si and SiO_2. In this contribution, Energy Filtered Scanning Transmission Electron Microscopy (EFSTEM) investigations on the morphology of phase separated Si in SiO_2 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 1 keV Si^+ implantation into 10 nm thick SiO_2 and by furnace annealing in N_2 (or N_2 + O_2). Varying fluences from 5 x 10^{15} to 2 x 10^{16} Si^+ cm^{-2} were used in order to adjust the Si excess in the SiO_2. For these conditions, 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, were elongated NCs are found in our computer ex-periment. 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 EFSTEM. 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 trough the growth project no. G5RD/2000/00320. [1] G. Ben Assayag, C. Bonafos, M. Carrada, A. Claverie, P. Normand, and D. Tsoukalas, *Appl.Phys.Lett.*82 (2003) 200. [2] T. Mueller, K.-H. Heinig, and W. Moeller, *Appl.Phys.Lett.*81 (2002) 3049.

4:15 PM R8.8
Heavy Ion Interactions in New Nanoscale Materials.
B W Jacobs[1], S P Song[1], V M Ayres[1], M A Crimp[2], R M Ronningen[3], A F Zeller[3], H C Shaw[4], J B Benavides[4] and J Plante[5]; [1]Electrical and Computer Engineering, Michigan State University, East Lansing, Michigan; [2]Chemical Engineering and Materials 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

radiation environment. The simulated space radiation experiments were performed at the National Superconducting Cyclotron Laboratory at Michigan State University. In these experiments, single wall carbon nanotubes (SW-CNT), multi-wall carbon nanotubes (MW-CNT), and tapered silicon nanowires (T-SiNW) were irradiated by energetic 86-Krypton heavy ions at the National Superconducting Cyclotron Laboratory (NSCL). Two additional sample types, electrospun carbon nanofibers (ES-CNF) and vapor-grown graphitic carbon fibers (VG-CF) were also studied. The choice of samples allowed us to investigate heavy ion interactions with multiple carbon wall structures: graphene single crystal (SW-CNT), nested graphene single crystal (MW-CNT), highly ordered organic networks (ES-CNF), and stacked graphite crystal platelets (VG-CF). Investigation of the silicon nanowires allowed comparisons between the behaviour of carbon versus silicon at the nanoscale. Pre and post-irradiated specimens were investigated for radiation-induced structural and chemical alterations. Scanning Electron Microscopy, Atomic Force Microscopy and Scanning Tunneling Microscopy were used to investigate changes to the external structure, with the choice depending on the size and conductivity of the sample. Transmission Electron Microscopy and High Resolution Transmission Electron Microscopy were used to investigate changes in the internal structure. Selected Area Diffraction was used to detect any departure from crystallinity. Micro Raman spectroscopy/Surface Enhanced Raman Spectroscopy and Fourier Transform InfraRed spectroscopy were used to investigate the molecular bonding present and to monitor the appearance of any defect induced peaks. The results of these experiments indicate swelling of the VG-CF consistent with a knock-on a-plane shrinkage/c-plane swelling mechanism. By contrast, multiple characterizations indicated little change in the SW-CNT. Such results indicate that carbon nanotube components and composites may have good heavy ion radiation resilience that would make them appropriate for deployment in space applications.

4:30 PM R8.9
Effects of Proton Irradiation on Oxidation of Carbon Nanotubes. Ananta Adhikari and Mengbing Huang; Physics, University at Albany-SUNY, Albany, New York.

The electronic properties of carbon nanotubes (CNTs)have been found to be affected strongly by oxygen exposure. This may pose a stability issue for the operation of CNT based devices. In this work, we investigate effects of ion beam irradiation on nanotube oxidation. A layer of single-walled or multiwalled CNTs supported by a Si substrate was first irradiated with protons with energy of 0.5-3.0 MeV to doses between 1e12-1e15 /cm2. Oxidation of CNTs was performed by heat treatment at 200-700 C in air or with an oxygen flow. The contents of carbon and oxygen in CNTs following ion beam irradiation and heat treatments were measured by ion beam analysis. The activation energies for CNT oxidation were extracted for various irradiation condictions, and were compared to the corresponding value for the oxidation of un-irradiated CNTs. This study may shed light on the mechanism for CNT oxidation.

4:45 PM R8.10
Characterization of Nanoclusters in MgO Created by Means of Metal Ion Implantation. Marijn Arnout van Huis[1], A. van Veen[1], H. Schut[1], B. J. Kooi[2] and J. Th.M. De Hosson[2]; [1]Interfaculty Reactor Institute, Delft University of Technology, Delft, Netherlands; [2]Materials Science Center, University of Groningen, Groningen, Netherlands.

Metal and semiconductor nanoclusters can easily be formed in MgO by metal ion implantation and subsequent thermal annealing. An overview is given of the optical and structural properties of Li, Cu, Zn, CdSe, Ag and Au nanoclusters in MgO. All metal nanoclusters show optical absorption in the visible range due to Mie plasmon resonance. Among the structural properties, we discuss the nanocluster size, the size dispersion, the crystal structure, the orientation relationship with the MgO and coherence strains. The techniques that are used for characterisation include optical absorption spectroscopy, Rutherford backscattering and channeling (RBS-C), X-ray diffraction (XRD), cross-sectional transmission electron microscopy (XTEM), and the positron beam analysis (PBA) techniques of Doppler broadening (DB) and two-dimensional angular correlation of annihilation radiation (2D-ACAR).

SESSION R9: Poster Session: Material Processing with Energetic Particle Beams
Chairs: D. Downey and L. Snead
Wednesday Evening, December 3, 2003
8:00 PM
Exhibition Hall D (Hynes)

R9.1
Nitride Formation in Transition Metals During High Dose-High Temperature Implantation. S. Maendl and B. Rauschenbach; Institut fuer Oberflaechenmodifizierung, Leipzig, Germany.

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 and enhancing its properties like hardness, 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 900 C, annealing, diffusion and phase transformations are facilitated. In the present contribution, nitrogen implantation at ion energies between 10 and 30 keV at fluences larger than 1018 cm-2 is investigated in molybdenum, titanium and austenitic steel (as a model for fcc 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 the experiments: nitrogen implantation in austenitic steel leads to lattice expansion and nitrogen in solid solution without phase formation, whereas 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 B1 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 could be observed. Despite a concentration plateau of 50 at.%, only a lattice expansion of the Ti was found with X-ray diffraction.

R9.2
Preparation and Patterning of GaSb Surfaces With Br-IBAE for Antimonide Based Molecular Beam Epitaxy. Shivashankar Vangala[1], B Krejca[1], K Krishnaswami[1], B Zhu[1], K Vaccaro[2], H Dauplaise[2], D Bliss[2] and W. D Goodhue[1]; [1]Photonics Center, Dept. of Physics & Applied Physics, University of Massachusetts, Lowell, Massachusetts; [2]Air Force Research Laboratory/SNHC, Hanscom AFB, Massachusetts.

In this paper, we demonstrate the use of Bromine Ion Beam Assisted Etching (Br-IBAE) 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 as-etched surface with a relatively thin thermally desorbable oxide to overgrow the surface with molecular beam epitaxy. The Br-IBAE 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 Br-IBAE 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 heater stage shows that Br-IBAE produces a mixed gallium and antimony oxide on (100) etched surfaces. The antimony oxides are desorbed between 100-300°C while gallium oxides are completely desorbed at 535°C, leaving a clean single-crystal GaSb surface for epitaxial growth. Upon oxide desorption, GaSb/AlGaSb epilayers were successfully grown on the GaSb surfaces using molecular beam epitaxy. Thus, the Br-IBAE 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.

R9.3
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 on 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 detonation of oxygen gas. A dens amorphous oxide layer of alumina formed on the Al (100) surface with 50,000 AO shots. Plan-view and cross-section samples were characterized under JEM 2010EF-FEG analyses electron microscope (AEM). High-resolution cross-section transmission electron microscopy (HRXTEM) shows the thin oxide film with thickness about 5 nm on the perfect crystal aluminum, revealing the passivation of Aluminum. HRXTEM shows the roughness 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 anode alumina of 700 nm was simultaneously exposed with Al (100) sample. HRXTEM shows the dense amorphous of Al oxide formed at the interface area and the

interface fluctuation at atomic level suggested that AO passed through the anode alumina layer reacting at the interface. The structure of the anode alumina was checked through both XTEM and plan-view, and no special structural change was found after AO passed through.

R9.4
Enhancement in Critical Current Density of MgB_2 Films Irradiated with 200 MeV Silver Ions. Sanjay Shinde[1], S. B. Ogale[1], J. Higgins[1], R. J. Choudhary[1], V. N. Kulkarni[1], T. Venkatesan[1], A. V. Pogrebnyakov[2], S. Y. Xu[2], Qi Li[2], X. X. Xi[2], J. M. Redwing[3] and D. Kanjilal[4]; [1]Center for Superconductivity Research, University of Maryland, College Park, Maryland; [2]Department of Physics and Materials Research Institute, The Pennsylvania State University, University Park, Pennsylvania; [3]Department of Materials Science and Engineering and Materials Research Institute, The Pennsylvania State University, University Park, Pennsylvania; [4]Nuclear Science Center, Aruna Asaf Ali Marg, New Delhi, India.

The effect of 200 MeV Ag ion irradiation, corresponding to an electronic energy loss of 16 keV/nm, on the temperature and field dependence of critical current density (Jc) of high quality MgB_2 thin films is studied. The films used for these studies were grown on 4H-SiC (0001) by a hybrid physical-chemical vapor deposition technique. These epitaxial films had Jc $\sim 10^7$ A/cm^2. After irradiation at a dose of 3 x 10^{11} ions/cm^2, no substantial changes in Jc are observed. However, about an order of magnitude increase in Jc is observed over a certain field range for the film irradiated at a dose of 10^{12} ions/cm^2. No morphological deformations associated with the columnar defects are observed in the atomic force microscopy studies. Our analysis suggests that the electronic energy loss in this case is much smaller than the threshold value for the columnar defect formation in MgB_2. As a result, columnar defects are not formed under irradiation conditions used in these studies. Defects clusters have been suggested to be responsible for the observed improvement in Jc. At lower dose, the defect concentration is small and defects do not offer strong pinning sites to vortices. At higher irradiation dose, increase in defect concentration enhances the vortices pinning. The work is supported under ONR Grant No. ONR-N000149611026.

R9.5
Temperature Dependence of Sputter Ripples on Cu(001) Surfaces. Wai Lun Chan and Eric Chason; Division of Engineering, Brown University, Providence, Rhode Island.

