SYMPOSIUM CM05

Fundamentals of Materials Property Changes Under Irradiation
November 26 - November 29, 2018

Symposium Organizers
Kazuto Arakawa, Shimane University
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Michael Short, Massachusetts Institute of Technology

* Invited Paper

SESSION CM05.01: Irradiation-Induced Point Defects and Diffusion
Session Chair: Michael Short
Monday Morning, November 26, 2018
Hynes, Level 2, Room 202

9:15 AM CM05.01.01
***In Situ* TEM of Formation Processes of Dislocation Loops in Tungsten Under Irradiation—Comparison Between Electron and Self-Ion Irradiations** Kazuto Arakawa; Shimane University, Matsue, Japan.

Nuclear-fission and fusion materials are degraded primarily due to the accumulation of radiation-produced lattice defects, such as point defects (self-interstitial-atoms (SIAs) and vacancies) and point-defect clusters (dislocation loops and cavities). In order to precisely predict the lifetimes of nuclear materials, accurate understanding of the origins of the defect accumulation—generation of defects and their subsequent dynamics—is crucial.

In-situ transmission electron microscopy (TEM) is a powerful technique for probing defect dynamics, in response to external stimuli such as irradiation under heating or cooling. As the irradiation sources for the in-situ TEM, electrons and ions are available. In the electron irradiation, only point defects are generated as the primary damage via knock-on displacement. In contrast, in the ion irradiation, point-defect clusters are also generated as the primary damage, which is called “collision cascade”, like neutron irradiation.

In the present study, we focus on the formation process of SIA dislocation loops in tungsten under irradiation. So far, we have revealed that the SIAs [1] and loops are intrinsically highly mobile and the loop-formation process must be governed by extrinsic “stabilizers” for them. In this study, we examine the loop stabilizers for 2000-keV electron irradiation using a high-voltage electron microscope in Osaka University in Japan and 500-keV W^+ self-ion irradiation using an ion-accelerators combined microscope in the JANNuS-Orsay facility in France. Through the comparison between these results, we try to extract the effects of collision cascade on the loop stabilization.

References
[1] T. Amino, K. Arakawa, and H. Mori, *Scientific Reports* 6 (2016) 26099.

9:30 AM CM05.01.02
Hot-Electron Mediated Atomic Diffusion in Proton-Irradiated MgO Cheng-Wei Lee and Andre Schleife; University of Illinois at Urbana-Champaign, Urbana, Illinois, United States.

Ionizing charged-particle radiation has exciting potential to modify material properties. In particular, swift heavy ions are known to either exacerbate or mitigate damage. Controlling the modification of a material using radiation relies on a quantitative understanding of fundamental interactions between particle radiation and target material.

Since high-energy projectiles significantly drive the electronic system of the target out of equilibrium, standard atomistic simulations based on the Born-Oppenheimer approximation are no longer valid. Therefore, knowledge of non-equilibrium electron-ion physics becomes crucial: Directly after excitation by the projectile ion, the electronic system of the target is in a highly excited, *non-thermalized* state. Subsequent thermalization and cooling takes tens to hundreds of femtoseconds and tens of picoseconds respectively, depending on the dominant scattering mechanism and the target material. However, it is currently not well understood whether and how non-thermalized excited carriers, as well as thermalized hot carriers, affect atomic diffusion, which is the critical knowledge to understand material property change via irradiation.

In order to achieve a quantitative description of atomic diffusion under particle radiation, we propose a parameter-free first-principles simulation framework that bridges time scales from ultrafast electron dynamics directly after impact, to atomic diffusion in the presence of hot electrons. First, we simulate electronic excitations during ion irradiation using real-time time-dependent density functional theory. We then extract the probability of finding electrons in excited electronic states as occupation numbers and use them as constraint in DFT-based nudged-elastic band simulations to compute migration barrier in the presence of hot carriers.

Here we apply this framework to magnesium oxide under proton irradiation [1]. We compare the migration barrier of an oxygen vacancy in the presence of (i) non-thermalized hot electrons, (ii) thermalized Fermi-distributed electrons, and (iii) an ionized oxygen vacancy. We found that in all three cases, the migration barriers are lower than for the electronic ground state by 1.33, 0.34, and 1.07 eV respectively. Neither thermalized hot electrons nor ionization of the point defect can fully explain the enhanced diffusion under non-equilibrium conditions, hinting at a novel hot-electron mediated diffusion mechanism.

Furthermore, our quantitative simulations show that this mechanism strongly depends on the projectile-ion velocity, opening the possibility of turning it on or off by varying the kinetic energy of the particle radiation. We predict that this should facilitate direct experimental observation of this effect and significantly advances current understanding of non-equilibrium electron-ion dynamics in materials under energetic particle radiation.

[1] C.-W. Lee and A. Schleife, (2018) arXiv:1806.00443

9:45 AM CM05.01.03
Helium Irradiated Cavity Formation and Defect Energetics in Ni-Based Binary Single-Phase Concentrated Solid Solution Alloys Zhe Fan[1], Shijun Zhao[1], Ke Jin[1], Di Chen[2], Yuri Osetsky[1], Yongqiang Wang[2], Hongbin Bei[1], Karren More[1] and Yanwen Zhang[1, 3]; [1]Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States; [2]Los Alamos National Laboratory, Los Alamos, New Mexico, United States; [3]The University of Tennessee, Knoxville, Knoxville, Tennessee, United States.

Binary single-phase concentrated solid solution alloys (SP-CSAs), including $Ni_{80}Co_{20}$, $Ni_{80}Fe_{20}$, $Ni_{80}Cr_{20}$, $Ni_{80}Pd_{20}$, and $Ni_{80}Mn_{20}$ (in atomic percentage), were irradiated with 200 keV He^+ ions at 500 ºC. He cavity size and density distribution were systematically investigated using transmission electron microscope. Here we show that alloying elements have a clear impact on He cavity formation. Cavity size is the smallest in $Ni_{80}Mn_{20}$ but the largest in $Ni_{80}Co_{20}$. Alloying elements could also substantially affect cavity density profile. In-depth examination of cavities at peak damage region (~ 500 nm) and at low damage region (~ 300 nm) demonstrates that cavity size is depth (damage) dependent. Competition between consumption and production of vacancies and He atoms could lead to varied cavity size. Density functional theory (DFT) calculations were performed to obtain the formation and migration energies of interstitials and vacancies. Combined experimental and simulation results show that smaller energy gap between interstitial and vacancy migration energies may lead to smaller cavity size and narrower size distribution observed in $Ni_{80}Mn_{20}$, comparing with $Ni_{80}Co_{20}$. The results of this study call attention to alloying effects of specific element on cavity formation and defect energetics in SP-CSAs, and could provide fundamental understanding to predict radiation effects in more complexed SP-CSAs, such as high entropy alloys.

10:00 AM BREAK

SESSION CM05.02: Radiation Defect-Solute Interactions
Session Chairs: Christophe Domain and Michael Short
Monday Morning, November 26, 2018
Hynes, Level 2, Room 202

10:30 AM *CM05.02.01
Atomic Simulation Insight of Extended Defect—Solute Properties in Metals Under Irradiation Christophe Domain[1] and Charlotte S. Becquart[2]; [1]EDF R&D, Moret-Sur-Loing, France; [2]UMET, Université de Lille, Villeneuve d'Ascq, France.

Under neutron or ion irradiation point defects and defect clusters are formed within the displacement cascades or by diffusion of defects under irradiation fluxes. The properties of these clusters have significant impact on the evolution of the microstructure under irradiation conditions. Furthermore, solutes within the alloys may affect the defect behaviour (their relative stability and their mobility) due to their more or less large interaction with them.
Atomic simulation allows to investigate properties of point defect clusters. DFT calculations are the most accurate available method to determine the impact of substitutional atoms representative of the alloying elements on the stability and mobility of clusters in particular for self interstitial clusters the mobility of which can be quite complex. The results we will present focus on Fe dilute alloys representative of reactor pressure vessel steels, tungsten representative of fusion divertors and zirconium representative of fuel cladding materials. The different possible structures small SIA clusters can adopt will be discussed, in particular the sessile and non parallel configurations in Fe, as well as the interstitial dislocation loop. The later has been experimentally observed when they are large enough. The dependence of solute interactions as a function of solute size, chemistry or magnetism will be discussed, as well as synergy effects between solutes. Furthermore, the formation of interstitial clusters in the displacement cascade obtained by molecular dynamics (using different EAM potentials) debris will be presented.
The data we obtained are essential / fundamental / necessary to model microstructure evolution using for instance kinetic Monte Carlo simulations.

11:00 AM CM05.02.02
Hydrogen Promoted Vacancy Diffusivity in Cu—First-Principles and Molecular Dynamics Study Junping Du[1, 2], W.T. Geng[2, 3], Kazuto Arakawa[4] and Shigenobu Ogata[2, 1]; [1]Center for Elements Strategy Initiative for Structural Materials, Kyoto University, Kyoto, Japan; [2]Department of Mechanical Science and Bioengineering, Osaka University, Osaka, Japan; [3]University of Science and Technology Beijing, Beijing, China; [4]Department of Materials Science, Faculty of Science and Engineering, Shimane University, Shimane, Japan.

The agglomeration of vacancies, which acts as one of the void nucleation and growth mechanisms, may cause ductile fracture in pure metals and radiation-damaged materials. It has been believed that diffusion of vacancy in metals is suppressed in hydrogen environment. The fact that excess hydrogen can enhance greatly the self-diffusion of atoms in metals has been explained by the appearance of superabundant vacancies, because the vacancy formation energy decreases substantially with increasing H concentration, while individual vacancy diffusion is supposed to be slowed down. Previous computational and theoretical studies suggest that the trapped H atoms in a H-vacancy complex impede the diffusion of vacancy by increasing the energy barrier of vacancy jumping. However, by performing first-principles calculations of appearance probability of vacancy-H configurations, the activation energy and attempt frequency of possible vacancy jumping pathways in face-centered cubic Cu, we find at certain H concentrations and temperatures, the diffusivity of vacancy is actually accelerated by H. The trapped H tends to increase the diffusion barrier of a vacancy and the environmental H tries to reduce it, whereas both of them enhance the diffusion attempt frequency. The molecular dynamics (MD) simulations of the vacancy diffusion in the Cu-H system have also been performed to demonstrate the promoting effect of H. The MD simulations of the vacancy diffusivity reveal an unharmonic effect extremely enhances the acceleration of vacancy diffusion by H. The uncovered H accelerated H-vacancy diffusion processes can advance our understanding of the H behavior in H-induced damage in metals.

11:15 AM *CM05.02.03
Formation Mechanism of Radiation-Induced Re and Os Precipitation in W and Their Influences on Mechanical Properties Hong-Bo Zhou, Yu-Hao Li, Ying Zhang and Guang-Hong Lu; Department of Physics, Beihang University, Beijing, China.

Tungsten (W) is one of the most promising candidates for plasma facing materials (PFMs) in future fusion reactors. Rhenium (Re) and Osmium (Os) are

not only the typical alloying elements but also the main productions of transmutation in W-PFMs. More importantly, Re and Os will aggregate and precipitate in W under high energy radiation, which substantially enhance the radiation hardening and embrittlement, leading to the great concerns for the life-limiting of W-PFM. So far, the formation mechanism of Re/Os-rich clusters in W as well as their influences on the mechanical properties remains to be fully elucidated.
We have investigated the interaction between Re/Os and defects in W using a first-principles method in combination with thermodynamic models in order to explore the precipitating mechanism of Re/Os under irradiation. It is found that the presence of defects can significantly reduce the total nucleation free energy change of Re/Os, and thus facilitate the nucleation of Re/Os in W. Kinetically, self-interstitial atom is shown to be easily trapped by substitutional Re/Os, and form W-Re/Os mixed dumbbell. Such W-Re/Os dumbbell combining with the substitutional Re/Os atom will transfer to high stable Re/Os-Re/Os dumbbell, which can serve as a trapping centre for subsequent W-Re/Os dumbbells, leading to the growth of Re/Os-rich clusters. Consequently, an interstitial-mediated migration and aggregation mechanism for Re and Os precipitation has been proposed.
To shed light on the effects of transmutation elements on the mechanical properties of W, we further have investigated the influences of Re on the motion of 1/2<111> screw dislocation in W. It is found that the influence of Re on the dislocation motion is directly related to the distribution of Re in W. For the state of Re dispersed distribution, the addition of Re will reduce the generalized stacking fault energy (GSFE) for both 1/2<111>{112} and 1/2<111>{110}, and improve the ductility of W. However, the influence of Re clusters (for the state of Re aggregation) on the dislocation motion is significantly different from that of dispersed Re. The presence of Re clusters will substantially increase the Peierls stress and energy, inhibiting the dislocation mobility. This will significantly exacerbate the irradiation hardening of W. Therefore, the radiation-induced precipitation of transmutation elements will degrade the mechanical properties of W.

11:45 AM CM05.02.04
Investigation of Hydrogen Isotope Distribution in Unirradiated and Neutron Irradiated Zircaloy-4 via Atom Probe Tomography Elizabeth J. Kautz and Arun Devaraj; Pacific Northwest National Laboratory, Richland, Washington, United States.

Tritium is a radioactive hydrogen isotope (^3H) used in various applications. Since tritium is not naturally abundant, it must be artificially generated with Tritium Producing Burnable Absorber Rods (TPBARs), which are specifically designed to produce and capture ^3H when irradiated with neutrons. At the center of each TPBAR, there is a lithium aluminate ($LiAlO_2$) ceramic pellet that produces tritium upon neutron irradiation, which is then absorbed by a Zircaloy-4 tube that surrounds the $LiAlO_2$ pellet [1]. Currently the amount of ^3H absorbed by the Zircaloy-4 getter, and the hydride phases formed are not well understood [2]. In order to improve predictive models and inform materials processing and design decisions, improved understanding of mechanisms responsible for hydrogen absorption and distribution in the Zircaloy-4 getter is needed. The overall goal of this work is to measure hydrogen isotopic ratios and spatial distribution in the Zircaloy-4 getter exposed to various environments in order to provide insight into how hydrogen is absorbed in the tritium production process. In this work, comparison of atom probe tomography results from as-received, hydrided, deuterated Zircaloy-4 samples was performed and compared to results from neutron irradiated Zircaloy-4. Data revealed several overlapping peaks in mass spectra, and non-uniformity in hydrogen distribution after exposure to hydrogen and deuterium gases. Additionally, sample preparation procedures and user-selected experimental parameters for pulsed-laser atom probe were studied in order to determine how various parameters impact hydrogen background, and hydrogen isotope content in all Zircaloy-4 samples analyzed. Laser energies of 80-200 pJ, at a pulse rate of 125 kHz were studied, and we found that measured hydrogen concentration decreased with increasing laser energy at a given pulse frequency. The work presented here is intended to serve as a baseline for application of atom probe tomography for the challenge of hydrogen isotope quantification in Zircaloy-4, with implications to other hydrogen-sensitive metal alloy systems.
References:

[1] A Devaraj, EJ Kautz, EA Vo; B Johnson, DJ Senor, J Hardy; "*Atom Probe Tomography for Detection and Quantification of Light Isotopes in TPBAR Components", PNNL-27132, January 2018.*

[2] D. J. Senor, "Recommendations for Tritium Science and Technology Research and Development in Support of the Tritium Readiness Campaign, TTP-7-084," PNNL22873, October 2013.

SESSION CM05.03: Chemical and Polymeric Changes Under Ionizing Radiation
Session Chairs: Kazuto Arakawa and Hidehiro Yasuda
Monday Afternoon, November 26, 2018
Hynes, Level 2, Room 202

1:30 PM CM05.03.01
Structural and Electronic Changes in Prototypical Catalysts upon X-Ray Irradiation Anna Regoutz[1], Amber Thompson[2], Alex M. Ganose[3], David O. Scanlon[3] and Claire Murray[4]; [1]Imperial College London, London, United Kingdom; [2]University of Oxford, Oxford, United Kingdom; [3]University College London, London, United Kingdom; [4]Diamond Light Source, Didcot, United Kingdom.

Interactions of X-rays with crystalline matter can induce a wide range of changes. Whilst some knowledge is available for biological systems and extended solids, practically nothing is known on the effect of ionising radiation on small molecules. However, they form the basis of a range of important technologies, e.g. catalysis. In small molecule crystals radiation damage can be understood as a three step process. Primary damage is caused by the direct interaction of the incident radiation with the sample. This is followed by secondary damage through electrons as well as species which are created during the initial damage. Finally, an extended collapse of the structure can occur based on a combination of a significant number of damage processes caused by energy deposition in the crystal.

Modern characterisation techniques make extensive use of X-rays to gain information on the properties of matter. Particularly modern microfocused laboratory sources and synchrotrons with their increased radiation dosages and often lower X-ray energies present a challenge. The move towards ever more powerful X-ray sources has increased the urgency to understand the influence of radiation damage. Whilst the observation of radiation damage in itself is useful to design strategies to prevent it, it is of even greater importance to understand the why and how of radiation damage in these materials. Lessons learned from radiation damage studies can in turn give vital information to understand a material's overall behaviour and stability.

Here, a combination of synchrotron-based X-ray powder diffraction (PXRD) and laboratory-based X-ray photoelectron spectroscopy (XPS) is used to provide insights into changes to the structure, to local chemical environments, and to the electronic structure of small molecular crystals. By combining results from both of these advanced techniques, structural changes can be directly correlated to changes of the chemical state of the metal, which also manifests itself in variations in the valence structure. A range of prototypical catalysts is investigated, based on the general formula of $M_xCOD_yX_z$, where

M=group 8-11 metals, COD=cyclooctadiene, and X=Cl, Br. By using appropriate timescales, the effects of radiation are followed continuously over long periods of time giving an insight into how radiation damage progresses. In order to understand the experimental observations in more detail, theoretical results from density functional theory calculations are employed. Differences in the behaviour of the materials will be discussed in the context of both structural and chemical characteristics.

The combination of diffraction and spectroscopy provides a powerful new way of following X-ray photon exposure effects on both structure and electronic structure. The characterisation processes developed are applicable beyond small molecule catalysts and the insights gained can be extended to other material systems, and inspire further investigations.

1:45 PM CM05.03.02
Evaluating Radical Initiators for Secondary Electron Optimization in Hafnium Oxide-Methacrylate EUV Photoresist Yasiel Cabrera, Eric Mattson, Kolade Oyekan, Yuxuan Wang and Yves J. Chabal; Department of Material Science, The University of Texas at Dallas, Richardson, Texas, United States.

Inorganic-organic hybrid nanoclusters are molecular compounds that have excellent photochemical properties for the newly emerging extreme ultraviolet lithography (EUVL). In particular, these systems have recently come into the spotlight of research due to their achievements in both high etch resistance and photosensitivity abilities thanks to their functional inorganic metal-oxide cores when exposed to ionizing radiation. In this work, we uncover the fundamental mechanisms of photoresists composed of hafnium-oxide core with terminal carboxylic acid ligands. A combination of *in situ* infrared (IR) spectroscopy and residual gas analyzer (RGA) measurements, together with density functional theory (DFT) provide mechanistic insight into each step of processing of the HfMAA system: post-application bake (PAB), 90 eV electron irradiation, and post-exposure bake (PEB). To understand the role of ligands on electron-induced chemistry, we added co-ligand to the HfMAA system -- hydroxybenzoic acid (HBA), and phenylacetic acid (PAA) -- and monitored the amount of alkyl CH produced after electron irradiation. We find that co-ligand films enhance crosslinking reactions, particularly for lower energy electrons (20eV). IR spectroscopy shows that similar amounts of CH are produced in the two systems, and analysis with RGA suggests that the ring radicals that are generated upon decarboxylation behave differently; we see the benzyl radical being released in the gas phase for PAA, while for HBA no phenyl radical is detected suggesting participation within the film.

2:00 PM *CM05.03.03
Reaction Processes by Electron-Orbital-Selective Excitation on Pt/SiO_x Interface Hidehiro Yasuda; Research Center for Ultra-High Voltage Electron Microscopy, Osaka University, Ibaraki, Japan.

When materials are atomic species-, site- or electronic orbital-selectively excited by photons with variable energy, bond breaking or reaction between specific atoms take place. It was confirmed in our group that a platinum silicide, Pt_2Si, was successfully formed at the platinum/silicon oxide interface kept at room temperature under 25–200 keV electron irradiation. This result shows that the reaction cannot be induced by simple thermal annealing under no-electron-irradiation conditions and takes place by bond breaking of Si-O and simultaneous bond formation of Si-Pt under electron irradiation. In the present study, the synthesis of platinum silicide at the platinum/silicon oxide interface by photo-excitation was investigated using synchrotron-radiation photo emission spectroscopy and transmission electron microscopy. After photo-excitation by 80 eV photons, valence band spectrum of silicon did not change, and remarkable changes were not recognized also in $Pt4f_{7/2}$ core level spectrum. On the other hand, in the case of photo-excitation by 140 eV photons, peak near the Si 3p level in the Si valence band spectrum shifts to higher energy, and a peak originating from Si3p-Pt5d bonds appears near the Fermi level. In $Pt4f_{7/2}$ core level spectrum, the peaks shift to higher energy by 1.2 eV and are similar to those which are obtained from Pt_2Si. These results indicate that valence band and $Pt4f_{7/2}$ core level spectra remarkably change during Pt2Si formation. As mentioned above, it was confirmed that Si 2p core level excitation plays an important role in Pt2Si silicide formation by reaction between silicon and platinum on Pt/SiO_x thin film interface, because the binding energy of Si 2p is approximately 99 eV. In order to produce Si-Pt bonds preferentially from Si-O-Pt bonds, simultaneous breaking of Si-O and O-Pt bonds and the consequent desorption of oxygen atoms and formation of Si-Pt bonds may be required by photo-excitation. It is suggested that a core level excitation mechanism related to the Knotek and Feibelman mechanism may play an important role in silicide formation within the solid.

2:30 PM CM05.03.04
Damage Efficiency of High-Energy Ions in Ultrathin Polymer Films Raquel S. Thomaz[1], Jean-Jacques Pireaux[3], Christina Trautmann[2] and Ricardo M. Papaleo[1]; [1]Catholic Univ of Rio Grande do Sul, Porto Alegre, Brazil; [2]Materials Research, GSI Helmholtz Centre, Darmstadt, Germany; [3]Université de Namur, Namur, Belgium.

In this contribution, we present recent results by our group aiming the investigation of the fundamental problem of damage efficiency of high-energy ions in polymers, under the spatial confinement conditions of ultrathin films. The identification and understanding of possible size-effects on the damage efficiency of energetic ions is crucial for several topics of interest, from radiation resistance and stability of nanomaterials and devices to biological damage at small scales. We followed the changes in radiation effects in two polymers (PMMA and PVC) as the thickness of supported films is systematically reduced from ~ 200 nm down to ~2nm to identify critical thicknesses below which the efficiency starts to deviate from bulk values. Two types of experiments were conducted using ions in an energy range from 2 MeV up to 2 GeV: one involving cratering produced by single ion impacts and another on measurements of bond-breaking rates, based on XPS spectroscopy investigations and average effects of high-fluence irradiations. Cratering efficiency decreases strongly with thickness below a critical size as large as 40nm in PMMA. Bond-breaking cross sections, in contrast, were insensitive to thickness reductions in both polymer films, even in layers as thin as 5nm. We will discuss why spatial confinement affects differently the damage efficiency of distinct types of effects, considering the degree of importance of long-range, cooperative effects of excited material along the ion tracks, and the changes in the radial profiles of deposited energy by secondary electrons in very thin layers.

2:45 PM CM05.03.05
Radiation Damage and Failure in Rubbers and Rubber Composites—Effect of Network Polydispersity Alireza Sarvestani[1, 2]; [1]Ohio University, Athens, Ohio, United States; [2]Mechanical Engineering, Mercer University, Macon, Georgia, United States.

Ionizing radiation is recognized as one of the major environmental factors affecting the performance, strength, and durability of polymeric compounds. However, the underlying mechanism by which radiation alters the internal structure of rubbers is not well understood. It is known that ionization initiates a variety of chemical reactions in polymers. Among others, crosslinking and scission are the most important effects that markedly change the mechanics and durability of elastomers. Depending upon the molecular structure of polymers and radiation intensity, the chains may either crosslink, with a resulting increase in the network modulus, or undergo rupture that leads to degradation and softening of the network. Scission is an oxidative process that presumably happens due to direct rearrangement of a backbone into two separate entities or loss of a side-group and consequent rearrangement. Crosslinking, on the other hand, in an abstraction process that occurs when two chains join and form a larger macromolecule. Hydrogen abstraction, for example, often takes place between two irradiated polymer chains providing a potential site for crosslinking between them. We developed a continuum micromechanical model that predicts the change in mechanical properties of (filled) elastomers subjected to high-energy radiation (e.g., gamma-rays, UV, or electron beams) and finite deformations. The model demonstrates that polydispersity in internal structure of rubber network controls the elasticity,

strength, and durability of rubbers subjected to irradiation. Accordingly, damage starts from scission of short strands and continues with radiation time, coupled with the magnitude of applied deformation.

3:00 PM BREAK

SESSION CM05.04: Thermal Property Changes Under Irradiation
Session Chairs: Kazuto Arakawa and Dorothy Duffy
Monday Afternoon, November 26, 2018
Hynes, Level 2, Room 202

3:30 PM CM05.04.01
The Effective Thermal Conductivity of U-10Mo Fuels with Fission (Xenon and Krypton) Gas Bubbles Present Rafi Iasir[1], Nickie J. Peters[2] and Karl D. Hammond[3]; [1]Nuclear Engineering Program, University of Missouri, Columbia, Missouri, United States; [2]University of Missouri Research Reactor Facility, Columbia, Missouri, United States; [3]Chemical Engineering, University of Missouri, Columbia, Missouri, United States.

Uranium alloyed with 10 wt% molybdenum (U-10Mo) is currently being developed as a potential high-density low-enrichment uranium (LEU) fuel for research nuclear reactors. Given the lower melting points of metals compared to ceramic fuels, control of the temperature—and therefore knowledge of the thermal conductivity—is important to reactor design and operation. Fission generates gas bubbles, metallic precipitates, and solutes in the fuel matrix which can change the thermal conductivity and cause swelling of the fuel. We studied the impact of distributed fission gas bubbles on the effective thermal conductivity of irradiated U-10Mo fuel using a two-dimensional finite element method (FEM). The effective thermal conductivity of the materials is calculated by solving the heat equation on a two-dimensional domain and estimating the mean temperature and heat flux. The effects of both intra- and inter-granular fission gas bubbles are discussed. A distribution representative of a gas bubble superlattice is used as a model of intra-granular bubbles, compared to less-uniform bubble arrangements. For inter-granular bubbles, the bubbles' spatial and size distributions were estimated from a two-dimensional scanning electron microscopy (SEM) image of fission gas bubbles that had collected on grain boundaries. The obtained results are compared with theoretical models and experimental results. The results show that the pressure inside the bubbles has minimal influence on the overall conductivity. The overall conductivity of a xenon–krypton mixture typical of fission gas is also negligibly different than that of pure xenon. Bubble arrangement is also insignificant unless a relatively wide bubble-free path through the metal exists. However, the area fraction of xenon bubbles has a significant impact on the overall thermal conductivity.

3:45 PM *CM05.04.02
Simulating Electronically-Driven Structural Dynamics in Silicon with Two-Temperature Molecular Dynamics and Electronic Temperature Dependent Forcefields Robert Darkins[1], Pui-Wai Ma[3], Samuel Murphy[2] and Dorothy Duffy[4]; [1]Dept. of Physics and London Centre for Nanotechnology, University College London, London, United Kingdom; [2]Department of Engineering, Lancaster University, Lancaster, United Kingdom; [3]Culham Centre for Fusion Energy, Abingdon, United Kingdom.

The structural evolution of materials following ultrafast laser irradiation is generally classified by two distinct regimes. At relatively low fluences thermal processes dominate, as energy transferred to the ions via electron-phonon coupling results in melting on thermal timescales. In contrast, at high fluences the dynamics are dominated by non-thermal processes. These processes drive the electrons out of thermal equilibrium with the nuclei, producing hot, transient electronic states that modify the interatomic potential energy surface. Such non-thermal processes can induce melting on sub picosecond timescales.
Two temperature molecular dynamics (2T-MD) has proved to be a very successful methodology[1] for modelling the low fluence regime, with excellent agreement between modelling and ultrafast electron diffraction experiments.[2] The modifications to the potential energy surface induced by high fluences have,however, proved more challenging for classical simulations. Such effects can be included in 2T-MD by the development of electronic temperature dependent forcefields that capture the dynamic effects of the modifications of the potential energy surface due to the electronic excitations.[3] However, as the potential energy surface changes dynamically during such simulations, care must be taken to ensure energy conservation.
We have developed a rigorous formulation of two-temperature molecular dynamics that ensures energy conservation in simulations that employ electronic-temperature-dependent forcefields.[4] We have also developed an electronic-temperature-dependent forcefield for silicon that faithfully reproduces the ab initio-derived thermodynamics of the diamond phase for high electronic temperatures, as well the structural dynamics observed experimentally under highly nonequilibrium conditions. We will present the details of the modelling methods, the electronic temperature dependent forcefield and the calculated atomistic dynamics of laser irradiated silicon films.

1. Z.B. Lin and L.V. Zhigilei Time-resolved diffraction profiles and atomic dynamics in short-pulse laser-induced structural transformations: Molecular dynamics study, Phys. Rev B 73, 184113, 2006
2. Y. Giret, N. Naruse, S. L. Daraszewicz, Y. Murooka, J. Yang, D. M. Duffy, A. L. Shluger, and K. Tanimura, Determination of transient atomic structure of laser-excited materials from time-resolved diffraction data, Appl. Phys, Lett. 103, 253107, 2013
3. S. T. Murphy,S . L. Daraszewicz, Y. Giret, M. Watkins, A. L. Shluger, K. Tanimura and D. M. Duffy Dynamical simulations of an electronically induced solid-solid phase transformation in tungsten, Phys., Rev, 92, 134110, 2015
4. R. Darkins, P.W. Ma, S.T. Murphy and D.M. Duffy, Simulating electronically-driven structural changes in silicon with two-temperature molecular dynamics , under review

4:15 PM CM05.04.03
Nanohillock Chain Formation under Grazing Angle SHI Irradiation by Molecular Dynamics Simulations Henrique Vazquez Muinos[1], M. Schleberger[2] and Flyura Djurabekova[1]; [1]University of Helsinki, Helsinki, Finland; [2]University of Duisburg-Essen, Duisburg-Essen, Germany.

It was shown previously that in layered crystals such as SrTiO3 or Mica, SHI irradiation under grazing incidence can produce chains of hillocks/grooves on the surface of the material [1-3]. These structures could be explained by the fact that at a small angle incidence, the ions travel long distances through high or low electron density pockets, giving rise to higher or lower local stopping power along the ion trajectory [1]. This hypothesis assumes that the electronic thermal conductivity does not wash away the inhomogenities of the local energy deposition before it is trasfered to the lattice, allowing the formation of the nanohillocks due to local melting. We develop a new approach to simulate SHI grazing incidence irradiation and apply it to verify the aforementioned hypothesis.
The new approach calculates the energy locally deposited by the ion based on the electronic density along the trajectory using CasP code and simulates the electronic energy redistribution and transfer to the lattice according to the two-temperature model. This energy is added to the atoms and simulated with

Molecular Dynamics (MD), producing structural changes in the material such as hillocks or grooves.
Simulations in SrTiO3 shows that low anlge irradiation produces strongly modulated electronic energy deposition along the ion track and that the electronic thermal conductivity is not capable of washing away the initial temperature inhomogenities. As a result, regions with higher energy deposition show stronger melting and give rise to nanohillocks. The simulated hillocks have similar length, interdistance and height as in the experiments and shows dependence on the irradiation angle and crystal structure. The hillocks and grooves observed on the surface are associated with molten and sublimated material, respectively.
This new method allows for the first time to simulate grazing anlge SHI irradiation realistically, taking into account the modulation of the stopping power due to the local electron density. The good agreement with experiments not only shows that the proposed method is capable of describing correctly the low angle SHI irradiation, but also strongly supports the hypothesis that the hillock chains form due to the varying local electron density along the ion track.

-[1] Akcöltekin, Ender, et al., Nature Nanotechnology 2.5 (2007): 290-294.
-[2] Gruber, Elisabeth, et al., Journal of Physics: Condensed Matter 28.40 (2016): 405001.
-[3] Aumayr, Friedrich, et al., Journal of Physics: Condensed Matter 23.39 (2011): 393001

4:30 PM CM05.04.04
Nanoscale Thermal Transport in Ion Irradiated Sapphire—Picosecond Time Domain Thermoreflectance Baurzhan Muminov[1, 2], Azat Abdullaev[1], Darkhan Alimzhanov[1], Jacques O'Connell[3], Vladimir Skuratov[4] and Zhandos Utegulov[1]; [1]Department of Physics, School of Science and Technology, Nazarbayev University, Astana, Kazakhstan; [2]Department of Mechanical Engineering, University of California, Riverside, Riverside, California, United States; [3]Centre for HRTEM, Nelson Mandela University, Port Elizabeth, South Africa; [4]Flerov Laboratory of Nuclear Reactions, Joint Institute for Nuclear Research, Dubna, Russian Federation.

Sapphire (α-Al_2O_3) is radiation resistive candidate inert matrix fuel host material for fission reactors, as well as for fusion reactors and for space station applications. The control of radiation-induced thermal conductivity degradation is a critical issue for nuclear and fusion reactor system design and validation.
We have studied nanoscale thermal conductivity *k* degradation in sapphire single crystals as a result of swift heavy ion (Xe, 167 MeV, ion fluence range 10^{12} – 10^{14} cm^{-2}) and slow light (He, 40 keV, 10^{15} cm^{-2}) ion irradiation. Cross-plane near-surface thermal transport measurements made by an ultrafast optical pump-probe technique called picosecond time domain thermo-reflectance (TDTR) [1, 2] were found to be in satisfactory agreement with semi-analytical thermal conduction modeling. The decay in through-plane *k* at high modulation frequencies in swift heavy ion (SHI) irradiated Al_2O_3 demonstrates a complex interplay between heat penetration depth, phonon mean free paths, spatial extent of SHI-induced latent tracks [3], and amorphization [4].
We demonstrate that TDTR is critical for the analysis of SHI-irradiated sapphire, especially at higher doses, even if virgin sapphire does not demonstrate modulation frequency-dependent thermal conductivity. We also establish using modulation frequency-dependent TDTR that variation in *k* across slow light ion (SLI) irradiated/virgin subsurface sapphire regions can be spatially profiled on the scale of hundreds of nanometers. Comparing the effects of SHI and SLI irradiations on thermal conductivity of sapphire, we conclude that SLIs tend to impart less damage to the structure and cause less decay of thermal transport even at high ion doses than HSIs do.
Funding by MES RK research grant (AP05130446) and state-targeted program (BR05236454) is acknowledged.

References:
[1] D. G. Cahill, Rev. Sci. Instrum. 75, 5119, (2004)
[2] R. Cheaito, C. S. Gorham, A. Misra, K. Hattar, P. E. Hopkins, J. Mater. Res., 30(9), 1403-1412, (2015)
[3] V.A. Skuratov, J. H.O'Connel,N.S.Kirilkin, J.Neethling, Nucl. Instr. Meth. B 326, 223–227, (2014)
[4] C. Grygiel, F, poisyt, M. Sall, H. Lebius, E. Balanzat, T. Madi, T. Been, D. Mairie, I. Monnet, Acta Materialia, 140, 157-167, (2017)

4:45 PM CM05.04.05
Uncertainty Quantification and Validation of Multiscale Models of the Effective Thermal Conductivity of UO_2 during Reactor Operation Michael R. Tonks[1], Jie Lian[2], Marina Sessim[1] and Xueyang Wu[1]; [1]University of Florida, Gainesville, Florida, United States; [2]Rensselaer Polytechnic Institute, Troy, New York, United States.

The microstructure of UO_2 changes significantly during reactor operation, including the generation of point defects, defect clusters, fission product formation, and more. These microstructure changes cause the thermal conductivity of UO_2, which is already low, to decrease even further. As part of the US Nuclear Energy Advanced Modeling and Simulation program, multiscale modeling and simulation have been used to develop a model of the thermal conductivity of UO_2 that is a function of the fuel microstructure. While this model has been shown to perform well in fuel performance simulations, further validation is needed. In this project we perform uncertainty quantification on both the mesoscale and macroscale thermal conductivity models. We then compare the predicted thermal conductivity distribution to the measured thermal conductivity of UO_2 samples fabricated to have various microstructures.

SESSION CM05.05: Multiscale Simulation and Characterization of Radiation Damage
Session Chairs: Chu Chun Fu and Thomas Schuler
Tuesday Morning, November 27, 2018
Hynes, Level 2, Room 202

8:30 AM *CM05.05.01
Strategies for Optimal Construction of Markov Chain Representations of Atomistic Dynamics and Their Application to Irradiated Materials Danny Perez and Thomas Swinburne; Los Alamos National Laboratory, Los Alamos, New Mexico, United States.

A common way of representing the long-time dynamics of materials is in terms of a Markov chain that specifies the transition rates for transitions between metastable states. Such chains can either be analyzed directly, used to generate trajectories using kinetic Monte Carlo, or upscaled into mesoscale models such as cluster dynamics. While a number of approaches have been proposed to infer such a representation from direct molecular dynamics (MD) simulations, challenges remain. For example, as chains inferred from a finite amount of MD will in general be incomplete, quantifying their completeness and propagating these uncertainties to observables of interest is extremely desirable. In addition, making the construction of the chain as computationally affordable as possible is paramount. In this work, we simultaneously address these two questions. We first quantify the local completeness of the chain in terms of Bayesian estimators of the yet-unobserved rate, and its global completeness in terms of the residence time of trajectories within the explored

subspace. We then systematically reduce the cost of creating the chain by leveraging an accelerated MD method, namely Temperature Accelerated Dynamics. We maximize the increase in residence time against the distribution of states in which additional MD is needed and the temperature at which these are respectively carried out. Using examples of defects that are relevant to the evolution of irradiated materials, we demonstrate that our approach is an efficient, fully automated, and massively-parallel scheme to efficiently explore the long-time behavior of materials.

9:00 AM CM05.05.02
Electronic Effects in Self-Ion Irradiated Tungsten—From *Ab Initio* to Experiment Andrea Sand[1], Rafi Ullah[2, 4], Kai H. Nordlund[1] and Alfredo A. Correa[3]; [1]Department of Physics, University of Helsinki, Helsinki, Finland; [2]CIC nanoGUNE, Donostia-San Sebastián, Spain; [3]Quantum Simulations Group, Lawrence Livermore National Laboratory, Livermore, California, United States; [4]Departamento de Fisica de Materiales, UPV/EHU, Donostia-San Sebastián, Spain.

Primary radiation damage formation from collision cascades has been simulated with molecular dynamics methods for several decades, yet despite early understanding that electronic effects may be significant in the highly non-equilibrium processes, such effects have proved difficult to incorporate into atomistic cascade simulations.

State-of-the-art cascade simulations now routinely include the energy losses caused by electronic stopping, but this is generally implemented through the use of a non-local friction term, with a cut-off velocity below which the stopping is considered negligible, and hence disregarded. However, in energetic cascades, the atoms with threshold velocities number in the thousands, and as a result the total energy losses change significantly with small changes in the cut-off value. We demonstrate the sensitivity of predictions of the primary damage to the choice of this essentially non-physical threshold parameter. Direct comparisons to *in-situ* ion irradiation and ion beam mixing experiments can be used to guide simulation methods, and we show that it is possible to find agreement for a number of cases. However, such comparisons are not possible in all materials, due to either a lack of reliable experimental data, or to the fundamental limitations of observing very small defects directly in an electron microscope. Hence there is a need to improve the treatment of electronic effects in molecular dynamics in order to increase the predictive capacity of cascade simulations.

A model for including electron-ion interactions without the use of a threshold, under a unified framework over the whole energy range relevant to cascade dynamics, has been suggested [A. Caro and M. Victoria, Phys. Rev. A **40** (1989)], but only recently implemented by Tamm and Correa [https://github.com/LLNL/USER-EPH] with a parametrization for nickel. The model describes both the electronic stopping in the high-energy regime, and electron-phonon coupling in the low-energy regime, with the magnitude of the coupling varying due to the local electronic density experienced by the ion. As a first step towards realizing such a model in the fusion-relevant material tungsten (W), we have performed real-time time dependent density functional theory (TDDFT) calculations of the energy losses of a W projectile in W. We show by direct comparison to experimental ion implantation ranges that the electronic stopping obtained in the <100> channel, predicted by TDDFT to be only a third of the value given by SRIM, is in fact in very good quantitative agreement with experimental values. These results provide evidence of the validity of the TDDFT method even for the heavy ion W, and open the way for constructing an electron density-dependent model of the electron-ion interaction for cascade simulations in W.

9:15 AM *CM05.05.03
Kinetics of Point Defects Under Irradiation—From Atomic to Cluster Scales Thomas Schuler[1], Luca Messina[2, 1], Maylise Nastar[1], Pascal Bellon[3], Robert S. Averback[3] and Dallas Trinkle[3]; [1]SRMP, CEA Saclay, Saclay, France; [2]KTH, Stockholm, Sweden; [3]MatSE, University of Illinois at Urbana-Champaign, Urbana, Illinois, United States.

Materials under irradiation experience an engaging competition between interrelated kinetic phenomena, namely the point defect creation rate and the long range diffusion, precipitation and elimination of atoms and defects. The modeling of such competition is hindered by the largely different time scales involved, hence requiring a multi-scale approach. We developed KineCluE, an open-source code that allows for computing cluster transport coefficients from atomic jump frequencies. These cluster transport coefficients—along with other parameters such as dissociation rates—can then be used as input parameters to cluster-based models such as cluster dynamics or object kinetic Monte Carlo to simulate micro-structure and point defect evolution over long timescales with accurate cluster kinetics. We employed this methodology to study and quantify the time-dependent effect of dilute solute additions on the fraction of inter-cascade recombined point defects. We found that point defect-solute flux coupling leads to a critical irradiation dose above which the solute effect vanishes, which was already observed experimentally. From this insight, we devised a general methodology to identify candidate solutes which increase point defect recombination under irradiation over extended periods of time. KineCluE also allows to take into account the effect of temperature, local strain, concentration and ballistic mixing on cluster kinetic properties. Some of these features will be presented in this talk.