Understanding pattern formation during low energy ion bombardment is a way to study surface transport under highly non-equilibrium conditions. We have recently used ion sputtering to create patterns on Cu(001) surfaces that have characteristics of the Bradley-Harper (B-H) instability. The ripples have a fixed wavelength, increase in amplitude exponentially in the early stages and their alignment is determined by the ion beam direction. Previous studies of B-H ripples have shown an Arrhenius temperature dependence consistent with the activation energy for surface diffusion. We observe similar behavior for Cu at low temperatures, but at high temperature (>190 °C) we find a much stronger temperature dependence for the ripple wavelength. We will compare it with the activation energy obtained from relaxation of ripples and discuss possible diffusional mechanisms that could explain this anomalous temperature dependence. This work was supported by the U.S. Department of Energy under contract DE-FG02-01ER45913.

R9.6
Study on the surface morphology and thermal stability of inclined ion beam treated a-C:H and a-SiOx alignment layer. Kyung Chan Kim[1], Han Jin Ahn[1], Soon Joon Rho[1], Hong koo Baik[1], Jeoung Yeon Hwang[2], Chang Joon Park[2] and Dae Shik Seo[2]; [1]Metallurgical Engineering, YONSEI University, Seoul, South Korea; [2]Electrical Engineering, YONSEI University, Seoul, South Korea.

We have investigated the surface morphology and thermal stability of a-C:H and a-SiOx thin films for liquid crystal display alignment layer. These films are respectively deposited by plasma enhanced chemical vapor deposition (PECVD) and/or RF magnetron sputtering system. These alignment layers are treated with Ar ion beam. The surface morphology and thermal stability of a-C:H and a-SiOx thin films are characterized by scanning electron microscopy, atomic force microscopy, and polarized optical microscopy and compared with that of polyimide film.

R9.7
Thermal stability of liquid crystal alignment layers induced by inorganic carbonated thin films exposed to inclined ion beam. Han Jin Ahn[1], Kyung Chan Kim[1], Soon Joon Rho[1], Hong Koo Baik[1], Jeoung Yeon Hwang[2], Chang Joon Park[2] and Dae Shik Seo[2]; [1]Metallugical system engineering, Yonsei Univ., Seoul, South Korea; [2]Electrical & Electronic Engineering, Yonsei Univ., Seoul, South Korea.

The thermal stability of liquid crystal alignment property between two kinds of inorganic carbonated thin films was investigated. These layers are hydrogenated amorphous carbon and amorphous carbon nitride thin films which are deposited at 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 polyimide and we can observed these results using the polarized optical microscopy (POM). Property of alignment layers are characterized by Raman, FT-IR and AFM.

R9.8
Al-N Bonding Formation on a-Al2O3(0001) by Using Low Energy Ion Beam at Room Temperature. Jong Yong Park[1], won-kook Choi[1], Yu. A. Ermakov[2] and Hyung-Jin Jung[1]; [1]Thin Film Materials Research center, Korea Institute of Science and Technology, seoul, South Korea; [2]Moscow Institute of Radio Engineering, Electronics & Automation, moscow, Russian Federation.

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 (O2, N2, Ar). The maximal ion current density ji = 1.2 mA/cm2 was obtained for O2 at discharge voltage Ud = 340 V, discharge current Id = 1A and flow rate q = 5.5 sccm. For all gases the dependences ji(q) and Ud(q) with constant Id = 1A were obtained. The ion energy distributions for all gases were obtained at different Ud. In average the ion energy was approximately 2/3 of the discharge voltage. a-Al2O3(0001) single crystal surface is irradiated by N2+ at beam potential 300 eV in the ion dosage range 5x10Î5/cm2-1x10Î8/cm2 at room temperature. After ion bombardment, chemical bonding on the modified sapphire surface was investigated by x-ray photoelectron spectroscopy. Below 1x10Î6/cm2, only non-bonded N1s peak at the binding energy 398.7 eV was found, but Al-O-N bonding was found up to 2x10Î7/cm2 which was located around 403 eV. As the ion dosage was increased up to 1x10Î8/cm2, the occurrence of Al-N bonding was identified at the dose higher than 5x10Î7/cm2 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 will be discussed as the temperature is varied.

R9.9
Properties of Ni+ Ion Implanted α- Al2O3 Single Crystals. X. Xiang[1], Xiaotao Zu[1], S. Zhu[2] and L.M. Wang[2]; [1]Department of Applied Physics, University of Electronic Science and Technology of China, Chengdu, Sichuan, China; [2]Department of Nuclear Engineering and Radiological Sciences, University of Michigan, Ann Arbor, Michigan.

Ion implantation as a versatile and powerful technique for forming nanostructures has shown considerable promise in modifying the near-surface mechanical, electrical, optical and magnetic properties. 64 keV Ni ion implantation was performed at room temperature up to a dose of 1 X 10^{17} cm^{-2}. The charge state, damage structure and UV-VIS absorption of implanted α-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^0 (metallic), which may contribute to the samples' 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 new broad absorption band centered at 400 nm appeared in the optical absorption spectra of implanted crystals. In contrast, an absorption band ranged from 240 to 280 nm, corresponding to F^+- and F-color centers, was observed in the absorption spectra of electron beam irradiated samples at the same dose. Therefore, the absorption band centered at 400 nm is believed to be from the Ni nanoparticles.

R9.10
On the Mechanism of Ion Irradiation Enhanced Exchange Bias in Magnetic Films. Stefan Poppe, Jurgen Fassbender and Burkard Hillebrands; Fachbereich Physik, University of Kaiserslautern, Kaiserslautern, Germany.

The effects of 5keV He ion bombardment on NiFe/FeMn exchange bias bilayers 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 limiting the effects of irradiation to specific parts of the layer stack. In addition,

the relevance of the exchange coupling between both 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.

R9.11
Abstract Withdrawn

R9.12
Dose and Isotope Effects in Low-Energy H/D Blistering of Silicon: Narrow Operational Window for Ion-Cutting at < 100 nm. Oussama Moutanabbir, Alexandre Giguere, Bernard Terreault and Guy Ross; INRS-EMT, Varennes, 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 doses of 1x10^{16} to 1x10^{17} cm^{-2}. They were subsequently subjected to rapid thermal annealing under vacuum and thermal desorption spectrometry was performed simultaneously. The resulting surface morphology was studied by atomic force microscopy. We discovered that: (1) there is not only a threshold dose but also a maximum dose for blistering; and (2) there is a giant isotope effect. At 1, 2 and 10 keV respectively, the hydrogen blistering dose "windows" are $(1-2)$, $(1.5-3)$, and $(2-4)$ in units of 10^{16} H cm^{-2}, but for deuterium at 5 keV it is $(4-8)$ X 10^{16} D cm^{-2}. Reflecting the higher 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 efficiency in applications. The absence of blisters at higher dose is associated with a sudden release of part of the gas by percolation through a porous layer. Future work includes infrared and RBS-channeling studies to understand the giant isotope effect, and assessment of the respective merits of H and D in ion-cutting and other applications.

R9.13
Structural and Magnetic Characterization of CoNi Nano-particles in Yttria-Stabilized Zirconia Single Crystals. Sha Zhu[1], Kai Sun[1], Qingyu Zhang[2], Xiaotao Zu[3], Lumin Wang[1] and Rodney C. Ewing[1]; [1]Department of Nuclear Engineering, University of Michigan, Ann Arbor, Michigan; [2]State Key laboratory for Materials Modification by Laser, Ion and Electron Beams, Dalian University of Technology, Dalian, Liaoning, China; [3]Department of Applied Physics, University of Electronic Science and Technology of China, Chendu, Sichuan, China.

Ion implantation has been used to synthesize magnetic CoNi nano-particles at room temperature in the near surface of yttria-stabilized zirconia (YSZ) single crystals for potential application in magneto-optical devices. Transmission electron microscopy (TEM) and superconducting quantum interference device (SQUID) magnetometer, as well as a vibrating sample magnetometer were utilized to characterize the structural and magnetic properties of the implanted layer. TEM analysis showed that the nano-particles 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.

R9.14
Inorganic-Organic Nanocomposite Systems for Microelectronic Applications. Marie-Isabelle Baraton[1] and Lhadi Merhari[2]; [1]SPCTS UMR CNRS 6638, University of Limoges, Limoges, France; [2]CERAMEC R&D, 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 nanocomposite resists for sub-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-nanostructure engineering.

R9.15
Ge Nanocrystal Formed Directly by High-Dose-Ion-Implantation. Tiecheng Lu[1,2,5], Yingqiu Zeng[1,2], Liru Shen[3], Libin Lin[1,2], Ping Zou[4] and Jingguo Yang[1]; [1]Department of Physics, Sichuan University, Chengdu, China; [2]Key Lab for Radiation Physics and Technology of Ministry of Education, Sichuan University, Chengdu; [3]Southwest Academy of Physics, Chengdu, China; [4]Analytic and Testing Center, Sichuan University, Chengdu, China; [5]International Center for Material Physics, Chinese Academy of Sciences, Chengdu, China.

Ge nanocrystals (nc-Ge) embedded in SiO_2 films were prepared directly by high dose Ge ion implantation into SiO_2 films for the first time. In the experiment, the implanting energy of 40keV , the dose from1×10^{16} to $1\times 10^{18} cm^{-2}$ and the substrate temperature lower than 250°C were applied. GIXRD and LRS were used to analysis 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 $1\times 10^{17} cm^{-2}$. With the implanting dose of Ge ions increasing, the ratio and size of nc-Ge in the film will enlarge.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 SiO_2 films receiving part of the kinetic energy of incident Ge ions so that a part of atoms in these clusters move and assemble to nc-Ge when a certain density of amorphous Ge clusters in SiO_2 films are reached .

R9.16
Formation of High Quality β-FeSi2 by Pre-Amorphization-Enhanced Atomic Mixing. Yuji Murakami[1], Atsushi Kenjo[1], Taizoh Sadoh[1], Tsuyoshi Yoshitake[2] and Masanobu Miyao[1]; [1]Department of Electronics, Kyushu University, Fukuoka, Fukuoka, Japan; [2]Department of Applied Science for Electronics and Materials, Kyushu University, Kasuga, 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-patterning technique is required. However, 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 silicidation 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 experiment, Si substrates were irradiated with 20 keV Ar^+ ions (dose: 2x10^{14}-5x10^{15} cm^{-2}) for pre-amorphization. For reference samples, some substrates were subsequently annealed at 800 °C for 2 h to recover damage [1]. Next, Fe films (thickness: 15 nm) 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 (5x10^{15} cm^{-2}). 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 or the increase in the supply 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 enhances the silicidation and improves the crystal quality of β-FeSi2. [1] Y. Murakami, H. Yamauchi, A. Kenjo, T. Sadoh, and M. Miyao, Solid State Phenomena **78 – 79** (2001) 341.

R9.17
Activation Behavior of Impurities Implante In Polycrystalline Silicon Films During Low Temperature Heat Treatment. Nobuyuki Ando[1], Toshiyuki Sameshima[1] and Yasunori Andoh[2]; [1]Tokyo Univ. of Agri. and Tech., Koganei, Tokyo, Japan; [2]Nissin Ion Equipment. Co., Ltd, Kyoto, Kyoto, Japan.

We discuss activation of impurity atoms doped in polycrystalline silicon films using the ion doping method. 50 nm-thick amorphous silicon films formed on glass substrates were first crystallized by 28-ns-pulsed XeCl excimer laser irradiation with a laser energy density of 360 mJ/cm^2. 1.0×10^{14}-cm^{-2}-phosphorus atoms were implanted into laser crystallized silicon films by the ion doping method at an accelerator 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 260°C in the air for 3 h. The electrical conductivity was 1.6×10^{-4} 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 1.7×10^{-2} S/cm after heat treatment at 260°C in the air for 3 h. Oxygen plasma had a effective role of activation of phosphorus atoms and carrier generation in polycrystalline silicon films. The crystalline volume ratio was also

investigated using measurements of the optical reflectivity spectra. The crystalline volume ratio was low of 0.2 for the as implanted state, while the laser crystallized silicon films was a crystalline volume ratio 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 reduced the disordered states and recovered 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.

R9.18
Electron Irradiation Effects on Poly-Si Thin Films Used for Solar Cells. Hua Liao[1,2,3], Libin Lin[1,2], Zuming Liu[3], Qiang Liu[1,2], Ying Xu[4] and Yuwen Zhao[4]; [1]Department of Physics, Sichuan University, Chengdu, China; [2]Key Laboratory for Radiation Physics and Technology of Education Ministry of China, Sichuan University, Chengdu, China; [3]Solar Energy Research Institute, Yunnan Normal University, Kunming, China; [4]Beijing 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 1×10^{14}/cm^2 to 1×10^{16} /cm^2 . 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, this is the main result from the effect of ionization; but after irradiated with high electron fluence, the resistivity of poly-Si thin films sharply increased, this is the result from the effect of displacement. And the mobility degradation shows approximate linear relation with the electron fluence.The results for parameters of poly-Si such as short-circuit current(Jsc), open-circuit voltage(Voc) transfer affeciency η also show the affects of electron fluence. All of these were discussed in detail.

R9.19
Magnetic Properties in Fe-Ni Invar alloys Irradiated with High-Energy Ions. Fumihisa Ono[1], S Komatsu[1], Y Chimi[2], N Ishikawa[2], T Kambara[3] and A Iwase[4]; [1]Department of Physics, Okayama University, Okayama, Japan; [2]Department of Materials Science, Japan Atomic Energy Institute, Tokai, Ibaraki, Japan; [3]Atomic Physics Laboratory, The Institute of Physical and Chemical Research, Wako, Saitama, Japan; [4]Research Institute for Advanced Science and Technology, Osaka Prefecture University, Sakai, Osaka, Japan.

Anomalously 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 and 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 increasing the ion beam energy. The high-density electronic excitation is considered to be responsible for the large modification of the ferromagnetism in Fe-Ni Invar alloys.

R9.20
Enhancement Effect of Photolominescence by Phosphorus Implantation in Si Nanocrystals. Joonkon Kim, H.J. Woo, H.W. Choi, G.D. Kim and W. Hong; Geochemical analysis center, Korea Institute of Geoscience and Mineral Resources, Daejon, South Korea.

Different from bulk silicon crystal, nano-sized Si crystalline embedded in silicon dioxide is known as an efficient photoluminescence (PL) center. In nano-crystilline Si, extonic electron-hole pair is considered to be attributed to radiation recombination. But the defects surrounding crystilline nc-Si suppress radiative recombination efficiency, which work as non-radiative decay paths. Hydrogen is usually utilized in order to en-capsulize the dangling bonds in the Si:SiO_2 interface, that dramatically enhances luminescence yield. Unfortunately because hydrogen has a relatively higher movility 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 1×10^{17} Si/cm^2 and by 440 keV P implantation with dose of (1 to 30) $\times$ 10^{15} P/cm^2. They were annealed at 1100°C for 2 hours in the Ar environment in the temperature range between 500° and 1100°. 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 emmission wavelength. Experimental data such as an enhancement effect of PL yield, decay time characteristics and thermal resistance both for the hydrogenated and phosphorus terminated nano-crystilline Si are shown, and the possible mechnism will be discussed.

R9.21
Thermal Stability of Thin Films of Ion Beam Deposited C_xN_y. David C Ingram[1], Asghar Kayani[1], William C Lanter[2] and Charles A DeJoseph[3]; [1]Physics and Astronomy, Ohio University, Athens, Ohio; [2]Innovative Scientific Solutions, Corp, Beavercreek, Ohio; [3]AFRL/PRPE, Air Force Research Laboratory, Wright-Patterson AFB, Ohio.

A dual ion beam deposition system has been used to deposit thin films of C_xN_y 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, rpg $1x10^{-7}$ 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^o C to determine the stability of the films as compared to those with much higher concentrations of hydrogen. C_xN_y 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^o C. Hydrogen is lost from the films and the optical, electrical and mechanical properties all change. Concomitant with the loss 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^o C. Further work is proceeding on determining any changes to the properties of the films before significant loss of nitrogen occurs.

R9.22
Trapping of Argon in Unbalanced Magnetron Sputter Deposited Films of $C_xN_yH_z$. Asghar Kayani and David C Ingram; Edwards Accelerator Laboratory, Ohio University, Athens, Ohio.

Unbalanced magnetron sputtering deposition of $C_xN_yH_z$ 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 ion 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.

R9.23
Nanocavity formation in metal oxides by ion implantation and thermal annealing. A. (Tom) van Veen[1,2], M.A. van Huis[1], H. Schut[1], B.J. Kooi[2] and J.Th.M. de Hosson[2]; [1]IRI, 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 stopped precipitates of the implanted species, and in the zones that mainly contain primary displacement defects nanocavities are formed. Requirement for the development of cavities and precipitates is a sufficiently high concentration (roughly >1 at %) corresponding to ion fluences > 10^{16}cm^{-2}. Positron beam analysis, THDS (Thermal Helium Desorption Spectrometry), and (X)TEM are useful tools to follow the development of the vacancy clusters. RBS and NDP (Neutron Depth Profiling) are used to monitor the depth profiles of the implanted species. An overview is given of recent studies on cavity formation in MgO, $MgAl_2O_4$, Al_2O_3, and ZrO_2 by light ion implantation (H, He), and in MgO by implantation with metallic ions, e.g. Cu, Zn, Ag, Au or by krypton. In all oxides cavities are formed by helium and hydrogen 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

at elevated temperature the bubbles loose the gas by permeation to the surface. In Al2O3 a different behavior is observed: bubbles grow larger but keep the helium to very high temperature (1600K). Thereafter the bubbles shrink by helium and vacancy dissociation. Metal ion implantation causes a zone of cavities between the surface and the implantation zone. During annealing the cavity zone develops in a different way than the implantation zone. In the latter (semi-)coherent precipitates are formed with no extra vacancies attached. After a further increase of the annealing temperature first the cavities dissolve and the precipitates survive. Nanocavities in the cubic metal oxides often adopt cubic or rectangular shapes. The 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.

R9.24

Anomalous Behavior of Gold Implanted $SrTiO_3$ (001) Single Crystal Surfaces. Vaithiyalingam Shutthanandan, Y. Zhang, J. S. Young, C. M. Wang, K. Barker, L. V. Saraf and S. Thevuthasan; Pacific Northwest National Lab, Richland, Washington.

Formation and nucleation of "ridge" like structures synthesized using MeV Au^{2+} implantation in $SrTiO_3$ 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^{2+}/nm^2 was implanted at 60^o off normal to the surface at 300 K and 973 K in $SrTiO_3$ (100) substrates. Measurements of the samples were conducted directly after implantation and following ex-situ annealing at 1475K in air for 10 hours. RBS measurements from 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 clustering. SEM micrographs obtained from the as 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 the average heights 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.

R9.25

Incorporation of supersaturated Fe centers in n-InP by high temperature ion implantation: effect on the microstructural and electrical properties. Tiziana Cesca[1], Andrea Gasparotto[1], Beatrice Fraboni[2] and Francesco Priolo[3]; [1]Dept. of Physics, INFM-University of Padova, Padova, Italy; [2]Dept. of Physics, INFM-University of Bologna, Bologna, Italy; [3]Dept. of Physics and Astronomy, INFM-University of Catania, Catania, Italy.

Fe is one of the most important transition metal impurities in InP-based materials. Thanks to its deep acceptor character it 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 an only slightly damaged crystal. The aim of this 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 implant-induced defects) to 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 DLTS-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 escape process is controlled by the substrate donor concentration. The possible extension of this study to ternary alloys, like e.g. InGaP and InGaAs, will also be considered.

R9.26

Electron Stimulated Oxygen Desorption Study of Materials for Low Temperature Solid Oxide Fuel Cells (SOFCs). Haiyan Chen[1], Yanfeng Chen[1], Thomas Orlando[1], Jian Dong[2] and Meilin Liu[2]; [1]Scool of Chemistry & Biochemistry, Georgia Institute of Technology, Atlanta, Georgia; [2]School 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 development of electrode 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 electrolytes, 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 O+ desorption with low energy electron (2-100 eV) excitation of SOFC materials under ultra high vacuum and at different temperatures. Imaging of the O+ desorption using a home made ion imaging system with a spatial resolution in the micrometer range is expected to shed light on the oxygen ion generation on grain boundaries where defect sites are abundant.

R9.27

The effect of ion implanatation temperature on the blistering and exfoliation in hydrogen implanted Si. Jung-Kun Lee[1], Ming Cai[2], SS Lau[2] and Michael Nastasi[1]; [1]Materials Science and Technology, Los Alamos National Laboratory, Los Alamos, New Mexico; [2]ECE department, University of California, San Diego, San Diego, California.

We have examined the role of ion implantation temperature on the nature of the blistering and exfoliation phenomenon in H implanted Si, which lead to the transfer of entire Si layer in Ion-Cut process. P-type <100> oriented Si substrates with the conductivity of 1 - 10 ohm-cm were implanted with 40 keV H+ at -140 oC or at room temperature. The implanted Si wafers were then bonded to acceptor Si wafers and annealed to induce exfoliation and layer transfer. The lattice damage and the hydrogen concentration of the as-implanted Si and transferred Si films were analyzed with Rutherford back scattering (RBS) in channeling mode and the elastic recoil detection (ERD), respectively. Compared with the -140 oC 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 implication of these observations on the fundamental physics underlying the blistering and exfoliation phenomena of H implanted Si will be discussed. Also, the electrical characteristics and its correlation with ion-solid interactions will be presented.