9:45 AM BREAK

SESSION CM05.06: New Methods of Radiation Damage Characterization
Session Chairs: Chu Chun Fu and Kai Nordlund
Tuesday Morning, November 27, 2018
Hynes, Level 2, Room 202

10:15 AM *CM05.06.01
Monitoring Microstructural Evolution in Metals with Nonlinear Ultrasound—Applications to Radiation-Induced Embrittlement Kathryn H. Matlack; University of Illinois at Urbana-Champaign, Urbana, Illinois, United States.

Material damage in structural components is driven by nano- and micro-structural evolution that occurs at small length scales and begins early in component life. In metals, these defects are known to cause measurable changes in the acoustic nonlinearity parameter. Physically, the interaction of an ultrasonic wave with nano- and micro-structural defects such as dislocations, precipitates, and micro-cracks, generates a second harmonic wave that is proportional to the acoustic nonlinearity parameter, an absolute and measurable material parameter. The acoustic nonlinearity parameter changes as the nano- and micro-structural features evolve in the material. Thus, through nonlinear ultrasound (NLU) measurements of the generated second harmonic wave, we can relate the ultrasonic signal to defect features. Recent research has shown that NLU is sensitive to microstructural changes due to radiation embrittlement in reactor pressure vessel (RPV) steels, precipitation in stainless steels due to thermal aging, fatigue damage in various metals, and stress corrosion cracking in steels, among many other examples. This talk will discuss how nonlinear ultrasonic techniques can be used as a nondestructive evaluation tool to monitor nano- and micro-scale defects and thus early-stage damage. It will focus on monitoring neutron radiation-induced embrittlement

in nuclear reactor steels and model components, in particular on experimental results of RPV samples with variations in neutron fluence levels, irradiation temperatures, material composition, and annealing. Opportunities for combining techniques for multi-scale detection, for using NLU for other material platforms and damage mechanisms, as well as using radiation-induced microstructural changes as a platform to study interactions between NLU and defects will be discussed.

10:45 AM CM05.06.02
Advanced Characterization of Irradiated Fuels and Materials at INL Jian Gan; Idaho National Laboratory, Idaho Falls, Idaho, United States.

Advanced characterization of the irradiated fuels and materials is crucial to help understanding the material and fuel property changes under irradiation. Microstructural defect evolution down to nanometer scale could strongly affect the material and fuel performance on macroscale. Radiation-induced material degradation include dimensional instability, hardening and embrittlement, intergranular cracking, radiation-enhanced chemical interaction at the interfaces and breakaway swelling. To mitigate the radiation damage, advanced characterization on irradiated microstructure, microchemistry, micromechanical property and local thermal property is necessary to identify the controlling mechanisms that are responsible to the degradations.

This presentation provides a summary of the advanced characterization capabilities at the Irradiation Materials Characterization Laboratory (IMCL), Materials and Fuels Complex (MFC), Idaho National Laboratory (INL). It highlights the recently established capabilities including shield sample preparation area (SSPA), shield confinement cells for two focused ion beam (FIB) systems, a shielded electron probe microanalysis (EPMA), the thermal property microscopy (TPM) along with non-shielded instruments like scanning electron microscopy (SEM), X-ray diffractometer, and transmission electron microscopy (TEM). Some examples on advanced characterizations on irradiated structural materials and fuels will be presented. It demonstrates the power of combining sample preparation of highly radioactive materials with the advanced characterization down to atomic resolutions within one facility.

11:00 AM *CM05.06.03
Possibility of Materials Modification by Dark Matter Particle Irradiation Kai H. Nordlund[1], Flyura Djurabekova[1], Andrea E. Sand[1] and Nader Mirabolfathi[2]; [1]University of Helsinki, Helsinki, Finland; [2]Department of Physics and Astronomy, Texas A&M University, College Station, Texas, United States.

Many astrophysical observations indicate that standard model particles compose only 5% of the matter in the universe. Understanding the nature of dark matter and dark energy, the remaining 85%, is of fundamental importance to cosmology, astrophysics, and high energy particle physics. There are a number of attempts for
direct detection of dark matter particles via an elastic interaction with detector nuclei. Astronomical observations indicate that dark matter forms a halo around our galaxy that is static or rotating much slower than the stars. Since our sun rotates around the center of the galaxy at a speed of 220 km/s, dark matter particles would, if they do interact with ordinary matter, give a momentum corresponding to this velocity to ordinary matter nuclei. Assuming dark matter particle masses of the order of 1 GeV/c^2, this would correspond to recoil energies of a few 100 eV, a typical ion irradiation energy. To date, the detectors developed could detect dark matter particles with masses > 10 GeV/c^2. In our recent work [1], we showed that potential dark matter particles in the mass range down to 200 MeV/c^2 could be detected by new kinds of single-electron resolution single crystal semiconductor detectors. The detector response can be calibrated with molecular dynamics simulations of low-energy self-recoils in the material. Moreover, since the threshold displacement energy depends on crystal direction, while the dark matter particles do not follow Earths rotation around its axis, the response of a single crystal detector should vary with the time of day. In this work, we used classical and time-dependent density functional theory molecular dynamics to calculate the response of the semiconductor detectors to dark matter recoils as a function of crystal direction, and using an analytical model translated this into a dependence of the signal on the time of the day. The diurnal variation could be a major benefit for distinguishing a dark matter particle signal from that of conventional particle physics standard model particles.

[1] F. Kadribasic, N. Mirabolfathi, K. Nordlund, A. E. Sand, E. Holmström, and F. Djurabekova, Phys. Rev. Lett 120, 111301 (2018)

11:30 AM CM05.06.04
3D-MEIS and Synchrotron XRD for Compositional and Structural Characterizations of Ion Implanted Si Fin-Shaped FDSOI Nanostructures, for the sub-22 nm Technological Nodes—3D *X*-MEIS Lucien W. Penlap Woguia[3], Denis Jalabert[1], Pierre François[3], Dario F. Sanchez[2], Samuel Tardif[1], Joel Eymery[1], François Rieutord[1], Frédéric Mazen[3] and Jean-Paul Barnes[3]; [1]Univ Grenoble Alpes, CEA, INAC-MEM,LEMMA, Grenoble, France; [2]Paul Scherrer Institut (PSI), SLS, microXAS, Villigen, Switzerland; [3]Univ Grenoble Alpes, CEA, LETI, Grenoble, France.

The miniaturization of integrated circuits (ICs) pushes the actors from the microelectronic industry towards the use of 3D architectures (e.g. FinFETs) and ultra-shallow junctions (USJs) for sub-22 nm nodes [1]. Doping must now be controlled in 3-D architectures and for this we need powerful characterization techniques capable of the depth profiling both implant induced damage and dopant concentration.

In this work, we prove the capability of the medium energy ion scattering (MEIS) technique to in-depth profile and quantify the implants inside the Fins, thanks to its excellent depth resolution (0.25 nm at the surface) and 3D simulations[3]. Even though the low lateral resolution of the beam does not allow the investigation of structures with much smaller dimensions, we overcame this challenge by developing suitable analysis protocols on arrays of Fins. We have discriminated the double contribution of the dopants, highlighted their profiles and the implanted doses at each individual part of the Fins. These simulations are possible using PowerMEIS, a unique software developed for 3D-MEIS[5] by our collaborators from UFRGS[4]. The methods adopted for inserting or into the samples studied in this project were plasma immersion ion implantation (PIII) and beamline (BL). The FDSOI 3D-patterns were obtained by e-beam lithography on SOI wafers. If MEIS can accurately probe defects in 2D FDSOI structures[2], it is however, not yet possible to do it within the Fins, which is crucial for the recrystallization processes for instance.

Grazing incidence x-ray diffraction (GIXRD) using an ESRF photon source was employed to investigate the impact of the two implantation methods in the crystal beneath the 3D implanted areas. The measurement of the reflexions at Q= (000) and Q= (220) allowed us to access, through modelling [6], to information regarding the shape, dimensions and damaged regions of the Fins. There were good agreements between MEIS, XRD and TEM regarding these parameters, since we need them to model the structure matrix for PowerMEIS simulations. Furthermore, GIXRD analyses provided information concerning the thicknesses of the damaged parts of the Fins and the dimensions of the crystalline areas at the Fin core. The correlation of the XRD and MEIS techniques allowed us to compare which method causes more implantation induced strain in the 3D line grating, as we did for 2D-FDSOI structures [2].

This work was performed on the Nano Characterization Plat-Form (PFNC)-CEA-LETI.

We are thankful to the Microscopy & ESRF-BM32 teams, Dario F. Sanchez (PSI) and Gabriel Marmitt (UFRGS)

[1] Van Den Berg et al., J. Vac. Sci. Technol. May/Jun 2000
[2] Lucien Penlap *et al*., '*Structural defects analyses in 2D-FDSOI nanostructures ion implanted with As.*' (To be published)
[3] Lucien Penlap et al., IUVSTA 2017
[4] Sortica, M. A. *et al.* http://dx.doi.org/10.1063/1.3266139
[5] D. F. Sanchez *et al*., http://dx.doi.org/10.1038/srep03414.
[6] T. Baumbach et al, J. Phys. Appl. (1999),

11:45 AM CM05.06.05
Towards High Throughput Quantification of Extended Irradiation Defects via Advanced-STEM-Based Machine Learning Yuanyuan Zhu[1], Brian Hutchinson[2], Graham Roberts[2], Simon Haile[2], Colin Ophus[3], Mychailo Toloczko[1] and Danny Edwards[1]; [1]Pacific Northwest National Lab, Richland, Washington, United States; [2]Western Washington University, Bellingham, Washington, United States; [3] Lawrence Berkeley National Laboratory, Berkeley, California, United States.

Transmission electron microscopy (TEM) is one of the most common characterization tools in the study of irradiation damage in nuclear materials. However, the effort to obtain statistically meaningful quantification of a variety types of extended irradiation defects, such as dislocation lines and loops, voids and bubbles, and various types of precipitates, is a labor-intensive and time-consuming task. In this work, we developed a (deep) convolutional neural network (CNN) model for recognition of extended irradiation defects, based on optimized TEM data.
Like most image processing methods, the quality of the input images governs the outcome of the feature classification. Additionally, for supervised CNN training typically used in image segmentation, the fidelity of the ground truth label determines the best achievable accuracy. To pave the way for reliable feature recognition, we first established an advanced diffraction contrast imaging scanning transmission electron microscopy (DCI STEM) technique capable of recording defect images with high clarity, free of bend contour artifacts. Based on these high-quality DCI STEM images, pixelwise CNN models were trained to segment three types of typical irradiation defects, dislocations, voids and precipitates, in a neutron-irradiated HT-9 ferritic/martensitic alloy as an example. Several CNN architectures, including a simple model, a VGG-based model and DenseNet modified versions of the two, were tested and evaluated for performance. To alleviate overfitting, we used a combination of data augmentation, batch normalization, Dropout and L2 regularization. The above CNN architectures were firstly trained using 100 random configurations of hyperparameters governing the learning behavior of the networks, and then these hyperparameters were further tuned by Bayesian optimization. This combined effort of improving image quality and automating feature classification offers a path forward to the high-throughput irradiation defects quantification needed for reactor lifetime prediction and more efficient alloy development.
This research is funded by the U.S. Department of Energy Office of Nuclear Energy's Nuclear Energy Enabling Technologies program project CFA 16-10570, Office of Fusion Energy Sciences under contract DE-AC05-76RL01830, and by the Molecular Foundry which is supported by the Office of Basic Energy Sciences, under Contract No. DE-AC02-05CH11231.

SESSION CM05.07: Mechanical Properties and Stresses Under Irradiation
Session Chairs: Pär Olsson and Hiroyasu Tanigawa
Tuesday Afternoon, November 27, 2018
Hynes, Level 2, Room 202

1:30 PM *CM05.07.01
Macroscopic Stresses and Strains Produced by Microscopic Radiation Defects in Reactor Components Sergei Dudarev[1, 2], Daniel Mason[1], Edmund Tarleton[2], Pui-Wai Ma[1, 3] and Andrea E. Sand[4]; [1]UK Atomic Energy Authority, Abingdon, United Kingdom; [2]Department of Materials, University of Oxford, Oxford, United Kingdom; [3]Department of Engineering, University of Oxford, Oxford, United Kingdom; [4]Department of Physics, University of Helsinki, Helsinki, Finland.

Predicting macroscopic strains, stresses and swelling in power plant components exposed to irradiation from the observed or computed defect and dislocation microstructure is a fundamental problem of fusion power plant design that has so far eluded a practical solution. We have discovered that the problem can be addressed and solved using the fact that elasticity equations involve no characteristic spatial scale and hence admit a mathematical treatment that is an extension to that developed for the evaluation of elastic fields of defects on the nanoscale. Strains, stresses and swelling can be determined using either the integral equation formalism where the source functions are defined by the density of relaxation volumes of defects, or they can be evaluated from the condition of elastic equilibrium with body forces computed from gradients of the density of defect relaxation volumes. We explore exact solutions of elasticity equations and also develop a general finite element method (FEM) implementation, applicable to a broad range of predictive simulations of strains and stresses induced by irradiation in materials and components of any geometry in fission or fusion nuclear power plants.

2:00 PM CM05.07.02
Microstructural and Micromechanical Investigation of Irradiation Effects in Beryllium Viacheslav Kuksenko[2, 1], Chris Densham[3], Patrick Hurh[4] and Steve Roberts[2]; [1]UK Atomic Energy Authority, Abingdon, United Kingdom; [2]University of Oxford, Oxford, United Kingdom; [3]Rutherford Appleton Laboratory, Dedcot, United Kingdom; [4]Fermi National Accelerator Laboratory, Batavia, Illinois, United States.

Beryllium is an essential material for reflectors and moderators in material testing nuclear reactors, plasma facing and neutron multiplier material for fusion reactor designs (ITER, DEMO), candidate material for target components in near-future multi-megawatt accelerator particle sources (LBNF), and it is under extensive investigation by fission, fusion reactors and proton accelerator facilities communities. Current work reports experimental results obtained on the beryllium sample irradiated at Fermi National Accelerator Laboratory, USA, by 120GeV protons over 7 years at about 50°C up to 0.5 dpa, and beryllium samples implanted with He ions at 50 and 200°C.
The microstructure was investigated by SEM/EBSD, STEM/EDX and Atom Probe Tomography, and irradiation induced hardening was measured by nanoindentation experiments.
Microstructural investigations revealed a highly inhomogeneous distribution of impurity elements in both unirradiated and irradiated conditions. Impurities were mainly localized in precipitates, and as segregations at grain boundary and dislocation lines. Low levels of Fe, Cu, Ni, C and O were also found to be homogeneously distributed in the beryllium matrix in non-irradiated state and after proton irradiation. In the proton irradiated beryllium, up to 440 appm of Li, derived from transmutation, was homogeneously distributed in solution in matrix.
Extremely high variation of nanoindentation hardness data was observed for grains with different crystallographic orientation in non-irradiated areas of the

beryllium sample. After irradiation, the average hardness was increased, while anisotropy of hardness was decreased.
Significant effect of irradiation on fracture properties of beryllium was noticed. The proton irradiated sample was deformed during the post-irradiation handling. Investigation of the produced cracks indicates that proton irradiation at 0.3 dpa level changes the fracture mode from transgranular cleavage to predominantly grain-boundary cracking. In the He implanted samples, microcantilevers were fabricated by focused ion beam milling and loaded via a conventional nanoindenter. Cantilevers were pre-notched so that the fracture properties of grain boundaries and basal cleavage plane, in both as-received and irradiated states, can be compared. Fracture load of both grain boundary and cleavage cantilevers increased significantly after irradiation. Deflection to fracture was found to be lower for cantilevers pre-notched in the basal cleavage plane, but the difference between two types of cantilevers was smaller in the irradiated state. The possible mechanisms of this behavior will be analyzed in combination with local properties data deduced via nanoindentation experiments and the observed microstructural changes.

2:15 PM *CM05.07.03
Tensile Deformation and Fracture Mechanism of Irradiated RAFM Steel Hiroyasu Tanigawa[1], Masami Ando[1], Yutai Katoh[2], Naoyuki Hashimoto[3] and Takuya Nagasaka[4]; [1]National Institutes for Quantum and Radiological Science and Technology, Rokkasho, Japan; [2]Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States; [3]Hokkaido University, Sapporo, Japan; [4]National Institute for Fusion Science, Toki, Japan.

Reduced-activation ferritic/martensitic steels (RAFMs), such as F82H (Fe-8Cr-2W-0.2V-0.04Ta), has been developed as the structural material of fusion in-vessel components which will suffer from high dose irradiation of 14 MeV fusion neutron. The most concerned issue of RAFM steel is hardening and embrittlement which appears as the loss of plasticity and ductile-brittle transition temperature (DBTT) shift by low-temperature irradiation below 350 degrees C. The mechanistic understandings of the phenomena are essential for the prediction of those irradiation induced mechanical property changes, and the impacts of microstructure feature changes have been investigated.
RAFM steels are fully tempered martensitic steels which have microstructures contain prior-austenitic grain (PAG) boundaries and MX precipitates which formed during normalization, martensite packet, block, and lath boundaries which formed during cooling, and $M_{23}C_6$ which formed during tempering. High-density dislocation in the matrix and fine precipitates on various boundaries gives the steel high irradiation and heat resistance. It has been reported that the major microstructural feature of RAFM steels irradiated at low temperatures is dislocation loop formation and evolution. However, this dislocation-loop evolution is not enough to explain hardening level which was observed in irradiated RAFM based on the Orowan equation.
In this study, the impact of three-dimensional morphology of martensite blocks, which is the minimum microstructural unit corresponds to the mechanical property, are discussed to investigate the deformation and fracture mechanism of irradiated RAFM steels. The three-dimensional SEM and EBSP analyses on tensile deformed unirradiated F82H, micro-tensile test on a single block in FIB, and TEM microstructural analyses on irradiated F82H are conducted. The impact of material mechanics on the tensile property, such as stress triaxiality, is discussed to interact the observed mechanical property and microstructure.

2:45 PM CM05.07.04
Micromechanical Study of Radiation and Temperature Effects on Localized Properties of SiC-SiC Fiber Composites Yevhen Zayachuk[1], David E. Armstrong[1], Arthur Hussey[1], Christian Deck[2] and Peter Hosemann[3]; [1]University of Oxford, Oxford, United Kingdom; [2]General Atomics, San Diego, California, United States; [3]University of California, Berkeley, Berkeley, California, United States.

Silicon carbide ceramics is a candidate material for the use in novel accident tolerant fuel (ATF) cladding designs. It is suggested to be used in the form of SiC-fiber reinforced SiC-matrix composite, and therefore in order to reliably predict behavior of fuel cladding it is necessary to understand mechanical properties of the individual constituents of the composite – matrix, fibers and, crucially, interphases, as well as how they are modified by radiation fields and elevated temperatures that fuel cladding is exposed to during the reactor's operation.

Micromechanical techniques are uniquely suited for determination of such localized properties, which can be rationalized by coupling the mechanical data and the microstructural information obtained by microscopy tools. In this contribution we present the results of the microcantilever fracture (at the interphases, within fibers and in the bulk matrix), fiber push-out and nanoindentation tests on SiC-SiC fiber composite. Samples were irradiated with Si and Ne ions up to 3.9 dpa at the temperatures of up to 750°C. Micromechanical tests were performed in the temperature range of up to 700°C.

Microstructure was investigated using transmission electron microscopy (TEM), with texture information obtained with transmission Kikuchi diffraction (TKD). It was found that in the matrix the preferred grain growth direction is <111>, while in the fibers no texture was observed. Both matrix and fiber feature extensive twinning.

Hardness of matrix and fibers, as measured by nanoindentation, didn't noticeably change as a function of dose, indicating that radiation damage in bulk SiC is minor. At the same time, cantilever testing indicated that the fracture strength of the interphase noticeably increased with the increase of dose, indicating that pyrolytic carbon that forms an interlayer is strongly affected by irradiation. On the other hand, measurements at elevated temperatures showed that the properties of matrix material significantly change with temperature – hardness decreases from ~45 GPa at room temperature to ~25 GPa at 700°C, and fracture strength decreases from ~22 GPa to ~12 GPa.

TEM was used for imaging of the crack paths in the cantilevers after fracture. It was found that in the matrix fracture is transgranular, while at the interphases it is following the fiber-interlayer boundary.

Fiber push-out measurements showed that there is a significant difference in the interfacial shear strength of the interphases, depending on where within a bundle the tested fiber is – changing from ~120 MPa at the periphery of a bundle to ~70 MPa in the center.

Experimental findings are discussed with the emphasis on the synergy of micromechanical and microstructural characterization, and how these enable better understanding and prediction of the properties of SiC fiber composites in advanced fission and fusion designs.

3:00 PM BREAK

3:30 PM CM05.08.01
Electrical Characterization of He-Ion Irradiated Pd/*n*-SiGe Schottky Diode Mamor Mohammed; Département de Physique, University Cadi Ayyad, Faculté Polydisciplinaire Safi, Safi, Morocco.