R9.28

Welding, Slicing, and Doping, of Carbon Nanotubes with Ion Beams. Raghuveer S Makala[1], P G Ganesan[1], A Cao[1], G Ramanath[1], M Marshall[2], J Mabon[2] and I Petrov[2]; [1]Materials Science & Engineering, Rensselaer Polytechnic Institute, Troy, New York; [2]Center for Microanalysis of Materials, University of Illinois, Urbana- Champaign, Illinois.

Carbon nanotubes have unique properties arising from their molecular dimensions 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 multiwalled carbon nanotubes (MWNTs) at preselected locations. Ga^+ ion beams with spot-sizes ranging from 300 nm to 1 μm were rastered at preselected sites in highly-oriented MWNTs arrays on silica, and MWNTs dispersed on electron-transparent grids. Scanning and transmission electron microscopy (SEM and TEM) characterization indicate that nanotubes dosed with 10^{13}- 10^{15} ions/cm^2 of 10 keV ions show no observable structural changes. Increasing the dose to $\sim 10^{17}$ ions/cm^2 results in the thinning of large diameter MWNTs and slicing of smaller diameter tubes, and the welding of overlapping nanotubes. High-resolution TEM and electron diffraction reveal that the irradiated areas the MWNT shells collapse into the hollow, transforming the nanotubes into amorphous nanorods. This is consistent with micro-Raman spectra from irradiated 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 $10^{15} \sim 10^{17}$ ions/cm^2, indicating that both ion dose and energy are factors that determine structural changes. Spatially resolved energy dispersive X-ray (EDX) spectroscopy shows that the irradiated sections of the MWNTs contain Ga, some of it in the form of Ga nanoparticles as indicated by TEM. Thus, in addition to welding and slicing nanotubes, our results also open up the possibility of using ion beams for creating compositionally modulated nanotube structures, or engineer high defect densities to enable facile site-selective attachment of other nanostructures via further chemical treatments. These features make ion-beam tailoring of nanotubes an attractive strategy for fabricating interconnected architectures of nanotubes.

R9.29

High-speed Machining with Cluster Ion Beams. Toshio Seki[1,2,3] and Jiro Matsuo[1]; [1]Quantum Science and Engineering Center, Kyoto University, Kyoto, Japan; [2]Collaborative Research Center for Nano-scale Machining with Advanced Quantum Beam Technology, Kyoto, Japan; [3]Collaborative Research Center for Cluster Ion Beam Process Technology, Kyoto, Japan.

A cluster is an aggregate of a few to several thousands atoms. When many atoms constituting a cluster ion bombard a local area, high-density energy deposition and multiple-collision processes are realized. Because of the interactions, cluster ion beam processes can produce high rate sputtering with low damage in comparison with monomer ion beam processes. Especially, it is expected that the extreme high rate sputtering can be realized with using reactive cluster ion beams. High current SF_6 cluster ion beams were generated with using recent high current cluster ion beam technique. The cluster size distribution was measured using Time-of-Flight (TOF) method and the mean size of cluster was about 500 molecules. Si substrates were irradiated with SF_6 cluster ions at the acceleration energy of 5-45 keV. Sputtering yield with SF_6 cluster ions was increased with acceleration energy and was about 2300 atoms/ion at 45 keV. The sputtering yield was about 1000 times higher than that of Ar monomer ions and was higher than that of Ar cluster ions. It was found that reactive sputtering occurred with SF_6 cluster ion irradiation. These results indicate that high-speed machining can be done with reactive cluster ion irradiation at high energy. This work is supported by 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. Alenka Razpet[1], Goran Possnert[1], Anders Johansson[1], Mohamed Abid[1] and Anders Hallen[2]; [1]Angstrom Laboratory, Uppsala University, Uppsala, Sweden; [2]Department of Microelectronics & IT, Royal Institute of Technology, Stockholm, Sweden.

Ordered nanoporous alumina [1] has recently been considered as a template for pattern transfer by broad 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 for production of structures with higher aspect ratios, light ions with MeV energies with larger penetration depth should be used. The aim of this contribution is to examine the transmission of alumina templates with sufficient thickness to mask such ions. A careful orientation of the pores in the direction of the incident beam is therefore needed due to the small opening angle for ions passing through the pores. Typical size of pores in the alumina foils was 50 nm, and foil thicknesses were around 2 μm. Foils with metal coating were also examined. Transmission through the foil and the energy of transmitted 2 MeV He+ ions were measured. Energy spectra were recorded for different target orientations with respect to the primary beam as in a traditional channeling experiment. In combination with conventional backscattering from alumina, the transmission energy spectra were used to evaluate the quality of foil templates for pattern transfer. [1] H. Masuda, K. Fukuda, Science 268 (1995), vol.268, 1466 [2] N. Matsuura, T. W. Simpson, I. V. Mitchell, X. Mei, P. Morales, H. E. Ruda, Appl. Phys. Lett. 81 (2002), 4826

R9.31

Preamorphization-Induced Defects in Shallow P+N Junctions Characterized by an AC Magnetic Field.
Moustapha Abdelaoui[1], Halima Mehor[1], Malika Idrissi-Benzohra[1], Mohamed Benzohra[1] and Francois Olivie[2]; [1]LEMI, University of Rouen, Mont Saint Aignan, France; [2]LAAS, CNRS, Toulouse, France.

Germanium implantation into silicon substrate is currently used to pre-amorphisize the crystalline structure in order to avoid boron channeling effects in shallow P+N junction manufacturing. Nevertheless, after boron doping and rapid thermal annealing, different defects are formed within the structure such as end of range defects which are created at the amorphous/crystalline interface. Our study concerns two types of shallow P+N junctions. These junctions were fabricated using low energy boron implantation at 3 KeV with a dose of 2e15 cm-2 into high-energy germanium preamorphized n-type crystalline silicon substrates at 2.2 MeV with a dose of 1e15 cm-2. In the first type, the preamorphization was performed at ambient temperature. In the second, the preamorphization was performed at nitrogen temperature. Boron doping was followed by a Rapid Thermal Annealing (RTA) step for 15 s at 950 C. TEM and DLTS techniques were used to characterize the defects formed in each structure. The impact of an ac magnetic field on the reverse current has been studied at a given bias, when sweeping the sample temperature. The measurements were performed under low frequency (less than 1 kHz) magnetic field of a Vrms value of 2000 G, with sample temperature varying between 100 and 300 K. The results show a high activity of defects at low frequencies (1 and 10 Hz) for the nitrogen preamorphized sample. Moreover, this activity is observed at about 200 K which corresponds to the peak of the DLTS spectra of such sample. However, the ambient preamorphized sample characterized by a lower concentration of defects seems to be insensitive to the ac magnetic field. Therefore, it appears that the preamorphization-induced defects influence strongly the response of the junction to an applied ac magnetic field.

R9.32

Correlation and Spectral-Density Roughness Analysis of Surfaces Processed With Gas-Cluster Ion Beams.
David B Fenner, Epion Corp, Billerica, Massachusetts.

Autocorrelation, height-difference correlation, and power spectral density are used to characterize various surfaces exposed to gas-cluster ion beam (GCIB), as well as for detailed comparison with statistical mechanism simulations by stochastic impact and surface diffusion models. Surfaces that are initially extremely smooth are roughened slightly by exposure to higher-energy GCIB, while slightly rough surfaces are smoothed to low residual levels by less aggressive GCIB processing. Examples of various microelectronic materials surfaces are shown for these two situations. Surface roughness over several decades in lag length and spatial frequency are always found to be essentially fractal in nature. Previous efforts to model GCIB effects on surfaces have had only limited success. The present work demonstrates a very close correspondance between detailed statistical analysis of AFM images from actual surfaces and the result of the same types of analysis of simulated surfaces. Phenomenological models with both continuum surface diffusion and Monte Carlo impact accumulations are presented. Accurate simulation of smoothing requires a combination of these models. The shape of the modeled individual cluster-impact craters is the primary determinant of the resulting surface fractals and the autocorrelation, height-difference correlation and power spectral density functions. Hurst parameters and correlation lengths are extracted from this analysis. Support by the NSF (DMI-0078580) is acknowledged.

R9.33

Local Modification of Microstructure and Properties by FIB-CVD. Heinz D Wanzenboeck[1], Stefan Harasek[1], Emmerich Bertagnolli[1], Peter Pongratz[2] and Herbert Hutter[3]; [1]Institute for Solid State Electronics, Vienna University of Technology, Vienna, Austria; [2]Institute for Solid State Physics, Vienna University of Technology, Vienna, Austria; [3]Institute for Chemical Technologies and Analytics, Vienna University of Technology, Vienna, Austria.

Ion-beam-assisted deposition utilizing a focused ion beam (FIB) is an well-appreciated method for nanostructuring of semiconductors. Focused ion beam (FIB) technology is widely applied as versatile tool for prototyping and re-engineering of microelectronics in the sub-μm regime. This ion-beam processing technology uses a focused beam that facilitates a locally confined interaction with the sample. The focused beams with a diameter down to 5 nm are successfully employed for local sputtering and for local deposition of metals as well as dielectrics. The deposition is based on a local chemical vapor deposition (CVD) that is induced by the energy of the ion beam. With an acceleration voltage between 10 and 30 keV the ion implantation as well as energetic aspects influence the substrate

material as well as the deposited material. All FIB processes are typically associated with ion implantation and microstructural changes due to atomic intermixing by the ions. This work uses advanced characterization techniques to quantify these effects the focused ion beam has on the substrate. The depth of the amorphisation 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 imaged. The chemical composition of the interface was obtained by a depth profile with secondary ion mass spectroscopy (SIMS). The observed results correlate with solicited Monte Carlo simulations of the dopand profiles. The morphological effects of locally confined implantation have been determined by atomic force microscopy (AFM) of the irradiated surface. The modification of material properties and electric characteristics 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 effect significant microstructural and property changes occurring in solids during energetic ion irradiation. This work offers a comprehensive outline of most recent experimental observations of ion radiation effects in different semiconductor materials.

R9.34

Nanoscale Surface Pattern Formation Via Sputter Erosion of Dielectric Surfaces. Sterling D. Fillmore[3], Randall L. Headrick[2] and Christopher C. Umbach[1]; [1]Materials Science and Eng., Cornell University, Ithaca, New York; [2]University of Vermont, Burlington, Vermont; [3]Brigham Young University, Provo, Utah.