There has been considerable interest in integrating high speed and novel devices made from $Si_{1-x}Ge_x$ materials, since the alloy is compatible with the silicon based technology. Ion implantation is now a common process in the mature semiconductor industry and is widely used during several electronic devices fabrication steps. In particular, ion implantation is used to improve the fast switches and the performance of photodiodes.
Moreover, it is well known that ion implantation into semiconductor materials has a profound influence on the structural and electronics properties of their surface and subsurface region. The ion implantation induces structural and electronic changes, which governs the characteristics of metal contacts formed on the semiconductor. In this presentation, we report on the electronic properties of He-ion irradiation induced defects, as determined by deep level transient spectroscopy (DLTS). In addition, we present the results obtained on temperature-dependent of the Schottky barrier height (SBHs) fabricated on He-ion irradiated *n*-$Si_{0.90}Ge_{0.1}$ and the impact of this irradiation on the conduction mechanism in Pd/*n*-$Si_{0.90}Ge_{0.10}$ Schottky barrier diodes (SBDs). The electrical properties of He-ion irradiated Pd/n-$Si_{0.9}Ge_{0.1}$ Schottky diodes were studied in a wide temperature range (100-300 K). It was found that the current flow is controlled mainly by thermionic emission. The Schottky barrier height (Φ_{bn}) and ideality factor (*n)* of Pd/n-$Si_{0.9}Ge_{0.1}$ Schottky diode have been studied as a function of temperature. A decrease of Φ_{bn} and an increase of *n* with decreasing temperature are observed. Additionally, linear dependence between the so-called temperature factor T_0 and temperature as well the well-known linear correlation between SBHs and ideality factors, Φ_{bn} (*n*), are observed and explained in terms of inhomogeneities due to the presence of He-ion irradiation induced defects and traps with associated energy level localized in the gap.

3:45 PM *CM05.08.02
Radiation Damage Effects on High-Temperature Superconductors in Fusion Conditions Brandon N. Sorbom[1], Penghui Cao[2], Zach Hartwig[2], Stephen Jepeal[2], Leigh Ann Kesler[2], Michael Short[2], Nick Strickland[3], Dennis Whyte[2] and Stuart Wimbush[3]; [1]Commonwealth Fusion Systems, Cambridge, Massachusetts, United States; [2]Massachusetts Institute of Technology, Cambridge, Massachusetts, United States; [3]Robinson Research Institute, Lower Hutt, New Zealand.

Recent advances in high temperature superconductors (HTS) have opened up a new parameter space for the design of tokamak fusion pilot plants. While previously the maximum on-axis field in a superconducting tokamak was limited to ~6 T, HTS allows tokamaks to be designed with on-axis fields in excess of 10 T, leading to smaller reactor designs, such as the ARC concept from MIT. For these designs, it is critical to determine the lifetime of modern HTS technology in an environment relevant to compact, high-field fusion reactors and develop strategies to mitigate damage from exposure to radiation. This damage has historically been quantified as the number of displacements per atom (dpa). While dpa can be used as a rough predictor of radiation effects, the irradiation conditions also play a key role in microscopic damage formation and macroscopic property changes, as demonstrated by recent work. As HTS is irradiated, a variety of changes occur within the superconducting crystal lattice, and competing effects on the achievable critical current density (Jc) of the superconductor emerge. On one hand, Jc can be lowered by the displacement of atoms and creation of defect clusters through the suppression of the critical temperature, amorphization of the lattice, degradation of intergrain current transfer, and disordering of intrinsic pinning sites. On the other hand, Jc can be increased by point defects and defect clusters acting as artificial pinning centers. The combined effect of these mechanisms can be a net increase or decrease in Jc. In order to better understand the microstructural changes that influence the macroscopic superconducting properties such as Jc, HTS samples (2G REBCO from SuperPower) were irradiated with 1.2 MeV proton beam in the DANTE accelerator facility at MIT. The degradation of these samples was then characterized under a wide variety of HTS operating conditions at the Robinson Research Institute in New Zealand. In order to guide and interpret the experimental studies, a simulation workflow was developed by combining DART (a binary collision approximation code), SRIM and MCNP (Monte Carlo codes for ions and neutrons/gammas, respectively), and LAMMPS (a molecular dynamics code). These simulations were performed to compare different ion energies and incident particle directions to determine the mechanisms behind the observed experimental results.

4:15 PM CM05.08.03
Effects of Ionizing Irradiation on Ferroelectric Thin Films Steven J. Brewer[1], Samuel C. Williams[2], Hanhan Zhou[3], Jacob L. Jones[3], Ryan Rudy[4], Maunel Rivas[4], Ronald G. Polcawich[4], Evan Glaser[5], Cory D. Cress[5] and Nazanin Bassiri-Gharb[1, 2]; [1]George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, Georgia, United States; [2]School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia, United States; [3]Department of Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina, United States; [4]U.S. Army Research Laboratory, Adelphi, Maryland, United States; [5]U.S. Naval Research Laboratory, Washington, District of Columbia, United States.

In recent years, the continuous thrust toward developing microelectronic devices with greater autonomy, reduced footprint size, and large-scale interconnection has necessitated high-performance materials capable of fulfilling multiple functional roles. Ferroelectric materials, and specifically lead zirconate titanate (PZT), boast large dielectric, polarization, and electromechanical responses, making them ideal for microelectromechanical system (MEMS) sensors and actuators, energy harvesters, multilayer ceramic capacitors (MLCC), ferroelectric logic elements and relays, *etc.* However, many of the most compelling applications for these types of devices – space travel, satellite communications, nuclear energy, and unmanned reconnaissance – require sustained operation in extremely demanding radiation-hostile environments. Radiation, both ionizing and displacive, has been shown to substantially degrade the functional responses of ferroelectric thin films, thus rendering the development of techniques for increased radiation tolerance of these materials critically important.
In this work, a multifaceted investigation towards understanding radiation interaction with PZT thin films and strategies towards increasing radiation hardness was undertaken. Specific focus was placed on an array of critical interfaces and interactions in the ferroelectric material and device. Specifically, we address the role of the electrode material, microstructural feature (columnar vs. equiaxed grains), the effects of doping (with Mn) modifying the mobility of internal interfaces (domain walls) and point defects, and crystallization interfaces. Furthermore, a phenomenological model was developed to quantify functional behavior with total ionization dose (TID), relying on the fact that radiation induces defects and defect interactions that modify functional material response. Fitting of functional response trends as a function of TID with the phenomenological model yields two important parameters describing (i) the global susceptibility to radiation-induced degradation by induced defects and (ii) the rate of defect saturation in the material. Extraction and comparison of these parameters allows for quantification of defect interactions as a function of microstructural and compositional variations in ferroelectric thin films.

4:30 PM CM05.08.04
Radiation Damage in REBCO Materials for Compact Fusion Reactors Rebecca Gray and Samuel Murphy; Lancaster University, Lancaster, United Kingdom.

The advent of High Temperature Superconducting magnetic tapes has accelerated the development of compact nuclear fusion reactors. The Rare-Earth

Barium Copper Oxide (REBCO) high temperature superconductors (HTS) offer high field strengths to be accessed at high temperatures (>70 K). During reactor operation high energy neutrons ejected from the plasma will damage the tapes ultimately limiting their lifetime. Experimental observation of the damage process at cryogenic temperatures is tricky without highly specialised facilities that are not currently available.

Atomistic simulation of the damage cascades enables informed choices of magnetic tapes to be made. As a first step to simulating the cascades, we present a new empirical pair potential for an idealised REBCO material based on the Buckingham form fitted using thermal expansion coefficients from Density Functional Theory (DFT). Using the new potential, we determine threshold displacement energies in YBa2Cu3O7 as a function of the atom type and direction. Finally, we perform radiation damage cascades at the operational temperature and compare with similar simulations performed at the temperature where experimental data is available. A detailed comparison of the remnant defect's population and distributions at different temperatures enable us to discuss the relevance of the available experimental data to operational conditions.

4:45 PM CM05.08.05
Charge Equilibration and Electronic Stopping for Silicon Projectiles in Silicon Cheng-Wei Lee and Andre Schleife; University of Illinois at Urbana-Champaign, Urbana, Illinois, United States.

Energetic-particle radiation is of technological interest for applications in nuclear energy, electronics in outer space, medicine, and fundamental research. As a result of the irradiation, damage forms and ultimately determines materials properties. Understanding the effects of highly energetic particle radiation is important, e.g. for improving radiation hardness and ion implantation to create quantum bits. While damage caused by irradiation is commonly simulated using Monte Carlo methods, including SRIM, this approach has severe limitations: The accuracy is poor for low projectile kinetic energies, for which band structure effects of the target compounds dominate. In addition, SRIM inherently assumes the target to be amorphous and overcoming this, e.g. using molecular dynamics simulations of primary knock-on atom events, requires accurate parametrizations of two-temperature models to account for the effect of electronic excitations.

This highlights that developing an understanding of the underlying interactions between charged, energetic particles and a material from first principles is highly important to predict evolution and dynamics of defects. Ehrenfest molecular dynamics and real-time time-dependent density functional theory have recently been shown to successfully describe electronic stopping during the early stages of radiation damage for light projectiles. At the same time, its capability to predict electronic stopping for heavy ions remains mostly unexamined.

Here we report our recent work on using this technique to compute electronic stopping of heavy (silicon) projectiles traversing silicon bulk crystals. We found a pronounced dependence of electronic stopping on the initial charge state of the projectile ion, which was not observed for light projectiles. Our analysis shows that this can be explained by accounting for dynamics of charge equilibration in the target, and we explicitly study the influence of the impact parameter as well as contributions of core and valence electrons. From our simulations we demonstrate that off-channeling trajectories as well as semi-core electrons are needed for a direct comparison to experiment.

Developing a consistent framework based on first principles is an essential part of a multi-scale simulation approach that can accurately predict damage formation after particle irradiation. Incorporating electronic friction, e.g. by deriving accurate parameters from our first-principles simulations, into classical molecular dynamics leads to predictive accuracy. With the growing interest in swift-heavy ion particle radiation that creates strong electronic excitations, the capability of predicting across a large projectile kinetic energy range is crucial. Finally, the strong dependence on the initial condition observed in our simulations may suggest a way to control the magnitude of electronic stopping and, thus, damage, e.g. in nanometer-thin films by varying the initial charge state of the projectile ion.

SESSION CM05.09: Comparisons Between Types of Ionizing Irradiation
Session Chair: Michael Short
Wednesday Morning, November 28, 2018
Hynes, Level 2, Room 202

9:00 AM CM05.09.01
Study the Effects of Localized Spot-by-Spot High Dose MeV Au and Ag into Silica John D. Demaree[2] and Daryush Ila[1]; [1]Fayetteville State University, Fayetteville, North Carolina, United States; [2]Weapons and Materials Research Directorate, US Army Research Laboratory, Aberdeen Proving Ground, Maryland, United States.

In this work we have studied the change in the optical properties of Infrasil (Heraeus high-purity optical quality fused quartz silica) before and after spot-by-spot implantation of 0.785 MeV Ag and 1.450 MeV Au ions using a National Electrostatics 5SDH-2 tandem accelerator. The ion beams were focused to spots roughly 2mm in diameter, and after a given fluence was delivered, the substrate was moved stepwise in horizontal and vertical directions in 0.5 mm increments across an area roughly 8mm x 8mm. The fluence delivered in each overlapping spot was calculated to produce a uniform total implantation doses of Au, Ag, and (sequentially) Au + Ag ranging from $10^{16}/cm^2$ to $10^{17}/cm^2$. The effects of this high dose spot-by-spot method on the optical absorption were then compared with traditional raster scan implantations, in which the beam is swept over the entire area quickly, and the entire area is implanted at once. We, also, used 3D wide area microscopy and 3D laser microscopy to study the optical changes in the silica due to this spot-by-spot high dose MeV ion implantation.
The uniformly implanted area, several millimeters by several millimeters across, was studied before and after annealing, using optical absorption photo spectrometry to assess the optical change in the material and evidence of Au and Ag nanocluster formation. Rutherford Backscattering Spectrometry (RBS) was used to confirm the implantation dose and the uniformity of the implanted area. We have observed, specifically in spot-by-spot Au implanted silica, evidence of a quadrupole interaction which produces widening of the Au nanocluster absorption band beyond 530nm, and which has been seen in past studies using traditional raster scanning followed by annealing. Also, an ordered change in the index of refraction of the host by 3D microscopy correlated to the stepwise implantation in horizontal and vertical directions in 0.5 mm increments, producing 3D embedded optical structures.
In this presentation we will compare the results obtained for both spot-by-spot implantation of Au and Ag into Infrasil with past raster scan implantations, and comment on the effect of this method on nanocluster formation and growth, as well as possible changes in the surface topography and 3D-well defined change in the index of refraction of this glassy material.

9:15 AM CM05.09.02
Use of Pure Iron and Fe-15Cr-16Ni Model Alloy to Study the Impact of Self-Ion Energy, Displacement Rate and Irradiation Temperature on

Charged Particle Simulation of Void Swelling Aaron J. French, Frank A. Garner and Lin Shao; Nuclear Engineering, Texas A&M University, College Station, Texas, United States.

Void swelling of iron-base alloys under neutron irradiation is known to be very sensitive to a wide variety of material and environmental variables. Additional sensitivities arise using charged particle simulation. To enhance the credibility of charged particle simulation of neutron-induced swelling it is necessary to isolate and quantify those variables associated with ion simulation from those that are material-specific or involve segregation and phase stability, especially under the influence of surface effects, injected interstitials and segregation along ion-induced gradients in dpa rates that are characteristic of ion irradiation. Additionally, it is important to assess the impact of the much higher rates of atomic displacement used in ion irradiation compared to neutron irradiation.

First, we used pure annealed bcc Fe as a model system to avoid complexity associated with radiation-induced segregation and precipitation, studying only void swelling and dislocation changes. Two sets of irradiations were conducted on iron. The first set involved irradiations with Fe ion energies of 1, 2, 3.5 and 5 MeV, all at comparable dpa rate ($1x10^{-4}$ dpa/s) and attained dpa peak level of 100 dpa, in order to separate the separate but synergistic effects of surface and injected interstitial on swelling. Moving from lower to higher ion energy the surface and injected interstitial effects were therefore progressively separated. These two effects are both known to be sensitive to the dpa rate and to contribute to the temperature shift phenomenon.

In the second iron set the synergistic effects of temperature and displacement rate on swelling, expressed in the well-known "temperature shift" concept, was studied, using 5 MeV Fe ions at peak dpa rates of $3x10^{-3}$, $1x10^{-4}$, and $3x10^{-4}$ dpa/s, to peak dpa values of 50, 75 and 100 dpa, and at irradiation temperatures of 375, 425, 475, and 525°C, respectively.

Finally, we repeated the temperature shift experiment on a pure annealed fcc Fe-15Cr-20Ni model alloy, but shifting the temperature range from 475 to 650°C, based on previous ion studies conducted on this alloy. The specimens used were drawn from the same batch used for dpa rate studies conducted in the FFTF fast reactor at 420°C where a transient shift was observed with changes in dpa rate. The lack of minor solutes (Si, P, C, especially) in this alloy preclude precipitation, but did result in some segregation of major elements along the ion depth profile.

The results provide significant insight on the complexities of using charged particle simulation at accelerated dpa rates to study neutron-induced void swelling, especially with respect to the temperature shift and transient shift phenomena.

9:30 AM CM05.09.03
Dynamics of Graphene Milling Under the Helium and Neon Ion Beams Alex Belianinov, Songkil Kim, Anton V. Ievlev, Ivan Vlassiouk, Matthew J. Burch, Ondrej Dyck, Xiahan Sang, Raymond R. Unocic, Sergei V. Kalinin, Stephen Jesse and Olga Ovchinnikova; Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States.

Graphene has been investigated thoroughly due to its excellent electronic, mechanical and thermal properties. This 2D material can be modified structurally, electronically and doped chemically, to utilize in the design of functional devices. Advances in ion beam-based imaging and nanofabrication techniques have offered a pathway to precisely manipulate 2D materials and offer a roadmap to create junctions, amorphized areas, and introduce dopants for new types of electronic devices. Helium ion microscope (HIM) offers "direct-write" capabilities, packaged in a machine capable of both imaging and nanofabrication with Helium and Neon gases, thus making it an excellent candidate for processing a wide range of 2D, and conventional materials. However, despite graphene's properties, and existing tools to take advantage of them; challenges remain in the development of workflows that can yield high-performance 2D electronic devices; where the damage at edges and the basal plane is minimized during the milling process.

In this study, we explore graphene milling by the helium and neon ion beams in order to control material's electronic and mechanical properties. We demonstrate localized formation, growth and coalescence of nanopores, by investigating different levels of defects in graphene via Scanning Transmission Electron Microscopy. Using advanced image data analytics, we illustrate different dynamic behaviors of graphene milling depending on the material's initial conditions. This work provides in-depth understanding of the graphene milling as it occurs, laying a foundation to develop new pathways to manufacturing 2D material based electronic devices.

Acknowledgement
This work was conducted at the Center for Nanophase Materials Sciences (CNMS), which is a U.S. Department of Energy (DOE) Office of Science User Facility.

9:45 AM BREAK

SESSION CM05.10: Irradiation-Induced Ordering and Disordering
Session Chairs: Bertrand Radiguet and Michael Short
Wednesday Morning, November 28, 2018
Hynes, Level 2, Room 202

10:15 AM CM05.10.01
Influence of the Enthalpy Landscape on the Irradiation-Induced Disordering of Minerals Mathieu Bauchy[1] and Anoop Krishnan[2]; [1]University of California, Los Angeles, Los Angeles, California, United States; [2]Department of Civil Engineering, Indian Institute of Technology Delhi, New Delhi, India.

Under irradiation, minerals tend to experience an accumulation of structural defects—which can ultimately lead to a disordered atomic network. Despite the critical importance of understanding and predicting irradiation-induced damage, the physical origin of the initiation and saturation of defects remains poorly understood. Here, based on molecular dynamics simulations of α-quartz, we show that the topography of the enthalpy landscape governs irradiation-induced disordering. Specifically, we show that such disordering differs from that observed upon vitrification in that, prior to saturation, irradiated quartz accesses forbidden regions of the enthalpy landscape, i.e., those that are inaccessible by simply heating and cooling. Furthermore, we demonstrate that damage saturates when the system accesses a local region of the enthalpy landscape corresponding to the configuration of an allowable liquid. At this stage, a sudden decrease in the heights of the energy barriers enhances relaxation, thereby preventing any further accumulation of defects and resulting in a defect-saturated disordered state.

10:30 AM CM05.10.02
Atomic Scale Modeling of the Effect of Forced Atomic Reactions on the Thermodynamic and Kinetic Properties of Fe-Based Alloys Under Irradiation Liangzhao Huang[1], Luca Messina[2], Thomas Schuler[1] and Maylise Nastar[1]; [1]DEN-Service de Recherches de Métallurgie Phisique, CEA, Université Paris-Saclay, Gif-sur-Yvette, France; [2]Nuclear Engineering, KTH Royal Institute of Technology, Stockholm, Sweden.

Irradiation drives materials far from equilibrium. Under sustained atomic reactions such as ballistic mixing forcing exchanges between neighboring atoms, standard thermodynamic and kinetic methods do not apply because of the loss of the microscopic detailed balance. However, the resolution of the microscopic Master Equation describing the transitions between different on-lattice configurations allows us to compute the dynamic chemical short range order (SRO) under stationary conditions. The latter depends on the atomic jump frequencies and is compared to the results of atomic kinetic Monte Carlo simulation. From the dynamic SRO computed by this theoretical approach, we define effective atomic jump frequencies, compute point defect flux coupling, and predict the solute redistribution. We analyze the effect of temperature and irradiation conditions (including ballistic mixing and recombination) on the thermodynamic and kinetic properties of a few iron-based binary alloys.

10:45 AM *CM05.10.03
Irradiation-Accelerated Phase Transformations for Low-Temperature Phase Diagram Development Julie D. Tucker[1], Fei Teng[1], Li-Jen Yu[2], Emmanuelle Marquis[2], Jia-Hong Ke[1] and David Sprouster[3]; [1]Oregon State University, Corvallis, Oregon, United States; [2]University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; [3]Brookhaven National Laboratory, Upton, New York, United States.

Low-temperature phase data is essential for long-term applications at intermediate temperatures such as energy production. Experimental data below 500°C is limited due to the long times needed for most phases to develop. First principles techniques are supporting the need for low temperature phase data but still require validation by experiments. Irradiation generates extra point defect, enhancing kinetics at lower temperatures and can be a tool for accelerating phase transformations. In this study, we use ion beam irradiation to enhance the formation of an ordered Ni_2Cr phase in the Ni-Cr-Fe system. Commercial alloys, such as alloys 625 and 690, are susceptible to mechanical property changes with thermal aging due to this ordered phase. Model and commercial alloys have been isothermally aged up to 10,000 hours and characterized via nanoindentation, atom probe tomography, synchrotron X-ray diffraction and transmission electron microscopy. Additionally, these alloys have been irradiated to 1.5 or 6 dpa to quantify the role of irradiation in accelerating the ordering kinetics. Preliminary results indicate change in stoichiometry do not change the ordering rate only the amount of ordered phase formed. Also, proton irradiation tends to accelerate the ordering process while Ni+ ion irradiation do not lead to ordering at the dose rates explored.

11:15 AM CM05.10.04
Theoretical Prediction of Void Superlattice Formation under Irradiation Yongfeng Zhang, Yipeng Gao and Jian Gan; Idaho National Laboratory, Idaho Falls, Idaho, United States.

Void and gas bubble superlattices have been widely observed in various types of materials under irradiation, with the formation mechanisms still open for debate. Here, rate theory based theoretical analysis coupling thermodynamics and kinetics show that the superlattice forms by superposition of vacancy concentration waves that develop upon the instability of a uniform field. The symmetry of superlattice is governed by anisotropic interstitial diffusion, and the superlattice parameter depends on the irradiation condition including temperature and dose rate. Dependent on the nature of anisotropic interstitial diffusion, various types of void superlattices are theoretically predicted including planar ordering, simple cubic, face-centered-cubic and body-centered-cubic. The theoretic predictions on both the superlattice symmetry and parameters are demonstrated by atomic kinetic Monte Carlo simulations and are consistent with previous experimental observations. The developed theory can be used to guide experimental design for tailored microstructure using irradiation. It may also have general applications in cases involving spontaneous phase transition and anisotropic diffusion reaction.

11:30 AM *CM05.10.05
Atomic Scale Quantification of Intergranular Segregation in Ferritic Thermally Aged or Irradiated Alloys and Steels Bertrand Radiguet[1], Philippe Pareige[1], Alfiia Akhatova[1], Leifeng Zhang[1], Patrick Todeschini[2] and Frederic Christien[3]; [1]Université de Rouen Normandie, Groupe de Physique des Matériaux, Saint Etienne du Rouvray, France; [2]MMC, EDF R&D, Moret sur Loing, France; [3]EMSE, Saint Etienne, France.

Phosphorous intergranular segregation can lower the cohesion between grains, resulting in steel embrittlement. Low alloyed bainitic steels used to build nuclear reactor pressure vessel (RPV) generally contain a small amount of phosphorus (in the range of 100 ppm). Continuous exposure to a low neutron dose rate irradiation at intermediate temperature (~300°C) results in radiation embrittlement of RPV steel. Since intergranular segregation of phosphorous can contribute to this embrittlement it is important to understand the effects of ageing conditions (temperature, irradiation dose), material composition and the grain boundary (GB) nature on the intensity of phosphorus intergranular segregation. Regarding to literature sources, it was revealed that the intergranular segregation values may strongly vary among different GBs. However, there is a lack of systematic studies in this field.
In order to get an accurate and representative description of the effect of GB nature different techniques are combined in this work. Atom Probe Tomography (APT) technique is utilized as the main tool and it is compared to Auger Spectroscopy for validation. GB geometry is determined from Transmission Kikuchi Diffraction (TKD) map.
Firstly, this approach is validated on a Fe-0.034at%P-0.01at%C model alloy. It is shown that radiation-induced segregation caused by phosphorus-interstitial complex is the dominant mechanism in under irradiation at 450°C with 10 MeV Fe5+ ions at a dose rate of 3 10-5 dpa/s . Also a higher phosphorus segregation at curved GBs in comparison with the straight one was found. This work has also shown that GBs with high Miller index planes has significantly higher phosphorus segregation than low index GB planes.
In a second step the approach is applied to a real RPV steel thermally aged or ion irradiated. APT analyses revealed that there was a considerable element segregation (C, P, Mn, Mo, Cr, Si, Ni…) for all boundary types. By taking into consideration all segregated chemical species, both interstitial and substitutional segregations were discussed with regard to GB types. Besides, the element segregation at carbide/matrix interfaces was also quantified. Comparison between as received and aged materials will be given.

SESSION CM05.11: Long Timescale Phenomena Resulting from Ionizing Radiation
Session Chairs: Kazuto Arakawa and Oleg Rofman
Wednesday Afternoon, November 28, 2018
Hynes, Level 2, Room 202

1:30 PM *CM05.011.01

The Effect of Neutron Irradiation, Deformation and Natural Aging on the Microstructural Changes and Properties of the Austenitic Reactor Steels Oleg Maksimkin[1], Kira Tsay[1], Oleg Rofman[2, 1] and Michael Short[3]; [1]Institute of Nuclear Physics, Almaty, Kazakhstan; [2]National University of Science and Technology MISiS, Moscow, Russian Federation; [3]Department of Nuclear Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States.

The current study explores physical characteristics of the austenitic stainless steels, constitutive materials of hexagonal fuel assembly shrouds, exposed in a BN-350 fast breeder reactor (Aktau, Kazakhstan). The 0.12C-18Cr-10Ni-Ti (AISI 321 an.) and 0.08C-16Cr-11Ni-3Mo (AISI 316 an.) steels were subject to high-dose neutron irradiation (0.2-59.0 dpa) and long-term post-irradiation storage. Evaluation of the microstructure and properties of the irradiated steels using electron microscopy, magnetometry and microhardness testing has initially revealed many interrelated irradiation- and stress-induced processes affecting the steels performance. The observed phenomena, including those during and after irradiation, were represented by swelling, fine defects evolution, phase transformations and denuded zones formation. Subsequent uniaxial tensile testing at different temperature conditions and strain states has helped to illustrate the importance of the deformation-induced changes taking place in the irradiated material. This knowledge is important to take into account during operational stages, for example, associated with loading and unloading of structural elements. The experimental stress-strain relationships were presented to estimate the effect of irradiation dose and temperature on the yield and ultimate strength of the irradiated austenitic steels. The deformation-induced changes to the microstructure give evidence of extensive transformation of paramagnetic γ-austenite to a ferromagnetic α-martensite phase. TEM study of the deformed samples also reveals the changes in voids shape and their arrangement towards stress direction. This work also presents the results of natural aging carried out over 15 years on the austenitic stainless steels, each with its own irradiation, stress state, and natural aging history. Natural aging is shown to reduce hardness in these steels by 10-25% and partially alleviate stress-induced hardening over this timescale, showing that materials evolve back towards equilibrium even at such a low temperature.

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2:00 PM CM05.011.02

Irradiation with Neutrons and Alfa Particles Reduces Dynamic Strain Aging in Armco Iron Mihail Merezhko[1], Diana Merezhko[1], Kira Tsay[1], Maxim Gussev[2], Oleg Maksimkin[1, 3], Michael Short[4, 3] and Frank A. Garner[5, 3]; [1]Institute of Nuclear Physics, Almaty, Kazakhstan; [2]Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States; [3]Moscow Engineering Physics Institute, Moscow, Russian Federation; [4]Department of Nuclear Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States; [5]Radiation Effects Consulting, Richland, Washington, United States.

Plastic deformation of metals and alloys containing light impurity atoms (for example, nitrogen or carbon) is often accompanied by jerky flow in mechanical tests at elevated temperatures (up to 400°C), with numerous load drops (serrations) appearing on the load-elongation curve. This phenomenon, known as the Porteven-le-Châtelier effect, is due to Dynamic Strain Aging (DSA) occurring in the material because of the interaction of solute atoms with mobile dislocations, temporarily arrested at obstacles. DSA in many cases leads to the reduced ductility and toughness, decreased ability to cold roll, etc. Irradiation leads to the appearance of radiation defects and their interactions with impurity atoms, reducing the concentration of these atoms in solid solution. These interactions significantly decrease the DSA process. It was shown [1] that with increasing irradiation dose of mild steel, the critical temperature for the onset of DSA serrations increased and the temperature range of "blue brittle" behavior narrowed. More precise understanding of the nature and magnitude of radiation defect interactions with the dislocations responsible for DSA can therefore help to mitigate its effects.
The present work is devoted to investigations of the effect of irradiation with neutrons and alpha particles on the mechanical properties and stored energy characteristics of Armco-iron. Tensile samples were irradiated with neutrons (maximum fluence 6×10^{18} n/cm^2, E>2.35 MeV, T<50°C) in the experimental WWR-K reactor core (6 MW water-pool nuclear research reactor) and alpha particles with an energy of 50 MeV in an isochronous cyclotron U-150 to a helium concentration of 10^{-2} at. % at <100°C. Uniaxial tensile tests were carried out in the temperature range of 20-300°C with two nominal strain rates, $\dot{\varepsilon}_1 = 8.33\times10^{-4}$ s^{-1} and $\dot{\varepsilon}_2 = 1.67\times10^{-3}$ s^{-1}. For each test temperature, the value of the critical strain energy density (Wc) was determined. In some cases, images of the surfaces were taken during tensile tests to study the features of deformation localization using digital image correlation approach.
As a result of the experiments, mechanical and energy characteristics were obtained, and DSA parameters were determined as a function of irradiation. It was determined that irradiating Armco-iron with neutrons and alpha particles suppressed DSA, decreased the amplitude of serrations, and increased the activation energy of the DSA process and the critical strain when serration occur on the curves. Decreasing DSA intensity led to increase in the plasticity and Wc of the material. Optical metallography and electron microscopy were used to study the evolution of radiation and deformation defects. The obtained experimental data can be used in the development of theoretical models of deformation aging, as well as the finding the ways and methods to reduce the negative effects of irradiation on structural materials.

[1] Murty, K.L., 1984. In *Fracture 84* (pp. 1385-1392).

2:15 PM CM05.011.03

Accelerated Materials Testing in Low Earth Orbit Kevin Heath and Lindsay Farrell; Alpha Space Test and Research Alliance, LLC, Houston, Texas, United States.

Alpha Space (AS) provides a turn key service that allows for testing of materials in an extreme environment, space. The AS Test Platform, the Materials International Space Station Experiment Flight Facility (MISSE), provides an environment that cannot be easily duplicated on the earth. The MISSE provides testing of materials in a vacuum, while simultaneously exposing the material to a radiation environment, UV-A through UV-C light, atomic Oxygen, and temperature cycling. The MISSE-FF allows for oxidation testing of a material utilizing atomic Oxygen, which is highly reactive with all materials. Ultra-violet light degradation testing on the MISSE-FF of polymer materials or coatings is provided at an accelerated rate, because the MISSE-FF exposes the materials to UV light at Air Mass Zero. The full extent of UV-A through UV-C is applied to the sample to determine degradation, which cannot be attained in the atmosphere because air absorbs 95% of the UV-B and almost 100% of UV-C wavelengths. The MISSE-FF provides radiation testing across the full spectrum of the naturally occurring radiation spectrum, Gamma Rays through proton/neutron emissions, to determine degradation of materials. The MISSE-FF provides the ability to limit the amount of molecular contamination that can occur with the samples being tested, providing a true test of the material. Thermal Cycling provided by the MISSE-FF occurs sixteen times a day, providing an accelerated test of the interface between the coatings and the substrate they are applied upon. The thermal cycling of samples on the MISSE-FF occurs between -60 Deg. C and 120 Deg. C per cycle, controllable using various different mounting structures to keep within the sample temperature parameters. Testing with the Alpha Space MISSE-FF provides the test environment described above simultaneously, mimicking the actual effects on materials by providing a real world environment that cannot be obtained in a cost effective manner in an earth bound laboratory. The MISSE-FF flight environment tests the cross-coupling effects on materials of the various input parameters from radiation, oxidation, UV, and temperature cycling. Testing of materials on the MISSE-FF is a continuous opportunity, with sample installation and removal on a six month to twelve month cycle. This continuous testing allows for Alpha Space to provide visual degradation data via high resolution pictures during the extended test period on orbit, and sample return for final comparisons between the virgin sample witness plates and

the post test samples. Alpha Space will also provide guidance to determine the best way to isolate the various effects of the environment on samples by isolating the input variables.

2:30 PM BREAK

SESSION CM05.12: Microstructural Stability Under Ionizing Irradiation
Session Chairs: Kazuto Arakawa and Camille Flament
Wednesday Afternoon, November 28, 2018
Hynes, Level 2, Room 202

3:30 PM CM05.12.01
Enhanced Twin Stability Against Irradiation in Nanotwinned Solid Solution Alloys Jin Li[1], Dongyue Xie[3], Sichuang Xue[1], Cuncai Fan[1], Youxing Chen[2], Haiyan Wang[1], Jian Wang[3] and Xinghang Zhang[1]; [1]Purdue University, West Lafayette, Indiana, United States; [2]University of Minnesota, Minneapolis, Minnesota, United States; [3]University of Nebraska-Lincoln, Lincoln, Nebraska, United States.

Face-centered cubic (FCC) metals are in general vulnerable to high-energy ion irradiation. Twin boundaries have been shown to improve the irradiation tolerance of FCC metals. However, nanotwins in monolithic metals are unstable during irradiation. In this study, we show that Fe solute can drastically improve irradiation stability of twin boundaries in Ag. By adding merely 1 at.% of Fe solute atoms into Ag matrix, ultra-high-density twins with an average twin thickness of ~ 3 nm form in Ag. *In situ* Kr ion irradiation studies show that defect size and density in $Ag_{99}Fe_1$ have been significantly reduced comparing with monolithic coarse-grained Ag and nanotwinned Ag. Furthermore, these extremely fine twins survived heavy ion irradiations. Density function theory calculations suggest that Fe solutes stabilize nanotwins by pinning twin boundaries. The mechanisms of enhanced radiation tolerance enabled by solute-twin boundary networks are discussed.

3:45 PM *CM05.12.02
Microstructural Evolution of Fe – 10 wt.% Cr Alloy Irradiated by Fe Ions with Carbon Implantation Camille Flament; DEN-Service de recherches de métallurgie physique, CEA Saclay, Gif sur Yvette, France.

Because of their high resistance to swelling and low ductile-brittle transition temperature, high chromium ferritic-martensitic (F-M) steels are promising candidates for structural materials of Gen. IV fast neutron reactors and for fusion. The presence of carbon in F-M steels can lead to the precipitation of carbides which may have significant impact on their mechanical properties. Submitted to high neutron flux, the study of their stability under irradiation is a crucial point for reactors lifetime. In order to better understand the mechanisms induced or enhanced by irradiation at fine scale, Fe-Cr model alloys representative of F-M steels have been widely studied. It is well-known that alloys with more than 10 wt.% of Cr are interesting for their resistance to corrosion but display brittleness at temperature below 500°C and after irradiation due to the precipitation of α' phase [1-3]. Nevertheless very few studies deal with the characterization of Fe-Cr-C model alloys and the evolution of carbides under irradiation.
This study proposes to characterize high purity Fe – 10 wt.% Cr alloy irradiated at high flux up to a damage of 110 dpa (SRIM2008 calculations (K.-P.)) with Fe ions at 500°C with C implantation, a way to simulate the enrichment in C observed in steels after years of irradiation in reactor. Observations by TEM after irradiation emphasize the coexistence of a_0<100> and $1/2a_0$<111> dislocation loops homogeneously distributed in the matrix as well as carbides in high density. The mean size of carbides is about 20 nm and they are homogeneously located in intragranular position in the irradiated zone. Observations in HR-TEM show two different morphologies and crystallographic structures: spherical carbides are compatible with $M_{23}C_6$with a face-centered cubic structure whereas ellipsoidal carbides display an orthorhombic structure close to the one of M_7C_3. APT analyses confirm the enrichment in C to about 0.5 wt.% and show segregation of Cr and C in the habit plane of dislocation loops. No α' precipitation is observed certainly due to the high density of sinks and C atoms implanted. This irradiated microstructure is compared to an un-irradiated Fe – 10Cr – 0.076C (wt.%) kept at room temperature for ten years. In that case, coarse intergranular carbides (> 200 nm) and finer intragranular carbides (< 150 nm) are observed. Selected area electron diffraction in TEM on several carbides show a face-centered cubic structure with a lattice parameter compatible with $M_{23}C_6$. Even though the C amount is different between both alloys, it is interesting to note that irradiation with C implantation creates a lot of small clusters of defects which enable a finer and denser microstructure of precipitates in Fe-Cr alloys compared to annealing in Fe-Cr-C alloys. It may impact the mechanical properties of alloys.
[1] O. Tissot et al., *Scr. Mater.* 122 (2016) 31.
[2] M. Bachhav et al., *Scr. Mater.* 74 (2014) 48.
[3] O. Tissot et al., *Mater. Res. Lett.*, 5 (2017) 117.

4:15 PM CM05.12.03
Stability of Carbides in Fe-Cr-C Systems Under Irradiation—An *Ab Initio* Based Study Chu Chun Fu[1], Maylise Nastar[1], Elric Barbe[1, 2] and Thomas Schuler[1]; [1]DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, Gif Sur Yvette, France; [2]DEN-Service de Recherches Métallurgiques Appliquées, CEA, Université Paris-Saclay, Gif sur Yvette, France.

Fe-Cr steels are promising candidates for structural materials in advanced fission and future fusion reactors. Possible presence of carbides in these systems is well known to have significant impact on their mechanical properties. Further, the stability of the carbides can be modified due to irradiation, as shown experimentally.
We address in this study mechanical, thermodynamic and kinetic properties of M_3C and $M_{23}C_6$, being respectively the most relevant carbide in α-Fe and in Fe-Cr alloys. It is known experimentally that distinct fracture mode occurs on these carbides, intra-precipitate for the former and interfacial for the latter. Under irradiation, partial amorphization and dissolution of $M_{23}C_6$, have been observed experimentally, together with the emergence of new carbide phases, changing mechanical properties of the materials.
To understand these features, density functional theory (DFT) calculations are applied to investigate the energetics, elastic moduli, and fracture properties of these carbides, as functions of the chemical composition (Fe versus Cr and the carbon concentration) in the carbides. Then, in order to evaluate the impact of irradiation, the stability of the carbides due to point-defect production and diffusion and the ballistic mixing are determined.

4:30 PM CM05.12.04
Additively Manufactured 316L Stainless Steel Behaviour Under Ion Irradiation Anne-Hélène Puichaud[1], Camille Flament[1], Fernando Lomello[2], Aziz Chniouel[2], Marie Loyer-Prost[1], Hicham Maskrot[2], Frédéric Schuster[3] and Jean-Luc Béchade[1]; [1]DEN-Service de Recherches de Métallurgie Physique, CEA, Gif-sur-Yvette, France; [2]DEN-Service d'Etudes Analytiques et de Réactivité des Surfaces, CEA, Gif-sur-Yvette, France; [3]CEA, Université Paris-Saclay, Gif-sur-Yvette, France.

Additive manufacturing (AM) is being extensively developed as a promising technology, and already exploited in various industries in particular in biomedical and aerospace applications ([1], [2]). However, the use of AM materials in nuclear applications still requires an in depth understanding of the materials response to irradiation, and little work has been done to date [3]. The long term objective of this work is to investigate possible applications of additively manufactured materials, here 316L type stainless steel, suitable for nuclear applications.
Stainless steel cubes were fabricated by selective laser melting (SLM) using commercial 316L powder, with AM fabricated materials studied as built, after a heat treatment (HT) and after a hot isostatic pressing (HIP). We performed an in depth microstructural characterisation of the as built, heat treated and HIP materials before irradiation using SEM, EBSD, TEM and nanoindentation. Fe^{5+} ion irradiations of the samples were then performed at the Joint Accelerators for Nano science and Nuclear Simulation (JANNuS, Paris Saclay, France) up to 3 dpa at 550 °C. Finally, microstructures and irradiation behaviours of the AM materials were compared to cold work 316L austenitic stainless steel.
The first results of the unirradiated materials show a high microstructural anisotropy for the AM as built and HT materials with elongated grain in the direction of fabrication and a close to α fibre texture. The HIP samples however present more equiaxial grains and a loss of the α fibre texture, closer to conventional 316L. Nanoporosity and segregation of elements (Mo, Si and Mn) were observed in the as-built and HT materials while the HIP samples did not show porosity but presented a high density of precipitates.
The microstructure and microchemistry of the irradiated materials were examined using a combination of TEM techniques to establish in particular the void swelling and precipitation behaviour under ion irradiation. The first microstructural characterisations at low dose show apparition of nanocavities, precipitates and a high density of dislocations.

[1] S. Sing, *et al.*, “Laser and electron–beam powder–bed additive manufacturing of metallic implants: A review on processes, materials and designs”, *J. Orthop. Res.*, vol. 34, no. 3, pp. 369–385, 2015.
[2] S. Singh, *et al*., “Material issues in additive manufacturing: A review”, *J. Manuf. Process.*, vol. 25, pp. 185–200, 2017.
[3] P. Freyer, *et al*., “Hot cell tensile testing of neutron irradiated additively manufactured type 316L stainless steel.” P*roceedings of the International Conference on Environmental Degradation of Materials in Nuclear Power Systems, Water Reactors*, the Minerals, Metals and Materials Society, 2018

SESSION CM05.13: Poster Session I: Fundamentals of Material Property Changes Under Irradiation
Session Chairs: Kazuto Arakawa and Michael Short
Wednesday Afternoon, November 28, 2018
8:00 PM - 10:00 PM
Hynes, Level 1, Hall B

CM05.13.01
Enhancement of Photoluminescent Properties in PBAT/MEH-PPV Blends Provoked by Gamma Radiation for Application in 3D Dosimetry João L. Souza[1], Thiago Schimitberger[1] and L.O. Faria[2]; [1]Nuclear Engineering, UFMG, Belo Horizonte, Brazil; [2]Materials, Centro de Desenvolvimento da Tecnologia Nuclear, Belo Horizonte, Brazil.