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 depends primarily on 1) the reduction of the surface viscosity 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 sapphire and for a LCD display glass (alkaline earth boroaluminosilicate). For ion energies between 500 eV and 1 keV, the wavelengths range from 25 to 50 nm for sapphire and from 50 to 80 nm for the glass. The wavelength varies with ion energy as a power law with a composition dependent exponent between 0.5 and 1. 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 Implantation in Cu3Au(100). Akbarali Rasulov[1] and Abdurauf Dzhurakhalov[2]; [1]Information Technology Dept., Fergana Polytechnical Institute, Fergana, Fergana region, Uzbekistan; [2]Theoretical Dept., Arifov Institute of Electronics, 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 channelling and implantation processes at low energy (<10keV) ion bombardment of Cu3Au(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 Cu3Au(100) the range of projectiles decreases, the relative contribution of elastic energy losses increase due to presence of Au atoms which lead to increasing the amplitude of trajectory oscillations of channeled particles. The angular and energy distributions of ions passing through thin (<5000A) single crystals have been calculated and studied in detail. The angular distributions of such ions in the case of composite crystals have been investigated in dependence on geometry and structure of the channel. In the case of Cu3Au(100) the half-width and range of angular distributions are wider and the number of dechannelled particles are significantly more than ones obtained for case of pure Cu(100) crystal. In the case of Cu3Au(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 differ for the cases of Cu(100) and Cu3Au(100), but the maximum of depth profiles is shifted to more deep layers in the case of Cu(100).

R9.36

Fast Neutral Ar Penetration duing Gas Cluster Ion Beam Irradiation to Magnetic Thin Films. Shigeru Kakuta[1,2], Toshio Seki[2,3], Shinji Sasaki[1,2], Kenji Furusawa[1,2], Takaaki Aoki[2,3] and Jiro Matsuo[3]; [1]Storage Technology Research Center, Hitachi, Ltd., Yokohama, Japan; [2]Collaborative Research Center of Nano-scale 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 neutrals have to be suppressed. Suppression of fast neutrals is important, since monomer ions can be easily suppressed with permanent magnet. In this paper, 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 acceleration voltage ranging from 3 to 20 kV were irradiated to 50 nm thick NiFe films deposited on Si wafers by Ar sputtering. Depth profiles of penetrated Ar were obtained through SIMS measurement with Cs ion 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 vertically 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 generated 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 obtained by SIMS.

R9.37

Heavy ion bombardment of electroformed Ni-Co alloys for stress release / mechanical properties enhancement. Iulia C. Muntele, Sergey Sarkisov, Claudiu I. Muntele and Daryush Ila; Physics, Alabama A&M 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 content 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 alloy produce a local annealing, reducing the stress and the amount of hydrogen and sulphur/sulphurous 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 Yamada[1], Shirabe Akita[1], Shingo Houzumi[2], Noriaki Toyoda[2] and Isao Yamada[2]; [1]Electrical Physics, Central Researech Institute of Electric Power Industry, Tokyo, Japan; [2]Laboratory of Advanced Science & Technolory for Industry, Himeji Institute of Technology, Hyogo, 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, 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. These features are useful for dry-etching of compound semiconductors. In this study, etching of GaAs and GaP with GCIB were studied as a function of ion dose and acceleration energy, and their sputtering yields. Cluster beams were formed by supersonic expansion of high pressure gas (1x10$\hat{6}$ 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 increased monotonically with increasing the ion dose from 1x10$\hat{1}$6 to 1x10$\hat{1}$7 ion/cm$\hat{2}$ at acceleration energy of 20 kV. The GaP

sputtering depth was higher than the GaAs sputtering depth in this range of ion dose. Also the sputtering depths of GaAs and GaP increased monotonically with the acceleration energy. Sputtering yields of GaAs and GaP were 40.9-173.7 and 75.3-178.3 atoms/ion for 10-25 kV, respectively. These sputtering yields were almost 10 to 30 times higher than those sputtered by Ar monomer ions. As Ar GCIB shows high sputtering yields with low-energy per atom (2.5 eV at an acceleration energy of 10 kV), the GCIB process is promising for fabrication of nano-structure on compound semiconductors.

R9.39
Position Controlled GaN Nano-Structures Fabricated by Low Energy Focused Ion Beam System. Takahiro Nagata[1], Parhat Ahmet[2], Takeyoshi Onuma[3], Takashi Koida[4], Shigefusa F Chichibu[3,4] and Toyohiro Chikyow[2,1]; [1]CREST, Japan Science and Technology Corporation (JST), Toyonaka, Osaka, Japan; [2]National Institute for Materials Science, Tukuba, Ibaraki, Japan; [3]Institute of Applied Physics and Graduate School of Pure and Applied Sciences, University of Tsukuba, Tukuba, Ibaraki, Japan; [4]NICP, ERATO, Japan Science and Technology Corporation (JST), Fujimi, Chiyoda, Japan.

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 the future optical devices and nano structured GaN has also a great potential to realize an innovative optical devices. However, ordered nano structures 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 systems have the ability to mill a few mono layers of a surface selectively by ion sputtering (nucleation site control) and can deposit materials via a ion-induced deposition (selective growth). The combination of these procedures can be used to fabricate the position controlled GaN three-dimensional nano-structures. 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 the substrate at 550 °C. The deposited Ga atoms migrated on the surface and were trapped at the nucleation sites to form Ga droplets. By the SEM observation, the Ga droplets of diameter 1 μm were found to be allocated every 2 μm periodically on the substrates. Ga organometallic precursors were also tried as Ga source for the ion beam assisted GaN deposition and similar result was obtained. To grow the GaN micro crystals from the droplets, NH_3 gas or excited atomic nitrogen sauces was supplied to the surface. The structure analysis for the GaN micro crystals and their optical properties are discussed in detail in the presentation.

R9.40
Abstract Withdrawn

R9.41
Radiation Damage Characterization in Ar^+ Implanted GaN. Igor Usov[1], Alex Kvit[2], Zachary Reitmeier[2] and Robert Davis[2]; [1]MST-STC, Los Alamos National Laboratory, Los Alamos, New Mexico; [2]Department of Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina.

Damage microstructure evolution in GaN films implanted with 150 keV Ar ions to a dose of 3e15 cm^{-2} as a function of implantation temperature was studied by cross-sectional TEM. After irradiation at room temperature, the implanted layer comprised mostly isolated point defects. Implantation at elevated temperatures significantly reduced the number of isolated point defects. Numerous partial dislocations and regions exhibiting strain-contrast were observed after implantation at 300 °C. Bombardment at 600 °C resulted in formation of a new type of defect. Along with the partial dislocations and the strained regions, precipitates composed of carbon and nitrogen were identified by EELS. These precipitates were formed in the vicinity of the Ar ions projected range where the amount of radiation damage was maximal. Therefore we believe that the high concentration of defects facilitated redistribution of carbon atoms introduced during the GaN film growth and resulted in the formation of precipitates. No precipitates were observed after implantation at 1000 °C. Consideration of the TEM results in conjunction with ion channeling data showed that presence of the precipitates correlated with "reverse annealing" damage accumulation mode which manifests itself as an increase of backscattering yield with the increase of implantation temperature. The results of our study indicated that carbon impurity in as-grown GaN films enhances the radiation damage accumulation rate and consequently it has to be taken into account when ion implantation doping of GaN is carried out.

SESSION R10: Advanced Processing and Characterization Techniques
Chairs: M. Terasawa and A. Vantomme
Thursday Morning, December 4, 2003
Room 306 (Hynes)

8:30 AM *R10.1
Xe Precipitates in Aluminum. Robert C. Birtcher[1], S E Donnelly[2], C W Allen[1], K Furuya[3], M Song[3], K Mitsuishi[3] and U Dahmen[4]; [1]Materials Science Department, Argonne National Laboratory, Argonne, Illinois; [2]Joule Physics Laboratory, University of Salford, Greater Manchester, M5 4WT, United Kingdom; [3]National Institute for Materials Science, Tsukuba, 313 Sakura, Japan; [4]National Center for Electron Microscopy, LBNL, Berkeley, California.

Real space, high-resolution transmission electron microscopy observations of Xe confined in nanometer size faceted cavities in Al yield information on both the inert gas and the cavity in which it is confined. Xe in such cavities can be liquid or an fcc solid. 1 MeV electron irradiation produces defects in the Al that cause atomic-level fluctuations of cavity facets. Crystalline Xe conforms by faulting to varying cavity shape. Xe within individual precipitates can undergo melting and recrystallization. At room temperature, fluid Xe (critical temperature 16C) confined in small faceted cavities in aluminum has up to three ordered layers of Xe atoms at the Al interface. Conceptually in a three-dimensionally confined system of sufficiently small size, three-dimensional ordering of the fluid may occur. Molecular dynamics simulations have revealed that fluid Xe confined to a small tetragonal volume would solidify in a body-centered cubic phase on compression. The Al/Xe interfacial tensions can be deduced from the largest Xe nanocrystal at 300 K by setting the corresponding calculated Laplace pressure equal to the equilibrium pressure for melting of Xe, obtained from empirical bulk compression data. These interfacial tension values are 1.05 J m-2 for {111} facets and 1.10 J m-2 for {200} facets. Because of the weak interactions, these values correspond to the surface tensions for Al at 300 K. Cavity shape changes lead to random precipitate motion and coalescence. There is no apparent elastic interaction between precipitates separated by as little as 0.5 nm. However, coalescence of close precipitates is enhanced by directed motion as a result of the differential displacement of Al atoms out of the volume between them. After coalescence, crystalline Xe conforms by plastic deformation without melting to changes in cavity shape. Cavity volume, not surface area, is conserved during coalescence, implying that cavity pressure is not determined solely by the interface tension.

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 crystallization in different glasses. However, the fundamental 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 cations, as 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 DMR0245702.

9:15 AM R10.3
Diffuse Electron Scattering by Individual Nanometer-sized Defects: Quantitative Measurements and Simulations. Marquis Kirk[1], Ray D Twesten[2], Zhongfu Zhou[3], Sergei L Dudarev[4], Adrian P Sutton[3,5] and Michael L Jenkins[3]; [1]Materials Science Division, Argonne National Laboratory, Argonne, Illinois; [2]Center for Microanalysis of Materials, University of Illinois, Urbana, Illinois; [3]Department of Materials, University of Oxford, Oxford, United

Kingdom; [4]UKAEA, Culham Science Centre, Abingdon, United Kingdom; [5]Laboratory of Computational Engineering, Helsinki University of Technology, Helsinki, Finland.

The atomic structure and interstitial or vacancy nature of individual nanometer-sized defects are determined by quantitative measurements and computer simulations of diffuse elastic electron scattering. 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 methods within the electron microscope, and is separated from Bragg scattering at weakly excited diffraction peaks. Computer simulations of kinematical elastic electron scattering from defect structures, modeled by both analytic 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. The sensitivity of this method to the diffraction 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 Science, under contracts W-31-109-ENG-38 (ANL) and DEFG02-91-ER45439 (UIUC).

9:30 AM R10.4
High-Resolution Spectrochemical Analysis of Columnar Defects formed in Bi2Sr2CaCu2Ox by Swift Heavy Ion Irradiation. Michitaka Terasawa[1], Fumihisa Kano[2], Tohru Mitamura[1], Tadashi Kambara[3], Yukichi Sasaki[4] and Yuichi Ikuhara[5]; [1]Laboratory of Advanced Science and Technology for Industry, Himeji Institute of Technology, Hyogo, Japan; [2]Power & Industrial Systems Research & Development Center, Toshiba Co., Yokohama, Kanagawa, Japan; [3]Atomic Physics, The Institute of Physical and Chemical Research Center, Wako, Saitama, Japan; [4]Micro-Structure Analysis Division, Japan Fine Ceramics Center, Nagoya, Japan; [5]Engineering Research Institute, The University of TikyoTokyo, Tokyo, Japan.

Single crystal of high temperature superconductor Bi2Sr2CaCu2Ox was irradiated with 3.5GeV Xe ions at room temperature up to 1.0X10E11ions/cm2. Significant enhancement of magnetization by the irradiation was confirmed. The irradiated specimens were studied by using a high resolution tansmission electron microscope with field emission gun (FE-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 spectrochemical analysis across the columnar defects revealed enrichment of Cu and depletion of Bi, 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 Helium Implantation. Vinay Venugopal, Leon J Seijbel and Barend J Thijsse; Laboratory of Materials Science, Delft University of Technology, Delft, Zuid Holland, Netherlands.

Thermal helium desorption spectrometry (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 metastable film/substrate systems. In this work we present results for thin Cu films (0.5-20 nm) deposited in UHV on Mo and Ta substrates by electron beam evaporation. These systems were selected to serve as model systems for investigating fcc films on bcc substrates and to increase 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 and at the Cu/metal interface. Subsequently, on heating the sample, helium release is seen not only by de-trapping from the defects but also as a result of two 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 and is strongly dependent on film thickness, is investigated. The differences between the Mo and Ta substrates and the influence of film thickness are discussed.

10:00 AM R10.6
Recovery Effect of Electron Induced Damage in 4H-SiC Schottky Diodes. Anna Daniela Cavallini[1], Antonio Castaldini[1], Lorenzo Rigutti[1], Filippo Nava[2], Pier Giorgio Fuochi[3] and Paolo Vanni[2]; [1]INFM and Dipartimento di Fisica, Universita' of Bologna, Bologna, Italy; [2]INFN and Dipartimento di Fisica, Universita' di Modena e Reggio Emilia, Modena, Italy; [3]Istituto ISOF, CNR, Bologna, Italy.

Deep level transient spectroscopy (DLTS) and capacitance-voltage (C-V) characteristics were used to investigate the effects of electron irradiation on the defect associated electronic levels in Schottky diodes on 4H silicon carbide epilayers grown by chemical vapour deposition. DLTS 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 - 0.63 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 DLTS temperature runs 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-0.70eV) 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. DLTS 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. Kannan Krishnaswami[1], S Vangala[1], L. P Allen[2], C Santeufemio[2], D Bliss[3], H Dauplaise[3], M Ospina[4], X Liu[4], J Whitten[4], C Sung[4] and W. D Goodhue[1]; [1]Photonics Center, Dept. of Phyiscs and Applied Physics, University of Massachusetts, Lowell, Massachusetts; [2]Epion Corporation, Billerica, Massachusetts; [3]Air Force Research Laboratory/SNHC, Hanscom AFB, Massachusetts; [4]Center for Advanced Materials, Univesity of Massachusetts, Lowell, Massachusetts.

Gas Cluster Ion Beam (GCIB) processing has recently emerged as a novel surface smoothing technique to improve the finish of chemical-mechanical polished (CMP) GaSb (100) and InSb (111) wafers. This technique is capable of removing CMP induced surface and sub-surface damage and smoothing the surface, while simultaneously producing a thin oxide layer that can desorb for epitaxial 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 2.8Å to 1.7Å with a dual energy, dual gas GCIB sequence incorporating CF_4/O_2 at 10 kV followed by O_2 at 3 kV. For the first time, we report a GCIB grown oxide layer, comprised of both 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 demonstrated smoothing by reducing the average roughness from 2.5Å to 1.6Å using oxygen gas clusters in a triple energy GCIB process with energies of 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 SF_6/O_2gas clusters in a triple energy GCIB process with energies 30 kV, 10 kV, and 3 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 epitaxial growth. These are 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. Noriaki Toyoda, Shingo Houzumi and Isao Yamada; LASTI, Himeji Institute of Technology, Kamigori, Hyogo, Japan.

It has been known from molecular dynamics simulations that cluster size plays important roles for damage formations. Even though the total acceleration or energy per atom are the same, the damage formations 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 ion-dose by size-selected cluster ion beams. Recently, we have developed a high-current cluster ion beam system with size separation functions at the first time. This system equipped a

permanent magnet with a magnetic flux density of 1.2T. There is a sliding detector and sample holder on a guiding rail perpendicular to the incoming cluster 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 and 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; NPTest, 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 the through oxide contrast mechanisms of the semiconductor doping profile to a permanent imaging capability. The developed methodology enables CAD/FIB-image alignment, 2-D doping profile imaging, and n-wells depth measurement. From the backside, the n-wells are first observed at a remaining silicon thickness ~4.5mm, which correlates to the implant simulation depth where n and p carrier concentrations are equal. When the wells are first exposed during the XeF2 assisted FIB trenching (bulk silicon removal), the wells appear bright with a contrast variation between n and p at about 5%{(Ip - In)/(Ip + In)}. During the deposition of oxide film, the wells become dark relative to the p-substrate, and then become brighter until a thickness ~130nm. It would appear that initially during this deposition step an ohmic contact phenomena dominates the capacitive effect. Then as the film thickness increases the capacitive effect dominates. At the optimized thickness (130nm), the wells appear white relative to the p-substrate with a contrast variation up to 85%. The ion beam range is ~60nm at 30 keV in SiO, which is less than its thickness. This phenomenon is then non-destructive to the subsurface well structure. The observed contrast can be explained by a differential charging of the MOS capacitor, created by the surface charges generated in the ion-oxide interaction volume, the FIB deposited oxide, and the underlying semiconductor either p-substrate or n-well. The recipes as well as the kinetics to observe and optimize this n-well contrast are to be discussed. The relative brightness level above the oxide on the p-substrate and n-wells are correlated with the energy structure of the MOS-like capacitor.

11:15 AM R10.10
Simulation of Focused Ion Beam Induced Damage Formation in Crystalline Silicon. Gerhard Hobler, Alois Lugstein, Wolfgang Brezna and Emmerich Bertagnolli; Inst. of Solid State Electronics, Vienna University of Technology, Wien, Austria.

Applications of focused ion beams (FIB) include circuit modification during the design and debugging of integrated circuits. A fundamental limit of the method is given by the degradation of active devices due to beam induced crystal damage. Simulation of damage formation during FIB processing allows to estimate the minimum distance between the beam and device active regions. In order to simulate FIB induced damage formation, we have extended our 1-D/2-D binary collision (BC) code IMSIL to allow surface movement due to sputtering. In contrast to other dynamic BC codes, the crystal structure of the target may be taken into account. In addition, beam-induced amorphization is considered. We show that channeling in crystalline silicon may produce damage tails that are a factor of two deeper at relevant defect concentrations than those obtained with the random target approximation. This result is unexpected since a beam-induced surface amorphous layer is present throughout the simulation. It shows that in crystalline targets a larger minimum distance between beam and device active regions must be obeyed than otherwise expected. To confim our simulations we have carried out experiments on milling a hole in the gate poly-Si of a MOSFET. In-situ monitoring of the drive current and intermitting charge pumping measurements reveal that electroactive defects are generated 300nm below the surface for a 50keV Ga beam, in agreement with simulation.

11:30 AM R10.11
Localised Charging Effects Resulting From Focused Ion Beam Processing of Non-Conductive Materials.
Marion A Stevens-Kalceff[1], Sergey Rubanov[1] and Paul R Munroe[2]; [1]School of Physics, University of New South Wales, Sydney, New South Wales, Australia; [2]School of Materials Science and Engineering, University of New South Wales, Sydney, New South Wales, Australia.

Ion induced charging effects in electrically insulating materials have been investigated using Scanning Surface Potential Microscopy (SSPM). SSPM is a specialized Atomic Force Microscopy technique in which long-range Coulomb forces between a conductive atomic force probe and a specimen enable the electrical potential at the specimen surface to be imaged with high spatial resolution. SSPM has been used to characterize non-conductive materials exposed to Gallium ion irradiation in a Focused Ion Beam system. Ion beam irradiation of poorly conducting materials may result in the trapping of charge at either pre-existing or ion irradiation induced defects, thereby inducing a localized electric field within the irradiated/ implanted micro-volume of specimen. Significant localized residual charging is observed within the Gallium implanted micro-volumes of non-conductive materials both prior to and following the onset of sputtering. The reproducible characteristic surface potentials associated with the ion implantation induced trapped charge have been successfully modelled using three-dimensional conformal Finite Element Analysis. This gives insight into the charging processes during implantation and milling and the resultant spatial distributions of the residual trapped charge. The degree of charging is influenced by a number of different self-regulating dynamic processes including implantation, non-stoichiometric sputtering from compounds, secondary electron emission, secondary electron trapping by irradiation induced defects, secondary ion re-attraction and trapping, etc. This work provides insight into the complex charging processes that occur during implantation and sputtering and the resultant spatial distributions of the residual trapped charge. The induced charging effects have implications for the focussed ion beam processing and microanalysis of non-conductive materials.

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

A diffractive structure was obtained by directly scanning on a glass substrate in an area of 25x20 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 geometric size were observed on glass after FIB scanning. The ripples can be used as diffractive grating. Wavelength and amplitude of the ripple was characterized by use of atomic force microscope (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 ultra violet (UV). However, physical properties of the glass maybe caused to a certain extent due to more or less Ga+ ion 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 Ga+, the implantation depth was calculated by TRIM software, which is commonly used for ion beam analysis. The compound percentage of the implanted Ga+ was measured using electron dispersion X-ray spectrometer (EDX).