When using high energy clinical beams for diseases treatments, the determination of the *dose distribution versus tissue depth* curves, before the patient irradiation, is significant for radiotherapy planning. The procedure allows medical physicists to accurately predict the dose that will only be enough to eliminate a tumor, without affecting the tissues near the region of treatment. In this context, the developing of 3D dosimetric systems capable to previously determine the dose distribution along the tissues affected by the radiation beam is a worldwide field of investigation. Nowadays, the best dosimetric systems commercially available for this application are the gel-based dosimeters such as PGD (Polymer Gel Dosimeter) and FGD (Fricke Gel Dosimeter). These gel dosimeters are tissue equivalent, with no angular dependence and with milimetric spatial resolution. Most 3D dosimeters are made of a continuous uniform medium which polymerizes upon irradiation. However, the small dose working range of these dosimeters (1-50 kGy) is a problem to be solved. In this work we investigate a new polymeric blend that, by means of radiation damage, can be proposed as a 3D photoluminescent radiation detector, which could operate in a much larger absorbed dose range (1 to 500 kGy). In this context, we have developed a polymeric blend made of poly(butylene adipate-co-terephthalate) copolymers (PBAT) and poly(2-methoxy-5(2'-ethylhexyloxy)-p-phenylenevinylene) copolymer MEH-PPV. Films of PBAT are non-photoluminescent polymers. However, after exposure to high doses of gamma radiation it shows high photoluminescence (PL) output, proportional to the exposed radiation dose. When excited with blue LED, its PL intensity at 490 nm (green) can be used for high gamma dose dosimetry [1]. MEH-PPV is a naturally photoluminescent polymer that, when in solution, undergoes a gradual color change, from red to colorless, when exposed to high gamma doses ranging from 0.5 to 500 kGy. Films of PBAT/MEH-PPV have been recently proposed for 2D high dose dosimetry [2]. In this paper we have produced blends of PBAT/MEH-PPV mixed with a plasticizer in order to produce 3D dosimeters, by using DINCH - 1,2-Cyclohexane dicarboxylic acid disononyl ester plasticizer. After gamma irradiation, the 3D samples in a cylinder form, changes its color from orange (lower doses) to light green (higher doses), for doses ranging from 1 kGy to 500 kGy, respectively. FTIR data revealed that the radio-induced aromatic amines in the binary system are responsible for the observed PL at 500 nm. The PL emission spectra demonstrate that the color change in the 3D polymeric cylinders is a combination of the variation in the green color intensity of PBAT with the decreased red color intensity of MEH-PPV. UV-Vis spectrometry, DSC and DRX analysis are used to complement the discussion about the radio-induced photoluminescent properties. PBAT/MEH-PPV blends are good candidates for 3D dosimetry and bio-imaging devices.

CM05.13.02
Ionising Radiation Effects in UK Nuclear Waste Glasses—An Assessment of Key Processes Aaron R. Daubney[2, 1]; [1]Dalton Nuclear Institute, Whitehaven, United Kingdom; [2]Chemistry, University of Manchester, Manchester, United Kingdom.

The current understanding of glass behavior after exposure to a multitude of ionising radiation fields (including alpha, beta and gamma) is under development by a growing international research effort. Understanding the physical mechanisms which cause deleterious (and sometimes even preferential) changes to a glass' microstructure will underpin future policy for the disposal of high-activity nuclear wastes.
By using ion beam and gamma irradiation facilities, an assessment of microstructural changes and their relation to glass mechanical and thermodynamic properties will be made.
Through coordinated research efforts, a picture of long-term glass behavior (over hundreds to thousands of years) is generated and so an understanding of key mechanisms and their application to amorphous, metastable materials such as glass are crucial. This agreement of physical mechanisms involved during multi-particle radiation fields and their relative impact to glass structure will also underpin atomistic simulations of glass corrosion processes.

CM05.13.03

Impact of Stored Mechanical Energy in Carbon Onion Resilience Under Space Radiation Gaurab Panda[1], Virginia M. Ayres[1], Harry Shaw[2], Kan Xie[1] and SK Bay[3]; [1]Michigan State University, East Lansing, Michigan, United States; [2]NASA Goddard Space Flight Center, Greenbelt, Michigan, United States; [3]Bahcesehir University, Istanbul, Turkey.

Nano-carbons are a promising new approach to resolve lubrication challenges in space including vacuum, radiation and non-terrestrial temperature regimes. Planar graphite, while an excellent lubricant on earth, undergoes structural collapse in vacuum and knock-on collision generated amorphitization in response to heavy ions, a key component of the solar wind. Space lubrication candidates: carbon onions and multi-walled carbon nanotubes have shown robust performance in vacuum environments and are under investigation by our group and others for radiation and temperature resilience [1, 2, 3].

The responses of carbon onions with increasing polygonal character due to increasing temperature growth conditions were investigated under heavy ion irradiation at the Facility for Rare Isotope Beams (FRIB) at Michigan State University. The heavy ions used in these experiments were primary beams of fully stripped Calcium-48, and Argon-40 with 140 or 70 MeV per nucleon kinetic energies. Stored elastic energy, and layer number were investigated using analysis of pre- and post- irradiation high-resolution transmission electron microscope (HRTEM) images. The study indicated that as the radiation dose increased, the carbon onions tended to store more mechanical energy, which reproduces a mechanical property of growth at a higher temperature. A key consequence was that rearrangements were enabled that included conversion of radial onions to planar graphite when the starting point material had sufficiently high stored mechanical energy. Increase in number of layers was not consistent and average numbers did not show much change. However, individual specimens and standard error of the mean values could support the interpretation of an increase.

Layer rearrangement could have both positive and negative implications for the
tribological performance of carbon onions in a heavy ion space environment.
Ongoing rearrangements into structures that retained the excellent tribological features of
the originals would be a self-healing way of dealing with radiation-induced defects. However, rearrangements that resulted in the formation of planar graphite could have negative
consequences for tribological performance. This suggests that for space lubrication applications, lower temperature synthesis carbon onions, while less polygonal and more defective, are more resilient to heavy ion radiation.
[1] R. A. Al-Duhaileb, K. Xie, V. M. Ayres, R. M. Ronningen, A. F. Zeller, T. Baumann, A. Hirata. In *Mater. Res. Soc. Symp. Proc. Vol.* **1407**, (2012).

[2] A Hirata, M Igarashi, T Kaito, *Tribol. Int.* **37**, 899, (2004).

[3] J. Kotakoski, A. V. Krasheninnikov, K. Nordlund. *Nucl. Instr. Meth. Phys. Res. B* **240**, 810, (2005).

CM05.13.04
Computational Design of Radiation Damage Tolerant Single-Phase Alloys Penghui Cao, Miaomiao Jin and Michael Short; Massachusetts Institute of Technology, Cambridge, Massachusetts, United States.

Understanding and predicting radiation damage are of central importance to develop radiation-tolerant structural materials for current and advanced nuclear systems. Single-phase solid solution alloys constitute attractive choices due to their promising mechanical properties and radiation tolerance. Here, by examining radiation-induced defect production and evolution in single-phase Ni-Fe alloys, we show that radiation damage resistance directly correlates with thermodynamic mixing energy. Defect numbers and sizes appear to first decrease with increasing Fe concentration, but then start to increase at the vicinity of equiatomic concentrations. The observation in damage reduction is further ascribed to the increasing heterogeneity of point defect migration across a complex potential energy landscape that results in enhancement of defect recombination. This new insight into the dynamical evolution of radiation defects implies a thermodynamic criterion for designing radiation-tolerant materials.

CM05.13.05
Photoirradiation-Induced Reversible Lattice Expansion in W-Doped TiO_2 Through the Change of Its Electronic Structure Fan Feng[1], Weiyi Yang[1], Shuang Gao[2], Linggang Zhu[3] and Qi Li[1]; [1]Institute of Metal Research, Chinese Academy of Sciences, Shenyang, China; [2]Graduate School at Shenzhen, Tsinghua University, Shenzhen, China; [3]Beihang University, Beijing, China.

The capability of reversible crystal lattice dimension changes on the order of 0.1% or above by external stimulations of applied force or voltage to impose external mechanical or electric forces on atoms forming the lattice had been observed in a lot of types of materials, including oxides, metals, polymers, and carbon nanostructures, which could be utilized as actuators or sensors for various technical applications. As an external stimulation, photoirradiation had been found to be effective to lead to reversible changes in materials, such as photocatalysis, photochromism, photoisomerization, and surface morphology change. In these processes, photoirradiation interacts with materials and electrons are excited internally to induce subsequent changes. If these photogenerated electrons could be designed to cause the material's internal electronic structure to change reversibly, it should also result in a reversible crystal lattice dimension change by light irradiation.

Recently, photostriction had been reported in several perovskite oxides due to the combination of the photovoltaic effect and the converse piezoelectric effect or the nonequilibrium of phonons. Here, we report that reversible lattice expansion comparable to those by applied force or voltage (on the order of 0.1% or above) can be induced by the on and off of UV-irradiation in an oxide of W-doped TiO_2 nanotube array through the reversible changes of its internal electronic structure by the accumulation and release of photogenerated electrons on W-dopants, respectively, which was different with the mechanism of previously reported photostriction. Furthermore, photoirriadation-induced optical absorbance property changes in both the visible to infrared and THz regions were also observed on this W-doped TiO_2 nanotube array.

This photoirradiation-induced reversible lattice expansion may also be present on other material systems by proper material design if they possess one component able to produce electrons upon photoirradiation and the other component able to accumulate photogenerated electrons to induce lattice changes and release them after the photoirradiation is off. Reversible optical, electric, and magnetic property changes could also be expected due to their reversible internal electronic structure changes. Various potential applications may be found for this kind of materials, including nanoscale, photo-driving actuators or detectors.

CM05.13.06
Ionization Induced Carbon Phase Changes in Graphite Lenore S. Miller[1], John D. Demaree[2], Kristopher D. Behler[2, 3], Zhiping Luo[1] and Daryush Ila[1]; [1]Fayetteville State University, Fayetteville, North Carolina, United States; [2]Weapons and Materials Research Directorate, US Army Research Laboratory, Aberdeen Proving Ground, Maryland, United States; [3]SURVICE Engineering Company, Belcamp, Maryland, United States.

We have studied changes in the surface of graphite before and after MeV ion bombardment, to assess the effect of ionization on the carbon phase and atomic bonding of carbon in HOPG, using X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, and 3D laser microscopy. We observed the hexagonal carbon ring structure of graphene sheets in graphite using AFM, to assess any changes in carbon bond length or distortion of the hexagonal lattice due to the passage of the heavily ionizing particles. Rutherford Backscattering Spectrometry (RBS) in conjunction with XPS were used to identify impurities in the material and at the surface, and their potential impact on graphite surface properties. RBS was used because most impurities are significantly heavier than carbon, and therefore they can be easily detected and quantified without any need for substrate background subtraction. XPS was used to confirm the RBS findings, identify any differences in the distribution of impurities in the bulk and at the surface of the material before and after MeV implantation. Ion induced changes in carbon bonding, including the transformation of graphitic sp2 bonding to amorphous or diamond-like sp3 bonds were measured using Raman spectroscopy, as well as using X-rays excited C KLL to characterize the carbon phase in various high purity HPOG bombarded transformation which may be explained by rapid thermal quenching following ion-induced excitation.

CM05.13.07

Accelerated Testing of Carbon Fiber-Reinforced Shape Memory/Epoxy Polymer Composites in Low Earth Orbit Space Joon Hyeok Jang[1], Seok Bin Hong[1], Jingyun Kim[2], Nam Seo Goo[3] and Woong-Ryeol Yu[1]; [1]Seoul National University, Seoul, Korea (the Republic of); [2]Kyung Hee University, Yongin, Korea (the Republic of); [3]Konkuk University, Seoul, Korea (the Republic of).

Carbon fiber reinforced shape memory polymer composites (CF-SMPCs) have been researched for space structural materials due to their high mechanical properties, lightweight, excellent shape deformability, and self-deployment properties. Long term durability of CF-SMPCs in the space environment should be guaranteed for their successful applications to aerospace engineering. In low earth orbit (LEO) space region, there are many factors, such as high vacuum, ultraviolet radiation (UV) and atomic oxygen(AO), that affect polymer matrix composites. Therefore, a predictive method is required to predict long-term properties of CF-SMPC considering these harsh environments and thus to design proper CF-SMPCs for aerospace engineering. In this study, CF-SMPCs made of CF and epoxy shape memory polymers were studied, focusing on their life prediction. First, acceleration tests were developed by exposing CF-SMPCs to LEO space environments (i.e., high vacuum, UV and AO) at elevated temperature in space environment chamber. Then, their storage moduli were measured using dynamic mechanical thermal analysis. Using time-temperature superposition principle (TTSP), a master curve was constructed to predict the long-term behavior of CF-SMPCs in LEO space. The long-term storage modulus was predicted by the linear product of the shift factors for time – three LEO environments and time - temperature superposition. Finally, a predictive model was developed to evaluate the durability of CF-SMPCs in aerospace.

CM05.13.08

Corrosion Protection Coatings for Depleted Uranium Volodymyr Lobaz[1], Martin Hruby[1], Peter Cernoch[1], Jiri Panek[1], Tomas Chmela[2] and Pavel Krupicka[2]; [1]Institute of Macromolecular Chemistry AS CR, Prague, Czechia; [2]UJP PRAHA a.s., Prague, Czechia.

The depleted uranium is still an indispensable material in numerous areas, from healthcare to arms industry; however its range of applications is limited by high reactivity and susceptibility to corrosion. The current state of art for the storage of depleted uranium stands on expensive and sophisticated procedures, as alloying with up to 20% of molybdenum or encapsulation in aluminum or steel containers. This project aims the reduction of the production costs and simplification of the technology for production and processing of depleted uranium based materials. Within current study we develop the coatings on depleted uranium stored for further reprocessing or already used in various radiation shielding applications.
For lower radiation doses, up to 100 kGy, the coatings are based on polymer materials, either in form of polymeric paints from poly(2-butyl-2-oxazoline), poly(2-phenyl-2-oxazoline), series of polyesters, or as two-component curable systems: polyurethanes based on isophorone diisocyanate (ID) with Krasol (K) or Polycarbonate (PC). The coatings were reinforced with inorganic fillers (e.g. modified graphene) to prevent the diffusion of water vapor and oxygen and stabilized with hindered amines BHT or Tinuvin 123 for radical scavenging.
The polyurethane layers were exposed to radiation from depleted uranium, and various doses of gamma or β^- radiation, and their chemical composition, thermal stability and mechanical properties were investigated by FTIR, EPR, TGA/DSC, and micro-hardness indentation. The gamma irradiation improved the thermal stability of polyurethane ID-K, but reduced for ID-PC; the glassing temperature is decreased for all polyurethane samples after every irradiation cycle. The harder polyurethane sample ID-K after irradiation become even harder and stiffer and demonstrated increased intensity of the hydroxyl (3600 cm^{-1}), carbonyl (1740 cm^{-1}) ether and ester (1500-1000 cm^{-1}) bands of FTIR spectra, usually assigned to oxidation products. It was assumed, that ID-K sample undergoes oxidation and additional cross-linking. The softer ID-PC polyurethane remained unchanged.
For higher radiation doses (in range of hundreds of MGy or higher) the entirely inorganic coating, based on low melting SnF_2-SnO-P_2O_5 glass is developed. The glass powder is sprayed on the metal surface, melted at 450°C to form the uniform layer, aged at 150°C for relaxation of strains and cooled to ambient temperature. The material contains 40 wt. % of tin, used for radiation shielding together with lead and copper.

Acknowledgements:
Financial support was provided by the Ministry of Industry and Trade of the Czech Republic (grant # FV10164).

CM05.13.09

Effects of X-Ray Irradiation on Amorphous Oxide Semiconductor Thin-Film Transistors Solah Park and Jang-Yeon Kwon; Yonsei University, Incheon, Korea (the Republic of).

In recent years, digital x-ray detectors have been used in the medical device market for miniaturization, portability and rapid information transmission. When driving indirectly, electric signal is amplified by using hydrogenated amorphous silicon Thin Film Transistors (a-Si:H TFT) on the detector panel. At this time, the detector panel is continuously exposed to the x-ray, and the elements therein are also affected by the x-ray.
The trend of x-ray detector market requires a high mobility device because it requires effective detection with low x-ray dose. TFT technology using oxide semiconductors (mobility of 10 cm^2/Vs) has already been applied to AMOLED in the field of display. It is a suitable alternative to solve problems such as low mobility and device reliability of existing a-Si:H TFT (mobility of 0.5 cm^2 / Vs). The application of oxide TFT technology in medical devices can give many advantages in the construction of digital X-ray radiography system structure that can realize high resolution and high aperture ratio based on high mobility. Therefore, it will make a great contribution to the development of smart medical device system. For this, the ionizing radiation effect studies are needed to utilize oxide semiconductor TFTs in medical devices. There is a lack of research on how each semiconductor device is affected by x-ray and how long it will last. Therefore, it is necessary to investigate the change of device characteristics after x-ray irradiation, and to study the lifetime and recovery of devices.
In this presentation, we investigated the effects of typical silicon and oxide TFTs used in displays on x-ray irradiation. In particular, we have investigated the effects of different crystalline states (amorphous or crystalline) on silicon and oxide, respectively. We investigated the effect and mechanism of each device according to x-ray dosage. This result is expected to contribute to the study of x-ray radiation damage due to the difference in crystal structure between silicon and oxide TFT and to develop medical industry (Radiography, Fluoroscopy, Dental etc.) and electronic device with tolerant in x-ray environment. Furthermore, it is expected to contribute greatly to research on x-ray industry technology for non-destructive testing (NDT) of facilities and buildings.

CM05.13.10
Experimental Determination of Diffusion Kinetics After Thermal Aging of FeCrNi Nanolayers Solène Rouland[1], Bertrand Radiguet[1], Alain Billard[2] and Philippe Pareige[1]; [1]Normandie Univ, UNIROUEN, INSA Rouen, CNRS, GPM, Rouen, France; [2]Institut FEMTO-ST, UMR 6174 CNRS, Univ. Bourgogne Franche-Comté, UTBM, Montbéliard, France.

GEMMA (GEneration IV Materials Maturity) European project aspires to validate structural materials and welded joints selected for GenIV demonstrators (e.g. ASTRID) under operating conditions by reliable experiments and simulations.

Austenitic stainless steels are candidates for both structures (316 L(N) steels) and cladding (AIM1-type steels). The 60-year life demonstration design and operating temperatures in the range of 400-550°C lead to long term ageing (thermal or irradiation ageing). This process is governed by thermodynamics and diffusion. Thus, to predict microstructural evolutions, an important step is to gain a better understanding of the diffusion kinetics properties in FeCrNi model alloys. At the typical range operating temperatures, diffusion properties of this ternary system aren't known for the moment either after thermal or irradiation ageing.

To investigate interdiffusion at low temperature under reasonable time, it has been shown [1] that decomposition or homogeneization of the stacking of composition modulated nanolayers can be used. This kind of material is synthetized by magnetron cosputtering of metallic targets at UTBM (France). Interdiffusion coefficients as a function of annealing time at low temperatures can be extracted from [2]:
- concentration profiles amplitude evolution obtained by elemental analysis techniques as Atom Probe Tomography (APT) and STEM-EDS/EELS ;
- the decay of satellite peaks intensity thanks to XRD.
These sinusoïdal modulations in composition can be described by their wavelength, corresponding to twice a layer thickness, and their amplitude. As diffusion kinetics are wavelength-dependent at this scale, different wavelengths have to be experimentally tested in order to extrapolate results for interdiffusion in a bulk material.

In this talk, the experimental results (APT, STEM, XRD) obtained on multilayers of different wavelengths before and after thermal ageing at different temperatures will be presented. The diffusion coefficients deduced from experimental results will be given.

[1] L. L. Chang et B. C. Giessen, Éd., *Synthetic modulated structures*. Orlando: Academic Press, 1985.
[2] K. N. Tu et R. Rosenberg, Éd., *Analytical techniques for thin films*. Boston: Academic Press, 1988.

CM05.13.11
Effect of Alloying Elements on Stacking Fault Tetrahedra (SFT) in Ni Alloys Gaurav Arora, Dilpuneet S. Aidhy and Anus Manzoor; University of Wyoming, Laramie, Wyoming, United States.

Formation of stacking fault tetrahedra (SFT) has been widely observed both experimentally and in molecular dynamics (MD) simulations in Ni. Using MD simulations, we show that SFT formation is arrested under tensile strain. This observation is explained by our density functional theory (DFT) calculations that show the decrease in the binding energy of SFT with increasing tensile strain. These predictions are qualitatively validated in Ni-Pd alloys. In particular, adding a large atom such as Pd leads to elongation of the Ni-Ni bonds; our MD simulations indeed show no SFT formation in Ni-Pd alloys. The lack of SFT formation has also been observed in irradiated Ni-Pd systems compared to pure Ni. We further elucidate the effect of strain on the energetics of loop and void formation. In particular, we find that while the vacancy binding energy is negative for SFT, it is positive for voids and loops. However, despite positive binding energy, voids are very difficult to form due to high formation energies. For example, the formation energy of a 10-vacancy void is approximately 9 eV. Thus, our results indicate that vacancy clustering and cluster sizes could be significantly reduced via choosing larger sized alloying elements and by applying tensile strain.

CM05.13.12
Object Kinetic Monte Carlo Modelling of Microstructure Evolution Under Irradiation in Zirconium Based on Atomistic Modelling of Point Defect Clusters Christophe Domain[1], Benjamin Christiaen[1], Ludovic Thuinet[2], Antoine Ambard[1] and Alexandre Legris[2]; [1]EDF R&D, Moret-Sur-Loing, France; [2]UMET, Université de Lille, Villeneuve d'Ascq, France.

Zirconium alloys are used to manufacture fuel cladding as well as fuel assemblies of pressurized water nuclear reactors. Under irradiation, they can show a dimensional change commonly called growth. Experimental observations have shown that above a threshold dose, these alloys are subject to accelerated growth called "breakaway". It has been established that the irradiation formation of <a> and <c> dislocation loops is responsible for the growth of irradiated zirconium alloys and that the appearance of <c> loops is correlated with this growth acceleration. In order to improve our understanding of the nucleation mechanisms of the <c> loops, object kinetic Monte Carlo modelling based on atomic simulations is used. Atomic-scale calculations based on the density functional theory (DFT) and empirical potentials are used to determine the properties of vacancy and self-interstitial clusters: stability and eigenstrain. In particular, DFT simulations have put in evidence the possible existence of different defect clusters (including non planar defects) with different properties prior to the formation of loops. These objects have been included, in addition to displacement cascade debris, in object kinetic Monte Carlo modelling of the microstructure evolution under irradiation. The calculated growth is compared to available experimental results.