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

1:30 PM *R11.1
Ion Beam Processing for Silicon-based Light Emission.
Wolfgang Skorupa[1], Jiaming Sun[1], Thomas Dekorsy[1], Manfred Helm[1], Lars Rebohle[2] and Thoralf Gebel[2]; [1]FWIM, Forschungszentrum Rossendorf e.V., Dresden, Germany; [2]nanoparc GmbH, Dresden, 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 FZR during the last years, (i) blue-violet (400 nm) light emitters based on metal-oxide-silicon (MOS) capacitors, and, (ii) infrared (~1 micron) light emitters based on pn-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 case we employed implantation 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 like 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 case we investigate the electroluminescence from ion-beam synthesized pn diodes as a function of the implantation dose. Low temperature electroluminescence investigations in combination with microstructural analysis reveals the relevance of local boron

oversaturation in combination with strain effects for efficient electroluminescence-which, of course, is only possible by ion implantation. A numerical model developed for 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 TiO_2 Films. C.F. Chow[1,3], K.H. Cheng[1,3], Y.W. Lai[1,3], K.W. Lo[1,3], Y. Gao[1,3], Q. Li[2,3], N. Ke[1,3], W.Y. Cheung[1,3] and S.P. Wong[1,3]; [1]Electronic Engineering, Chinese University of Hong Kong, Shatin, Hong Kong; [2]Physics, Chinese University of Hong Kong, Shatin, Hong Kong; [3]Materials Science & Technology Research Center, Chinese University of Hong Kong, Shatin, Hong Kong.

In this work, TiO_2 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 $4x10^{15}$ cm^{-2} to $1x10^{17}$ cm^{-2}. Annealing was performed in vacuum at 600°C for 2h. The cobalt and iron composition and distribution in these implanted TiO_2 films were studied using Rutherford backscattering spectrometry. The microstructures were studied using transmission electron microscopy and x-ray diffractometry. 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 M_S values for the Co- and Fe-implanted samples ranged from 0.5 to 1.7 μ_B/Co atom and from 0.5 to 1.6 μ_B/Fe atom, respectively, both exhibiting an oscillatory dependence on the implantation dose. The coercivity values ranged from 100 Oe to 500 Oe for the Co-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: CUHK4216/00E and CUHK4221/00E).

2:15 PM R11.3
Microstructures and Electron Field Emission Properties of Ion Beam Synthesized and Modified SiC Thin Layers. S.P. Wong[1,3], W.M. Tsang[1,3], Y.W. Lai[1,3], W.Y. Cheung[1,3], N. Ke[1,3] and J.K.N. Lindner[2]; [1]Electronic Engineering, Chinese University of Hong Kong, Shatin, Hong Kong; [2]Institut fur Physik, University of Augsburg, Augsburg, Germany; [3]Materials 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 1V/μm could be obtained from ion beam synthesized (IBS) SiC/Si heterostructures [1]. More recently, by correlating the FE properties with the surface morphology and local surface conductivity, it was demonstrated that there were two distinct electric field enhancement mechanisms for electron FE from these IBS SiC samples [2]. Inspired 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 were 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 enhancement mechanisms will be discussed. This work is supported in part by the Research Grants Council of Hong Kong SAR (Ref. CUHK4200/01E) and by the Germany-Hong Kong Joint Research Scheme of RGC, Hong Kong SAR and DAAD, Germany. [1] D. Chen *etal*, Appl. Phys. Lett. 72, 1926 (1998). [2] W.M. Tsang *etal*, 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 Renk[1], Paula P Provencio[1], Somuri V Prasad[1] and Michael O Thompson[2]; [1]Sandia National Laboratories, Albuquerque, New Mexico; [2]Cornell 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 ~200ns ion pulse produces fast melt and cool cycles, leading to grain refinement and formation of metastable alloys. Titanium alloy substrates, with and without sputter-deposited metal coatings, were treated using nitrogen and other ion beams, producing cooling rates of up to 10^9K/sec. The fluences used produce a melted layer several microns thick, with ablation produced at the highest doses. The microstructure of treated samples was investigated by electron diffraction (SAD) and both bright field and dark field cross-sectional TEM (XTEM). Compositional changes were measured by nanobeam energy dispersive 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 friction and wear behavior. In both cases, improvements in friction and wear behavior are observed, compared to both untreated and uncoated/treated 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 VO_2 Thin Film. Libin Lin[1,2] and Tiecheng Lu[1,2]; [1]Department of Physics, Sichuan University, Chengdu, China; [2]Key Laboratory for Radiation Physics and Technology of Education Ministry of China, Sichuan University, Chengdu, China.

VO_2 thin films with special phase-transition properties prepared by vacuum evaporation combined with vacuum deoxidation were irradiated by proton beam with fluence of 1×10^{11}/cm^2 -1×10^{14}/cm^2 and energy of 7.6MeV. After irradiation, the samples were annealed at different temperature. Before and after irradiation, both phase transition properties and crystalline structures are characterized by X-ray diffraction and X-ray photonelectron spectroscopy, UV-VIS transmittance and Raman spectroscopy. The results indicate that after irradiation, VO_2 thin films can also be transferred from the phase of anatase to rutile, but the phase-transition temperature and the width of phase-transition hysteresis changed as well as the valence of V ion and the crystalline structure changed. The results of Raman spectroscopy measurement show the disturbation of OH clusters induced by protons .

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

Nanopatterned thin films are of crucial importance for magnetic storage technology. Ion irradiation based techniques exhibit the potential to produce improved storage media, since it becomes possible to tailor the magnetic parameters on a nanometer scale without a modification of the surface topography. The achievable storage 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 of magnetic films. Both examples show that research covering the interaction between ion beams and magnetic films are of important technological relevance. Due to the reduced symmetry of thin metallic films and multilayers their magnetic properties often depend on surface and interface effects, for example induced magnetic anisotropies or magnetic coupling phenomena. The material choice allows to adjust these parameters to some extent. In addition the structural ordering of alloys is important for their magnetic properties and hence relevant for technological applications. He ion irradiation in an energy regime between 1 - 50 kV is ideally suited to tailor and control the structural and thereby also the magnetic properties of thin magnetic systems after their preparation. In this energy range He ions penetrate the magnetic films, which are typically a few nanometer thick, completely and modify the strucutral order due to the energy impact on a very local scale. Since this interaction is very short range direct ion writing or ion irradiation through a resist mask allows to pattern the magnetic properties on a micro- or nanometer scale. It is especially important to highlight that the magnetic properties are patterned without any modification of the surface topography.

4:00 PM R11.7
Optimizing the Fracture Toughness of Brittle Materials by Ion Implantation. J Gregory Swadener[1], Michael I Baskes[1], Thomas E Felter[2], Chris J Wetteland[1], Joseph R Tesmer[1], Xinghang Zhang[1] and Michael Nastasi[1]; [1]MST-8, Los Alamos National

Laboratory, Los Alamos, New Mexico; [2]Lawrence Livermore National Laboratory, Livermore, California.

We have conducted a combined experimental and molecular dynamics (MD) investigation to determine how ion beams can be used to greatly increase fracture toughness in brittle materials. In the MD simulations on silicon, ion implantation produced displacement spikes leading to the formation of clusters of disordered atoms. The presence of these disordered regions allowed silicon to deform plastically as a crack approached, blunting the crack tip and arresting crack growth. The MD calculations predict that fracture toughness increases with the amount of disorder and can be increased by a factor of 3 or more. This newly discovered toughening mechanism can also explain earlier experimental observations of increased fracture toughness in irradiated ceramics. In order to corroborate the MD results, silicon specimens have been implanted with Ne and Xe ions. The fracture experiments along with RBS-C and TEM analyses confirm that the fracture toughness of ion implanted silicon increases by a factor of 3 when the material just becomes amorphous. The combined experimental and atomistic method has enabled us to examine the details of fracture at the atomic scale, revealing how the fracture process converts energy from potential energy in the strained lattice into kinetic energy, surface energy and energy loss through distortions of the crystalline lattice. Research sponsored by the Office of Basic Energy Sciences, U. S. Department of Energy. The work by TEF 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.

4:15 PM R11.8
Electrical Properties of Rutile Single Crystal Irradiated by High-Fluence-Reactor-Neutron. Tiecheng Lu[1,3], Libin Lin[1], Gang Cheng[1], Chunpei Zhao[2] and Yunfei Tian[2]; [1]Department of Physics, Sichuan University, Chengdu, China; [2]Analytic and Testing Center, Sichuan University, Chengdu; [3]International Center for Materials Physics, Chinese Academy of Sciences, Shenyang.

Electrical properties of high fluence neutron irradiated rutile (TiO_2) single crystals has been investigated for the first time. Stoichiomatric rutile is one kind of good insulator of high dielectric constant. But it can be dramatically changed into n-type semiconductor due to oxygen insufficiency by annealing under reduction phenomenon or ion radiation, etc. It may be used to radiation dosage detecting material. In this paper, the colorless rutile single crystal turned into deep blue after irradiated by high-fluence-reactor-neutron of $10^{19}cm^{-2}$ and its electrical property presented large change, from high insulator to normal semiconductor. The relationship of sample resistance with temperature (low temperature, room temperature and high temperature) and the effect of annealing atmosphere(in air or in vacuum) on the electrical property of sample have been studies. The results showed that sample presents semiconductor properties at low temperature. At high temperature, it is oxidized into colorless insulator in air condition. In 10^{-4} Pa vacuum condition, it presents conductance behavior of dot defects without oxidation. The excitation energies of the defects are 0.06 and 0.12eV, corresponding to H^+ and Ti^{3+}, respectively.The electrical conductance mechanism of sample has been also discussed.

4:30 PM R11.9
Ion beam induced luminescence of Al2O3 in tens keV-hundred MeV range. Vladimir Skuratov, Flerov lab.of nuclear reactions, Joint Institute for Nuclear Research, Dubna, Russian Federation.

"In-situ" measurement of optical absorption and luminescence has proved to be a useful tool for characterizing of radiation damage accumulation in solids under energetic particle bombardment. Several papers have been devoted to study the spectral content of light emission from single crystal alumina enhanced by heavy ions at various energies. At the same time, many features of ion beam induced luminescence of Al2O3 are not yet fully understood. In this paper we report on results concerning detailed study of the luminescence generated in Al2O3 by multicharged heavy ions ranging in mass and energy from He+2 (40 keV) to Bi+51 (710 MeV). Luminescence spectra were registered at 80K and 300K under irradiation on ion beam line for applied research of U-400 FLNR JINR cyclotron (E= 1 - 3.5 MeV/amu) and experimental set-up based on ECR ion source (40 - 300 keV). "In-situ" measurements were followed by postradiation optical examinations. The peculiarities of variation of the luminescence intensity in F and F+-bands with damage dose at different excitation density levels are discussed.