SESSION CM05.14: Surface Effects of Ionizing Radiation
Session Chairs: Fabio Di Fonzo and Chu Chun Fu
Thursday Morning, November 29, 2018
Hynes, Level 2, Room 202

8:15 AM CM05.14.01
Kinetic Study on the Evolution of Nanoceramic Coatings Under Heavy Ions Irradiation Matteo Vanazzi[1, 2], Luca Ceseracciu[1], Marco Beghi[2], Gaelle Gutierrez[3], Celine Cabet[3], Jing Hu[4], Meimei Li[4] and Fabio Di Fonzo[1]; [1]Istituto Italiano di Tecnologia, Milan, Italy; [2]Energy Department, Politecnico di Milano, Milan, Italy; [3]CEA, Paris-Saclay, France; [4]Argonne National Laboratory, Argonne, Illinois, United States.

In order to qualify innovative materials for structural components and coatings, their radiation resistance must be assured. In this framework, irradiations studies with neutrons present overwhelming complications related to cost, availability and experimental time needed to reach significant levels of radiation

damage. Ions irradiation has been proposed as a valid alternative to produce comparable and accessible data. Specifically, heavy ions in the MeV energy range are quite appropriate to simulate neutrons due to the low Electronic to Nuclear Stopping Power (ENSP). However, the comparison of the relative effects for neutrons and heavy ions presents intrinsic difficulties and many data are required to make it reliable. In the previous studies, we have reported on the evolution of amorphous-nanoceramic Alumina (Al_2O_3) coatings under heavy ions irradiations. The material was irradiated up to 450 displacements per atom (dpa), showing a general radiation-induced crystallization trend. In this work, we employ 12 MeV Au ions to irradiated Al_2O_3 coatings up to 3 dpa. In opposition to earlier experiments, here we concentrate on the low dpa regime, to evaluate carefully the first stages of crystallization and to obtain radiation damage values more compatible with neutrons tests. Moreover, irradiations are now performed at different temperatures (namely 400, 500 and 600 °C) in order to decouple the thermal contribution from the radiation-induced effects. A comprehensive analysis of the irradiated samples is accomplished by X-Ray Diffractometry (XRD), Transmission Electron Microscopy (TEM), Scanning-TEM (STEM) and Nano-indentation (NI). Generally, the evolution seems strictly temperature-dependent, with no structural changes at 400 °C. For the higher temperatures, results show again an intense crystallization process - even at very low dpa levels - with the formation of different crystalline phases, in relation to the test conditions. A preliminary kinetic model is proposed, based on the experimental data, and the grain-growth-related parameters are calculated. From a mechanical point of view, an evident size-effect is manifested. The formation and growth of nanometric crystalline domains increase rapidly the hardness, in accordance with the Hall-Petch relationship. In particular, for the initial stages of irradiations, an inverse Hall-Petch mechanism is observed, with a reported maximum hardness of about 27 GPa (ultra-hardness). To support and confirmed these evidences, irradiation tests are repeated with in-situ TEM tandem apparatus. Further tests are carried out with 1 MeV Kr ions on free-standing Alumina films, to collect dynamically microstructural changes and phases transformation. To conclude, an extensive characterization campaign is performed on ions irradiated-Al_2O_3 coatings. Tuning different experimental conditions (like temperature, dpa, ions), a consistent and coherent picture of the Alumina evolution under irradiation is produced.

8:30 AM CM05.14.02
Analysis of Helium Segregation on Surfaces of Tungsten at Different Levels of Helium Ion Irradiation Lin Hu[1], Asanka Weerasinghe[1], Karl D. Hammond[2], Brian D. Wirth[3] and Dimitrios Maroudas[1]; [1]Chemical Engineering, University of Massachusetts Amherst, Amherst, Massachusetts, United States; [2]Chemical Engineering, University of Missouri–St. Louis, Columbia, Missouri, United States; [3]Nuclear Engineering, The University of Tennessee, Knoxville, Tennessee, United States.

Plasma facing components (PFCs) in nuclear fusion reactors are exposed to intense plasma heat and particle fluxes. The implantation of helium (He) atoms into these materials impacts significantly the evolution of their surface morphology and near-surface structure. In tungsten (W), a promising PFC material because of its thermomechanical properties, interstitial He atoms are very mobile and aggregate to form clusters of various sizes. Small, mobile helium clusters (He_n, $1 \leq n \leq 7$) are attracted to the tungsten surface due to an elastic interaction force that drives surface segregation, and their diffusional transport mediates the dynamics of surface morphology and near-surface microstructure.

Here, using atomistic simulations based on a reliable many-body interatomic potential, we explore helium segregation on surfaces of tungsten that has been exposed to different levels of He ion irradiation. At higher helium fluence, mobile helium clusters are subjected to cluster-defect interactions in addition to cluster-surface interactions, which complicate cluster dynamics beyond the dilute limit of helium content in the PFC material. We characterize in detail configurations generated by large-scale molecular-dynamics simulations of implanted helium evolution in plasma-exposed tungsten with W(100), W(110), W(111), and W(211) surfaces facing the plasma. We examine the effects of varying helium fluence due to increased plasma exposure of the tungsten PFC by performing systematic molecular-statics computations of small helium cluster energetics near the above low-Miller-index W surfaces as a function of distance (depth) of the cluster center from the surface on a grid of lateral locations on the surface. We analyze the defect interactions that mediate the energetics of small helium clusters migrating to the surface, taking into account that the migrating cluster also is subjected to the stress fields generated by larger helium bubbles, as well as other small clusters, and quantify the strength of these interactions for different levels of He irradiation. The outcome of this analysis is the systematic parameterization of mobile helium cluster energetics at varying levels of He irradiation through functional forms that include contributions from cluster-cluster and cluster-bubble interactions as well as cluster-surface interactions. Such parameterizations are important for developing atomistically-informed, hierarchical multiscale models of helium cluster dynamics in PFC materials.

8:45 AM CM05.14.03
Harsh Environments of Fast Neutrons and Extreme Temperature Effects on Amorphous Fe-Based Nano-Coatings on Steel Substrate Ilyas Savkliyildiz[1, 2], Enver Koray Akdoğan[3], Zhong Zhong[4] and Nikolaos Simos[4]; [1]Selçuk University, Konya, Turkey; [2]Konya Technical University, Konya, Turkey; [3]Rutgers, The State University of New Jersey, Piscataway, New Jersey, United States; [4]Brookhaven National Lab, Upton, New York, United States.

Protective coatings on next generation nuclear reactor steels shows safe operation behavior at high temperatures and fast neutrons. The integrated studies include fast neutron irradiation, macroscopic post-irradiation evaluation, scanning electron microscopy and energy dispersive X-ray diffraction (EDXRD) to investigate irradiation-induced macroscale physio-mechanical changes in the nanocoating/substrate structures. At extreme temperatures, phase evolution and effect on crystallization/amorphization is mapped with EDXRD technique throughout the coating. With modest neutron doses of ~$2x10^{18}$ n/cm^2, the loss of ductility in an amorphous Fe-alloy coating on a steel substrate due to high temperature is prevented. At the higher neutron dose of ~$2x10^{19}$ n/cm^2, radiation-induced embrittlement behavior is observed on Fe-alloy nanostructured coating with macroscopic stress-strain analysis which implies ductility loss in the coating-substrate structure. Neutron irradiation displayed remarkable oxidation resistance of the protective Fe-based amorphous coating, which is attributed to the formation of the Fe_2B phase in the coating. In-situ 3D space resolved EDXRD study revealed an increase amorphous-to-crystalline transition in the amorphous Fe-alloy at elevated temperatures. On the surface of the coating, mostly α-Fe phase is observed but these α-Fe phase transformed into γ-Fe phase close substrate interface. This phenomena is attributed to carbon diffusion from steel substrate to Fe based coating at high temperature annealing process. Electron microscopy was carried out to sustain the radiation-induced suppression of crystallization in the amorphous Fe-alloy nanostructured coating.

9:00 AM CM05.14.04
Nanoceramic Coatings—An Enabling Technology for Future Generation Nuclear Systems Fabio Di Fonzo, Erkka J. Frankberg, Francisco Garcìa Ferré, Daniele Iadicicco, Boris Paladino and Matteo Vanazzi; Istituto Italiano di Tecnologia, Milano, Italy.

In the framework of conceptually innovative nuclear reactors, next generation systems are meant to outperform current ones, by providing disruptive solutions in terms of non-proliferation, fuel cycle efficiency, radioactive waste management and safety. However, the development of future power plants is directly linked to the availability of suitable materials. The greatest challenges in this sense arise from the extremely harsh environments and the intense radiation fields to which materials will be exposed during operation. Among the other candidates, ceramic coatings are a promising solution to tackle these issues. Indeed, the deposition of ceramic coatings on traditional structural materials can provide surface engineering without affecting structural integrity. It is worth highlighting that protective coatings are already being considered as a near-term option for accident tolerant fuel (ATF) for Light Water Reactors (LWRs) while, in the case of Generation-IV (GIV) concepts and fusion systems, coatings could be used to mitigate high-temperature corrosion and tritium permeation. Here, we present a brief summary of the activities performed by the Center for Nano Science and Technology of the Istituto Italiano di

Tecnologia, on the materials for advanced nuclear systems. Engineered coatings are grown on relevant structural alloys such as 1515-Ti, EUROFER-97, ZIRLO® and Zircaloy-4. Coatings are designed and processed by different methods, namely Pulsed Laser Deposition (PLD) and Magnetron Sputtering (MS). In respect to GIV systems - specifically Lead reactors - Alumina (Al_2O_3) layers have been characterized as anti-corrosion radiation-resistant barriers. In particular, the compatibility of PLD-grown Al_2O_3 in molten Lead has been proven in up to 5000 hours exposure time tests, without degradation. For what concerns fusion reactors, Yttria (Y_2O_3) as well as Alumina coatings have been evaluated as possible solutions against Lead-Lithium corrosion and Tritium permeation. Indeed, the obtained Tritium permeation reduction is in the order of 10^4-10^5 while the requirements indicate reduction values of about 1000. Nevertheless, Al_2O_3 coatings have been tested also under heavy ions irradiation, at damage levels relevant for fusion and fast reactors. The ceramic film has preserved again its integrity and stability, evolving structurally from an amorphous to an almost-completely crystalline state. Last but not least, a combined approach has been investigated for ATF claddings. An optimized multi-layered structure of metallic Chromium and transitional metal oxides has been tested in autoclave systems, simulating standard and accidental condition. Results show a strong improvement in terms of high temperature oxidation resistance. To conclude, engineered coatings represent promising candidates to face the major issues related to future nuclear technologies and allow the design of innovative and economically attractive power plants.

9:15 AM CM05.14.05
Studies of Electron Beam Damage on γ-FeOOH Nanoparticles Yulia Trushkina, Cheuk-Wai Tai and German Salazar-Alvarez; Stockholm University, Stockholm, Sweden.

It is known that electron beam in transmission electron microscopy (TEM) can cause a damage of a material in various ways, i.e. a change of surface and structure of a specimen. In the case of lepidocrocite (γ-FeOOH) nanoparticles, electron beam damage is an obstacle to obtain full information about the structure from TEM measurements.

In this work we study lepidocrocite whiskers ($2,5\times6\times200$ nm^3) prepared through oxidation of a green rust precursor. TEM observations show that within 10 minutes lepidocrocite structure undergoes changes under electron irradiation starting at electron dose 171 $e^-/Å^2/s$. Analysis of the final structure indicates that the structure dehydroxylates topotactically to produce maghemite (γ-Fe_2O_3).

In this talk I will present the investigation and quantification of beam damage on lepidocrocite nanoparticles. Results from high-resolution TEM and EELS (e.g., thickness change vs dose) with and without cooling will be presented. We suggest that beam damage mechanisms for lepidocrocite nanoparticles are displacement damage and heating.

9:30 AM CM05.14.06
Nanoscale Chemical Phenomena Using HIM-SIMS Alex Belianinov, Songkil Kim, Artem Trofimov, Matthew J. Burch and Olga Ovchinnikova; Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States.

The key to advancing materials in a broad range of scientific sectors is to understand, and subsequently control, (i) the structure as well as (ii) the chemistry of surfaces and interfaces. However, significant gaps in characterization techniques hamper simultaneous chemical and physical characterization of materials with high spatial resolution and high chemical sensitivity.
This work will illustrate recent nanoscale results on imaging and chemical analysis of conductive and nonconductive surfaces using a tool that combines high resolution imaging and milling with high spatial resolution chemically sensitive approaches – a Helium Ion Microscope (HIM) with a secondary ion mass spectrometer (SIMS). This multimodal chemical imaging methodology transcends inherent individual instrument limitations, data volumes, and complicated analyses originating from an ex-situ combinatorial approach.

Data will be presented on conductive and non-conductive chemical standards as well as scientifically relevant organic-inorganic perovskite (HOIPs) materials. Ionization efficiency, sputtering, fragment detection, and other salient features of the HIM and the SIMS tools will also be presented and discussed. Overall, a combined HIM-SIMS platform offers significant potential to visualize and map active interfaces, by intertwining imaging, nanoscale elemental characterization, and data analytics; to better grasp the physical properties of materials and the mechanistic physics-chemistry interplay behind their properties.
Acknowledgements
This work was conducted at the Center for Nanophase Materials Sciences, which is a Department of Energy (DOE) Office of Science User Facility

9:45 AM BREAK

SESSION CM05.15: Radiation Resistant Material Design
Session Chairs: Chu Chun Fu and Yanwen Zhang
Thursday Morning, November 29, 2018
Hynes, Level 2, Room 202

10:15 AM *CM05.15.01
Current Understanding of Irradiation-Induced Defect Production and Microstructural Evolution in Tunable Concentrated Solid-Solution Alloys Yanwen Zhang[1], Shijun Zhao[1], Yuri Osetsky[1], Hongbin Bei[1] and William J. Weber[2, 1]; [1]Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States; [2]The University of Tennessee, Knoxville, Knoxville, Tennessee, United States.

Multicomponent concentrated solid solution alloys (CSAs) offers tunable chemical complexity. The random arrangement of multiple elemental species on a regular lattice (fcc or bcc) results in unique site-to-site lattice distortions and local disordered chemical environments. Control of chemical complexity can be achieved by substitute transition metal elements within the same period or the same group. The requirements for an alloy system with increasing chemical complexity (e.g., variation of electronic structure disorder or magnetic frustration) can be fulfilled, for example, in fcc Ni with addition of other elements, primarily 3*d*–transition metals (e.g., Cr, Mn, Fe and Co). The composition of this fcc CSA system (e.g., binary, ternary, quaternary and quinternary) can be at or near equiatomic concentrations, or at concentrations with one or two elemental species in large variation within solubility limits. In the case of high entropy alloys (HEAs), e.g. NiCoFeCrMn and NiCoFeCrPd, extreme chemical complexity leads to substantially reduced electron, phonon and magnon mean free paths; modified coupling strengths; and complex formation energies and migration barriers. In contrast to traditional dilute alloys, these energies have broad distributions. Moreover, defect–defect interaction strengths, such that interstitials, vacancies and defect clusters produced by displacement collisions, may create their own distributions that can be strongly affected by the intrinsic site-to-site complex disordered states. Recent

results [1-5] show that tuning compositional disorder in CSAs represents a powerful tool to dramatically affect defect energetics that ultimately enhances radiation tolerance. In this presentation, current understanding on defect dynamics and microstructure evolution will be discussed through closely integrated theoretical, computational, and experimental studies.

Work supported by the Energy Dissipation to Defect Evolution Center (EDDE), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science.

References

1. C. Lu, et al., *Nat. Commun.* **7** (2016) 13564
2. S. Zhao, et al., *Phys.Chem.Chem.Phys*. **18** (2016)24043.
3. Y. Zhang, et al., *Curr. Opin. Solid State Mater. Sci.* **21** (2017) 221-237.
4. Y. Zhang, et al., *Nat. Commun.* **6** (2015) 8736
5. S. Zhao, et al., *Phys. Rev. Materials* **2** (2018) 013602.

10:45 AM CM05.15.02

Absorption of Radiation-Induced Point Defects at Crystal/Amorphous, Metal/Covalent Interfaces Sanket S. Navale and Michael J. Demkowicz; Materials Science and Engineering, Texas A&M University, College Station, Texas, United States.

We use atomistic simulations to investigate the interaction of radiation-induced point defects with interfaces between crystalline metals and amorphous covalently-bonded solids. We select the gold (Au)/silicon (Si) binary system as a model material and construct interface models along different facets of crystalline Au and with amorphous Si (a-Si) created at different quench rates. We compute formation energies of vacancies and helium interstitials as a function of position relative to the interface and find that Au/a-Si interfaces are strong traps for defects originating from both Au and a-Si. Our work suggests that crystal/amorphous, metal/covalent interfaces, such as those found in iron/silicon oxycarbide (Fe/SiOC) composites may be as affective at removing radiation-induced point defects as interfaces in polycrystalline metals composites.

11:00 AM *CM05.15.03

Helium Nanochannels and Future Prospects for Damage-Free Helium Outgassing from Metals Michael J. Demkowicz; Texas A&M University, College Station, Texas, United States.

In this talk, I will present the recent finding that helium (He) implanted into certain metal nanocomposites spontaneously forms networks of elongated channels, rather than a field of isolated, equiaxed precipitates. Thanks to many years of prior research—performed in large part using ion implantation and ion beam analysis facilities—we now have a complete explanation for the physical mechanisms underlying this surprising departure from classical He behavior in metals. I will explain these mechanisms and, on their basis, discuss prospects for technological applications of metal nanocomposites as He-resistant materials to be used in nuclear energy.

11:30 AM CM05.15.04

Displacive Annihilation of Point Defects in Body-Centered-Cubic Metals Qing-Jie Li[1], Ju Li[2] and Evan Ma[1]; [1]Johns Hopkins University, Baltimore, Maryland, United States; [2]Massachusetts Institute of Technology, Cambridge, Massachusetts, United States.

Irradiation often generates excess point defects well beyond the equilibrium concentration in a crystal. Annihilation or annealing of these point defects plays an important role in keeping materials from accumulating damage. Here, using atomistic simulations, we demonstrate that screw dislocations in body-centered-cubic (BCC) metals often transport point defects along the line sense direction, efficiently annihilating point defects either at interfaces or with their opposite counterparts. This ‘displacive annihilation’ mechanism stems from the capability of screw dislocation to decompose point defects into cross-kinks, a reverse process to creating point defects via cross-kink pinch-off. We speculate that, under appropriate conditions, 'displacive annihilation' may overwhelm 'displacive accumulation' to heal the material, and we call this ‘displacive annealing’. Our findings shed new light on the defect-property relations in BCC metals subjected to irradiation.

11:45 AM CM05.15.05

Nanotube/Nanowire as Effective Defect Sinks in Metals—Atomistic Simulations and *In Situ* Ion Radiation Transmission Electron Microscopy Kang Pyo So[1], Penghui Cao[1], Yang Yang[1], JongGil Park[2], Mingda Li[1], Jing Hu[3], Meimei Li[3], Young Hee Lee[1], Michael Short[1] and Ju Li[1]; [1]Massachusetts Institute of Technology, Cambridge, Massachusetts, United States; [2]Sungkyunkwan University, Suwon, Korea (the Republic of); [3]Argonne National Laboratory, Argonne, Illinois, United States.

The accumulation of defects during irradiation leads to material property degradation modes such as embrittlement and swelling, eventually causing material failure. Effective and efficient removal of defects is of crucial importance to design radiation damage-tolerant materials. Here, by biasing defect migration pathways via carbon nanotube (CNT) infiltration, we present a greatly enhanced damage-tolerant Al-CNT composite with defect storage measured to be one order of magnitude lower than that in pure, irradiated Al. Furthermore, extreme-value statistics (largest size) of defect clusters are significantly changed in the presence of CNT. *In situ* ion irradiation transmission electron microscopy (TEM) experiments and atomistic simulations together reveal the dynamic evolution and convergent diffusion of radiation-induced defects to CNTs, facilitating defect recombination and enhancing radiation tolerance. The occurrence of CNT-biased defect convergent migration is tuned by the thermodynamic driving force of stress gradient in Al matrix due to the CNT phase transformation. This approach to controlling defect migration using 1D interface engineering creates a new opportunity to enhance the properties of nuclear materials.

SESSION CM05.16: Crafting Materials with Ionizing Radiation
Session Chairs: Pär Olsson and Jeroen Van Kan
Thursday Afternoon, November 29, 2018
Hynes, Level 2, Room 202

1:30 PM CM05.16.01

Formation of Porous Silicon by Means of Low Energy Oxygen Bombardment Angelica Hernandez, Rene Asomoza-Palacio, Georgina Ramirez and Yuriy Kudriavtsev; CINVESTAV, Mexico City, Mexico.