SESSION R12: Sputtering, Ion Beam Mixing and Assisted Deposition
Chair: B. X. Liu and K.-H. Henig
Friday Morning, December 5, 2003
Room 306 (Hynes)

8:30 AM *R12.1
Range and mixing distributions of low-energy carbon ions as a base for subplantation growth models. Guenther Dollinger[1], Peter Neumaier[1], Andreas Bergmaier[1], Lutz Goergens[1], W. Eckstein[2], Reiner Fischer[2], Hofsaess Hans[3], H.U. Jaeger[4], H. Kroeger[3] and Carsten Ronning[3]; [1]Physik Department E12, TU Muenchen, Garching, Germany; [2]Centre for Interdisciplinary Plasma Science, Max-Planck-Institut fuer Plasmaphysik, Garching, Germany; [3]II.Physikalisches Institut, Universitaet Goettingen, Garching, Germany; [4]Institut fuer Ionenstrahlphysik und Materialforschung, Forschungszentrum Rossendorf e.V, Dresden, Germany.

Subplantation was early recognised as being the basic process in low-energy ion growth of diamondlike materials and has also to be considered for the description of bias enhanced diamond nucleation. A number of theories modelling the evolution of diamondlike phases have been proposed. However, the precise details of the subplantation and relaxation processes remain unclear. The problem in testing the complex models is that experimental information other than film structure versus ion energy is missing to a large extent. Mixing and range distributions of low-energy carbon ions are ideal data to model diamond-like film growth. Here, we present measurements of range and mixing distributions for carbon ions at energies in the relevant energy range between 12 eV and 692 eV in carbon. The substrates are grown at the identical energies using 12C ions by mass separated ion beam deposition. Less than a monolayer of 13C was implanted each for the range distributions and as a marker layer for mixing profiles. The 13C depth profiles are measured by high-resolution elastic recoil detection (ERD). These data are directly compared to calculations based on the binary collision approximation (TRIDYN) and to molecular dynamics (MD) simulations which consider atomic interactions on a time scale up to 15 ps including the thermal-spike phase. Addititionally, mixing distributions are derived from a transport calculation based on the measured range distributions. The measured range profiles show bimodal structures for energies below 200 eV which are significantly broader than the calculated profiles. The mixing profiles are also significantly broader than respective TRIDYN and MD calculations at these low energy. However, mixing profiles are in good agreement with transport calculations based on the measured range profiles showing the relevance of the measured range structures. Three reasons for the observed differences between the measured and theoretical range and mixing distributions are discussed in the paper: thermal induced self diffusion during thermal spike, mobility solely of the deposited ion after the collisional stage and a 3-dimensional surface structure of the carbon films on atomic scale. The experiment allows a crucial test for models of the subplantation scheme and may serve as input for improved calculations.

9:00 AM *R12.2
Hard Coatings Design by Hyperthermal Ion Processing. Wolfhard Moeller, Institute of Ion Beam Physics and Materials Research, Forschungszentrum Rossendorf, Dresden, Germany.

It has been known since long that the properties of thin films are significantly influenced by ion bombardment which is inherent to the specific processes of deposition, thus giving possibilities to tailor the films for specific applications. However, the understanding of the corresponding mechanism on an atomic level is still at its infancy and far from a general predictive modelling, although an increasing number of well-tailored experiments have been performed more recently. In addition, new theoretical tools such as molecular dynamics computer simulation have become applicable which are supplementary to simple analytical models of the film growth and properties. The paper will review these developments for the examples of carbon based coatings and selected nitride films. Recent experimental findings, which in particular make use of real-time in-situ diagnostics during film growth, will be correlated with theoretical modelling and simulation. The role of ion bombardment for the formation of phases, film crystallinity and texture will be discussed with special emphasis on the generation and release of internal stress, and on interface engineering. Deposition processes involving pulsed ion bombardment appear to be particularly promising in this area.

9:30 AM R12.3
Sputter-Induced Carbon Nanotube Formation. Thomas A. Westrich[1], Steven C. Seel[1], Jerrold A. Floro[1] and Thomas A. Friedmann[2]; [1]Surface and Interface Sciences, Sandia National Laboratories, Albuquerque, New Mexico; [2]Nanostructure and Semiconductor Physics, Sandia National Laboratories, Albuquerque, New Mexico.

We have produced dense arrays of nanotube-like features by argon ion sputtering of graphite targets at intermediate temperatures (below 550°C). Typical ion bombardment conditions include incident energies in the 0.5-2 keV range, doses up to $2E19/cm^2$, and dose rates of $1mA/cm^2$. The resulting tubes have diameters ranging from 15-50 nm, and lengths of order 300-3000 nm, and the arrays can be as dense

as 1E10/cm^2. The mean tube dimensions and the areal density both increase with dose. Tube morphology improves with target temperature during sputtering. We will discuss the effect of energetic hydrogen on the formation kinetics of sputter-induced nanotubes, and the effect of bombardment conditions on the detailed atomic structure of individual tubes from transmission electron microscopy measurements. This work was partially supported by the DOE Office of Basic Energy Sciences. Sandia is a multiprogram laboratory of the United States Department of Energy operated by Sandia Corporation, a Lockheed Martin Company, under contract DE-AC04-94AL85000.

9:45 AM R12.4
Pattern Formation in Ar-sputtered InP and Sample Rotation. Gih Sheng Lau, Jisheng Pan and Jian Wei Chai; MSCL, 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 with varying beam energies, beam currents and rotating 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.

10:15 AM *R12.5
Ion Beam Assisted Deposition. James K. Hirvonen, WMRD-MC, 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 important influence ion bombardment has on coating properties when present during vapor deposition processing. The optical coating community was among the first to adopt the process in the form of concurrent , low energy, 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 as 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.

10:45 AM R12.6
Formation of Gold Nanoclusters in the Au-Silica Thin Films Deposited by Ion Beam Assisted Deposition. Jinghao He, Carmine A. Carosella, Syed B. Qadri, James A. Sprague, David L. Knies, Rhonda M. Stroud, Kenneth S. Grabowski and Graham K. Hubler; Naval Reseach Laboratory, Washington DC, District of Columbia.

Gold nanoclusters in silica are prepared using electron beam evaporation of gold and silica 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.

11:00 AM R12.7
Deposition of metallic nanowires by electron- and ion-beam assisted decomposition. Vidyut Gopal, Eric A Stach and Velimir R Radmilovic; National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, California.

Crucial to nanotechnology 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 of a metal organic precursor 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 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 spectroscopy (EDS) as well as by the surface sensitive technique of 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 limit 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 nanoscale building blocks such as semiconducting nanowires and nanotubes.

11:15 AM R12.8
Lateral Templating for Guided Self-Organization of Sputter Ripple Morphologies. Alexandre Cuenat[2,1], Henry George[1], Vidya Ramaswamy[1], Kee-Chul Chang[3], Jack Blakely[3] and Michael J Aziz[1]; [1]Division of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts; [2]Si-Ge Nanostructures Lab, CRMC2 - CNRS, Marseille, France; [3]Materials Science Center, Cornell University, Ithaca, New York.

We study the influence of a patterned substrate on self-organized ripples spontaneously appearing during uniform irradiation with low energy Ar ions. We show that the long-range order of the ripples can be greatly enhanced by imposing lateral boundary conditions on the sputter instability. The self-organization can be controlled by changing the size of pre-patterned regions made on the substrate. Conditions to control and guide the self-organization are discussed. The effect of nonlinearities in the model for ripple evolution is discussed in the presence of boundaries. These observations demonstrate the usefulness of lateral templating to guide the self-organization of surface nanofeatures.

11:30 AM R12.9
Two Dimensional Diffusion Effects and Defect Evolution in Ion Implanted Silicon Nanostructures. Susan M Kluth[1,3], David Alvarez[2,4,5], Stefan Trellenkamp[1], Juergen Moers[1], Steffi Lenk[1], Patrick Kluth[1,3], Johannes Kretz[2], Wilfried Vandervorst[5,6] and Siegfried Mantl[1]; [1]Institut fuer Schichten und Grenzflaechen, Forschungszentrum Juelich, Juelich, Germany; [2]Corporate Research Nano Devices, Infineon Technologies AG, Munich, Germany; [3]Department of Electronic Materials Engineering, Australian National University, Canberra, Australian Capital Territory, Australia; [4]Failure Analysis, Infineon Technologies AG, Munich, Germany; [5]Materials and Components Analysis, IMEC, Leuven, Belgium; [6]Katholieke Universiteit Leuven, Leuven, Belgium.

Several future CMOS devices such as double gate transistors are based on nanostructured Si. Ion implantation is a likely candidate for the introduction of dopants, due to its highly established technology. However, only limited investigation into implantation of nanostructure targets has been carried out. It is well established that implantation generates an elevated Si self interstitial point defect population which leads to transient enhanced diffusion (TED) of dopants such as B and the formation of extended defects. Significant evidence has been adduced to suggest that both TED and defect formation are influenced by surface proximity. As lateral dimensions of implanted structures decrease, the availability of free surfaces increases, facilitating the enhanced annihilation of point defects at the surface. Consequently, dopant diffusion and defect formation in nanostructured silicon should differ significantly from that in bulk materials. Etching masks were produced either by electron-beam lithography using a three-layer resist or a spacer method. Fields of 25-125 nm wide, 300 nm high Si nanostructures were then generated using reactive ion etching with an HBr plasma. 1 keV, 1x10^{15} at.cm^{-2} B implants into 125 nm wide, 300 nm high Si nanostructures have been characterized following a 1050°C spike anneal in N_2. Scanning spreading resistance microscopy, which makes use of an atomic force microscopy tip biased relative to a semiconductor sample is a promising method for the analysis of 2D dopant profiles on a nanometer scale. A curved diffusion front has been observed. B in the center of the ridge diffuses further than at the sides. A similar effect has been observed in SUPREM-IV simulations. It is attributed to a reduction in TED close to the vertical surfaces due to recombination of excess Si self interstitials. For narrower structures, simulations indicate that the junction depth will be determined by the dimensions. Defect evolution is also under investigation.

11:45 AM R12.10
The influence of ion beam energy on thin film growth: Co on Si(111). Koen Vanormelingen, Bart Degroote, Mehmet Cakmak, Stefaan Cottenier and Andre Vantomme; Instituut voor kern- en stralingsfysica, Leuven, Belgium.

The technique used to deposit a thin film often influences its properties significantly. Frequently the difference in deposition energy plays a crucial role, e.g. Chemical Vapor Deposition (absorption), Molecular Beam Epitaxy (10-100 meV) or sputtering (exhibiting a broad distribution, of the order of 2-10 eV). We studied this energy dependence systematically using low energy ion beams, and focused on the initial layer growth for a metal-semiconductor system. We investigated the growth of an ultra-thin Co film on a Si(111) substrate using two techniques: low energy ion deposition (LEID) and MBE. In LEID, an isotopically pure ion beam with energy of 50 keV is

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 ($\sim$ 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 ($\sim$2 ML) we investigated the influence of the deposition energy on the surface morphology. Depositions with LEID 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 $\sim$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.