We studied the morphology evolution of silicon surfaces under ion bombardment by utilizing diatomic oxygen ions (O_2^+) with low energy (0.5 - 2.0 keV). Besides, the ion bombardment was performed at room temperature by varying the ion fluence. Ripple and pyramid-like morphologies were observed on Si surfaces after the bombardment with an ion beam energy of 1 keV and 2 keV, respectively. It was detected the coarsening of the ripple and pyramids structures accordingly with the increment of the ion fluence. 0.5 keV oxygen ion irradiation results in the formation of a porous Si (PSi). The morphological, structural and optical properties of porous Si (PSi) were studied in detail in this work. The pores size and depth were characterized by atomic force microscopy for the different ion fluences used. Raman spectra was acquired from the PSi in order to study the changes in the crystal lattice. On the other hand, the PSi was characterized by photoluminescence spectroscopy and we observed emission in the visible range when the excitation wavelength was 325 nm.
In this work we show a simple procedure for pSi fabrication as an alternative to the well-known chemical etching of silicon.

1:45 PM *CM05.16.02
Focused MeV Proton Beams for 3D Nano-Lithography and DNA Nanofluidics in Resist and Graphene Jeroen A. Van Kan[1] and Tanmoy Basu[2]; [1]Centre for Ion Beam Applications, Department of Physics, National University of Singapore, Singapore, Singapore; [2]Centre for Advanced 2D Materials, Faculty of Science, National University of Singapore, Singapore, Singapore.

In microscopy the wavelength of the probe is a critical parameter in achieving high resolution. Microscopies using charged particles have a natural advantage as the wavelength is much smaller than the size of an atom. A good example is electron microscopy, here atomic resolution has been achieved for very thin samples. One limitation is the rather rapid spread of the beam after penetrating into a sample due to electron – electron scattering. Proton microscopy on the other hand is an attractive addition to the available microscopies. A fast incoming proton mainly interacts with substrate electrons. Due to the mass mismatch between a proton and an electron there is very little energy transfer to substrate electrons and most of them get just enough energy to break bonds resulting in a project range of a few nm. Consequently the proton beam practically follows a straight path, except at the end of its range where nuclear interaction starts to play a larger role causing the beam to spread more. In order to make full use of the potential of proton probes in microscopy and lithography it is important to understand proton interactions in material.
Two dimensional (2D) materials provide a good platform to study the effect of ion irradiation from a fundamental point of view. In particular, graphene, an atomically thin layer of carbon atoms, has become a promising candidate for ion irradiation studies due to its potential application in nanofluidics, DNA translocation, water desalination and catalysis.
Looking into three dimensions (3D), proton beam writing (PBW) provides a platform to study the effect of ion irradiation in resist materials. PBW employs a focused MeV proton beam which is scanned in a predetermined pattern over a resist, which is subsequently chemically developed.
The main weak point is the ion source performance, i.e. the brightness is typically several million times less compared to electron beam sources. Recent test with on chip ion sources has shown great potential, opening up the way to improve the ion beam brightness by a million times.
In this talk I will give an update on defect formation in graphene using different ion species and different energies (1 keV – 2 MeV). As well as an update on the applications into PBW, especially in the area of nanofluidics where we developed a new platform to image single stranded DNA molecules, used in large scale genomic mapping. Finally I will discuss our progress in the development of our new ion source, aiming for single digit nanometer proton beam spot size.

We kindly acknowledge NRF-Singapore for their support: NRF-CRP13-2014-03 and NRF-CRP13-2014-04.

2:15 PM CM05.16.03
Blister Formation at Subritical Doses in Tungsten Irradiated by MvE Protons Inbal Gavish Segev[2], Ido Silverman[3], Guy Makov[2] and Eyal Yahel[1]; [1]NRCN, Beer-Sheva, Israel; [2]Materials Engineering, Ben-Gurion University of the Negev, Beer-Sheva, Israel; [3]SNRC, Yavne, Israel.

Tungsten samples were irradiated by 2.2 MeV protons at the Soreq Applied Research Accelerator Facility (SARAF) to doses of the order of 10^{17}protons/cm^2 which are below the reported critical threshold for blister formation derived from keV range irradiation studies. Large, well-developed blisters are observed indicating that for MeV range protons the critical threshold is at least an order of magnitude lower than the lowest value reported previously. The effects of fluence, flux, and corresponding temperature on the distribution and characteristics of the obtained blisters were studied. FIB cross sections of several blisters exposed their depth and structure.

2:30 PM CM05.16.04
Feedback-Based Automated Fabrication in a Scanning Transmission Electron Microscope Ondrej Dyck[1, 2], Sergei V. Kalinin[1, 2] and Stephen Jesse[1, 2]; [1]Center for Nanophase Materials Science, Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States; [2]Institute for Functional Imaging of Materials, Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States.

In recent years, a surprising number of examples of electron beam-induced transformations have been observed in the scanning transmission electron microscope (STEM). Such transformations set the stage for harnessing the electron beam as a fabrication tool at the atomic scale, however most of these demonstrations are performed “by hand”. In the development of a tool set for atomic manipulation, feedback-based automated beam control and real-time image analysis are needed to improve the consistency, throughput, and executability of various processes. Here, we present the development of feedback-based tools which interface with the microscope through a custom scan control system. We demonstrate automation-enhanced control of crystallization, amorphization, and dopant movement. To accomplish this, we must address the challenge of detecting material alterations while concurrently attempting to manipulate the material. Because the same electron beam is used for imaging and manipulation we explore techniques to generate meaningful sample information during manipulation and use rapid, sparse scanning coupled with real-time image analysis to extract sample information with minimum beam exposure. These experiments represent the first steps toward transforming the modern STEM from a characterization to a fabrication platform.

2:45 PM CM05.16.05
Towards a Vertical Nanopillar-Based Single Electron Transistor—A High-Temperature Ion Beam Irradiation Approach Xiaomo Xu[1, 2], Karl-Heinz Heinig[1], Wolfhard Möller[1], Ahmed Gharbi[3], Raluca Tiron[3], Hans-jürgen Engelmann[1], Lothar Bischoff[1], Thomas Pruefer[1], René Hübner[1], Stefan Facsko[1], Gregor Hlawacek[1] and Johannes von Borany[1]; [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany; [2]Faculty of Physics, Technische Universität Dresden, Dresden, Germany; [3]CEA-LETI, Grenoble, France.

We propose an ion irradiation based method to fabricate a single Si nanocrystal embedded in a Si(001)/SiO_2/Si nanopillar layer stack as a prerequisite for manufacturing a CMOS-compatible, room-temperature Si single electron transistor. After either 50 keV broad beam Si^+ or 25 keV focused Ne^+ beam from a helium ion microscope (HIM) irradiation of the nanopillars (with diameter of 35 nm and height of 70 nm) at room temperature with a medium fluence (2e16 ions/cm^2), strong plastic deformation has been observed which hinders further device integration. This differs from predictions made by the Monte-

Carlo based simulations using the program TRI3DYN. We assume that it is the result from the ion beam induced amophisation of Si accompanied by the ion hammering effect. The amorphous nano-structure behaves viscously and the surface capillary force dictates the final shape. To confirm such a theory, ion irradiation at elevated temperatures (up to 672 K) has been performed and no plastic deformation was observed under these conditions. Bright-field transmission electron microscopy micrographs confirmed the crystallinity of the substrate and nanopillars after HT-irradiation.
When a semiconductor material such as silicon is heated above its amorphisation critical temperature during ion irradiation, it stays crystalline due to an interplay between ion damage and dynamic annealing process. Viscous flow does not occur for the crystalline nano-structures and the shape remains intact. This effect has been observed previously mainly for swift heavy ions and energies higher than 100 keV. Such high-temperature irradiation, when carried out on a nanopillar with $Si/SiO_2/Si$ layer stack, would induce ion beam mixing without suffering from the plastic deformation of the nanostructure. Due to a limited mixing volume, single Si-NCs would form in a subsequent rapid thermal annealing process via Oswald ripening and serve as a basic structure of a gate-all-around single electron transistor device.
This work is supported by the European Union's H-2020 research project 'IONS4SET' under Grant Agreement No. 688072.

3:00 PM BREAK

SESSION CM05.17: In Situ Studies of Radiation Damage
Session Chairs: Grace Burke and Pär Olsson
Thursday Afternoon, November 29, 2018
Hynes, Level 2, Room 202

3:15 PM CM05.17.01
***In Situ* Studies of Nanoporous Niobium During Dealloying and Irradiation** Maria Kosmidou[1], Nicolas J. Briot[1], Nathan J. Madden[2], Remi Dingreville[3], Jessica A. Krogstad[2], Khalid Hattar[3], John Balk[1] and Azin Akbari[1]; [1]University of Kentucky, Lexington, Kentucky, United States; [2]University of Illinois at Urbana-Champaign, Urbana-Champaign, Illinois, United States; [3]Sandia National Laboratories, Albuquerque, New Mexico, United States.

Nanoporous materials are potentially advantageous in radiation environments, due to the high amount of ligament surface area that can act as a sink for defects produced during irradiation. A special technique, thermal dealloying in vacuum, is utilized for the formation of nanoporous refractory metals. In-situ thermal dealloying experiments in the TEM are performed on Nb-Mg alloys for fabrication of nanoporous niobium (np-Nb), where the precursor alloy composition range and dealloying temperature are the main parameters for controlling morphology and residual Mg in the final nanoporous structure. Subsequently, heavy irradiation of np-Nb at different energies and varying total ion dose are performed on samples inside the TEM, creating defect structure within ligaments, as well as possible changes in the overall porous network structure. This presentation will address the formation of np-Nb and its behavior during heavy ion irradiation, with emphasis on the ability of nanoporous structures to accommodate radiation damage.

3:30 PM CM05.17.02
***In Situ* Measurement of the Dislocation Density of Steel During Plastic Deformation Using Ultrasound** Vicente Salinas[1, 2], Claudio Aguilar[4], Rodrigo Espinoza[3], Fernando Lund[1] and Nicolás Mujica[1]; [1]Physics Department, Universidad de Chile, Santiago, Chile; [2]Núcleo de Matemáticas, Física y Estadística, Facultad de Ciencias, Universidad Mayor, Santiago, Chile; [3]Departamento de Ingeniería Química, Biotecnología y Materiales, Universidad de Chile, Santiago, Chile; [4]Departamento de Ingeniería Metalúrgica y Materiales, Universidad Técnica Federico Santa María, Valparaíso, Chile.

We report results of local measurements of the speed of transverse waves in 304L steel under standard testing conditions, continuously as a function of applied load. The result, as expected, is independent of stress in the elastic regime, but there is a clear change, consistent with a proliferation of dislocations, as soon as the yield strength is reached. To interpret the results, we use a theoretical model that blames the change in wave speed on the interaction of elastic waves with oscillating dislocation segments. The relevant formulae quantitatively relate the change in wave velocity with dislocation density Λ and segment length L, thus obtaining a continuous relation between dislocation density and externally applied stress.

The experimental results are compared in some detail with similar measurements obtained with aluminum [1]. The change in velocity as a function of applied stress is smaller in steel than in aluminum, consistent with a higher Peierls barrier.

The theory can be worked out replacing the dislocation segments by dislocation loops [2]. Similar formulae result, in which the dislocation segment length is replaced by the dislocation loop radius. Available STEM images of dislocation loops in FeCrAl after neutron irradiation [3] suggest a density of dislocation loops sufficient to provide a measurable signal. Ultrasound could thus become a non destructive measuring tool for dislocation density in fuel cladding alloys.

[1] V. Salinas et al., Int. J. Plasticity 97 (2017) 178-193.
[2] N. Rodríguez et al., J. Appl. Phys. 106 (2009) 054910.
[3] K. G. Field et al., J. Nucl. Mater. 495 (2017) 20-26.

3:45 PM CM05.17.03
A New Solid Solution Approach for the Study of Self-Irradiation Damage in Non-Radioactive Materials Tzvi Tempelman[2], Michael Shandalov[1], Yuval Golan[2] and Eyal Yahel[1]; [1]Physics, NRCN, Beer-Sheva, Israel; [2]Materials Engineering, Ben Gurion University of the Negev, Beer-Sheva, Israel.

We present a new method to produce a model system for the study of radiation damage in non-radioactive materials. The method is based on homogeneous incorporation of ^{228}Th ions in PbS thin films using a small volume chemical bath deposition (CBD) technique. Controlled doping of the thin films with minute amounts of a-emitting radioactive elements such as thorium is expected to provide a unique path for studying self-irradiation damage in materials without the need of sealed enclosures, such as gloveboxes and hot cells.
We developed CBD process for controlled doping of PbS thin films with active ^{228}Th and stable ^{232}Th isotopes [1]. The ^{228}Th-doped films were characterized using x-ray powder diffraction (XRD), which indicated a single phase material. Film morphology and thickness were determined using scanning electron microscopy (SEM). Energy dispersive spectroscopy (EDS) mapping in the analytical transmission electron microscope (A-TEM), x-ray photoelectron spectroscopy (XPS) depth profiles and a-autoradiography indicated that the Th ions were homogeneously distributed throughout the films, suggesting Pb substitution by Th ions in the crystal lattice. Electrical resistivity studies were performed and decay-event damage accumulation was measured, followed by isochronal annealing, which presented two defect relaxation stages and additional sub-stages [2]. Photoluminescence (PL) studies of emissive defect states created in the bandgap due to self-irradiation are on the way. This is the first report on self-irradiating damage studies in IV-VI

semiconductors and the resulting films present a novel method for the analysis of dilute defect systems in materials.

[1] T. Templeman, M. Shandalov, V. Ezersky, E. Yahel, G. Sarusi, Y. Golan, "Enhanced SWIR Absorption in Chemical Bath Deposited PbS Thin Films Alloyed with Thorium and Oxygen", *RSC Advances*,**6** (2016) 88077.
[2] T. Templeman, M. Shandalov, E. Yahel, M. Schmidt, I. Kelson and Y. Golan, "A New Solid Solution Approach for the Study of Self-Irradiating Damage in non-Radioactive Materials", *Scientific Reports*, **7** (2017) 2780.

4:00 PM CM05.17.04
***In Situ* Irradiation of Carbide Based Hybrides—Challenges and Differences** Karl R. Whittle[1], Tanagorn Kwamman[2], Glyn Cobourne[1], W Mark Rainforth[2] and Philip D. Edmondson[3]; [1]University of Liverpool, Liverpool, United Kingdom; [2]The University of Sheffield, Sheffield, United Kingdom; [3]Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States.

Binary carbide hybrids based on TiC and SiC, with mixed properties of both single carbided, have been proposed for application within nuclear reactor cores. For such applications to be viable, their response to irradation induced damage, must be more fully understood. To achieve this a selection of different TiC-SiC mixtures have been irradiated in situ, at the IVEM facility at Argonne National Laboratory, followed by high resolution electron imaging and diffraction at the University of Liverpool, and Oak Ridge National Laboratory. This analysis has indicated that there is a behavourial change with variation in composition, with increasing TiC content giving rise to a system that is more resiliant to increasing levels of damage.

4:15 PM CM05.17.05
***In Situ* Characterization of Single Ion Strikes in Single Crystal Silicon** Anthony Monterrosa, James Stewart, Patrick Price, Remi Dingreville and Khalid Hattar; Sandia National Laboratory, Albuquerque, New Mexico, United States.

Understanding the evolution of damage cascades caused by energetic particle strikes has proven difficult for experimental studies. Individual cascade events occur over an extremely limited spatial and temporal scale, which has left most of their exploration to modeling efforts. However, recent in-situ transmission electron microscopy developments have begun to close this gap, allowing for detailed experimental studies of damage cascades. In-situ and ex-situ irradiations were performed at the Sandia Ion Beam Laboratory with Au ions ranging from 46 keV to 1 MeV on single crystal silicon to explore a wide range of cascade morphologies. Procession electron diffraction (PED) was used to experimentally measure the changes in volumetric strain induced by single cascade events by measuring changes in the diffraction spot area. The experimental results were coupled with a molecular dynamics (MD), which simulated the radiation damage events and provided the size, shape, and composition of the defect damage, along with virtual selected area electron diffraction (SAED) patterns. Information from a single damage cascade can be acquired through direct comparison between the experimental diffraction patterns and the virtual SAED patterns. Additionally, the coupling of the in-situ ion beam with a dynamic transmission electron microscope (DTEM) can provide the unique capability to experimentally probe the collapse of the damage cascade on a nanosecond timescale.

4:30 PM *CM05.17.06
Using Advanced Analytical TEM to Study Irradiation-Induced Microstructural Evolution in Fe- and Ni-Base Alloys Grace Burke[1] and Joven Lim[2]; [1]Materials Performance Centre, University of Manchester, Manchester, United Kingdom; [2]UKAEA Materials Research Facility, Didcot, United Kingdom.

The requirement to predict long-term behavior of alloys used in nuclear power systems requires the ability to generate high irradiation-induced damage levels in these alloys and the ability to characterise the nanoscale changes in the microstructure leading to changes in mechanical properties. These nanoscale changes in microstructure lead to the evolution of a variety of features including solute-enriched clusters, segregation, precipitation and defects that directly affect the properties of materials. Neutrons, ions and protons all promote these nanoscale changes. Thus, the ability to generate high dose damage levels using ions or protons represents a potential route to producing microstructures that have similar characteristics to those generated by neutrons. The characterisation of these nanoscale features provides data essential for fundamental modelling efforts. This presentation will discuss advanced analytical electron microscopy studies of microstructural evolution in several Fe-base and Ni-base alloys.

SESSION CM05.18: Poster Session II: Fundamentals of Material Property Changes Under Irradiation
Session Chairs: Kazuto Arakawa, Chu Chun Fu, Pär Olsson and Michael Short
Thursday Afternoon, November 29, 2018
8:00 PM - 10:00 PM
Hynes, Level 1, Hall B

CM05.18.01
Particle Irradiation Induced Defects in High Temperature Superconductor Prashanta M. Niraula[1], Eiman Bokari[1], Shahid Iqbal[1], Lisa Paulius[1], Matthew Smylie[2], Ulrich Welp[2], Wai-Kwong Kwok[2] and Asghar Kayani[1]; [1]Physics, Western Michigan University, Kalamazoo, Michigan, United States; [2]Argonne National Laboratory, Lemont, Illinois, United States.

Particle irradiation technique can be used to induce defects in High Temperature Superconductor (HTS) such as $Y_1Ba_2Cu_3O_{7-x}$ (YBCO). These defects can act as pinning centers to restrict the motion of magnetic flux vortices, which as a result can increases the critical current density (J_c). Depending on the mass and energy of the particle and the properties of the target material, irradiation enables the creation of defects with well-controlled density and topology, such as points, clusters, collision cascades or linear tracks. Furthermore, irradiation allows for the combination of defects with different morphologies or to add to pre-existing defects at densities that are interesting for vortex pinning, all without changing the chemistry of the sample. This creates the so-called mixed pinning landscapes that have proven very effective in vortex pinning, particularly in high magnetic fields. In this work, HTS coated conductors containing Barium zirconate nanorods as pre-existing defects were irradiated with 50 MeV copper ions at angles of 0º, 15ºand 30º from the crystallographic c-axis. We observed moderate enhancement of J_c at 5 K at high fields in samples irradiated at 30º and a suppression in others.

CM05.18.02
Photoluminescence Properties in Aliphatic-Aromatic Biodegradable Polymers Induced by Low Energy Radiation Elisete L. Cunha[2], Thiago Schimitberger[2], Victor A. Rosas[1] and L.O. Faria[1]; [1]Materials, Centro de Desenvolvimento da Tecnologia Nuclear, Belo Horizonte, Brazil; [2]Nuclear Engineering, Federal University of Minas Gerais, Belo Horizonte, Brazil.

Poly(butylene adipate-co-terephthalate) (PBAT) is a biodegradable aliphatic-aromatic copolyester. The radio induction of photoluminescence (PL) properties in PBAT, after exposure to high doses of gamma radiation, was firstly reported by T. Schimitberger *et al.* (2014). The material shows the highest photo-stimulated luminescence emission when excited with a light-emitting diode (LED) source at wavelengths ranging from 370 to 405 nm. These new PL properties may have great potential for applications in *in vitro* imaging of human cancer, bio-imaging devices and radiation dosimetry. However, most of these applications are possible just for biocompatible materials. In this context, PBAT-based polymer nanocomposites have been reported to present biocompatibility features. Also, recently, films of PBAT irradiated with ultraviolet light (UV) in the presence of O_2 gas atmosphere has proved to have bioactivity. This characteristic increases with the time of exposure of the films to the UV irradiation in atmosphere of O_2(g), due to the functionalization with the insertion of polar groups on their surface.
In this paper, we report the radio induction of photoluminescence (PL) properties in PBAT, after exposure to low energy UV radiation. In this investigation, films of PBAT produced by using the *wire-bar coating* technique were exposed to UV for periods of time ranging from 50 to 1,000 hours. For comparison purposes, the irradiations were performed under air and O_2(g) atmospheres. PL emission, UV-Vis and FTIR spectrometry were used to characterize the relationship between *UV doses x PL Intensities* and to reveal the mechanisms behind the post-irradiation PL character in PBAT samples. Peak fitting of FTIR data using Gaussian lines indicates the radio induction of molecules attached to aromatic hydrocarbons via chain scission. The high quantum yield emission of UV-induced PL near 500 nm, observed in PBAT, is a very interesting finding because it involves the development of a new cheap biodegradable photoluminescent polymer that
could find applications in radiation dosimetry and bio-imaging.
References

[1] Schimitberger, Thiago; Bianchi, Rodrigo F.; Curti, Priscila S.; Faria, Luiz O**.** Photoluminescence Properties in Aliphatic-Aromatic Biodegradable Polymers Induced by Gamma Radiation. IEEE Transactions on Nuclear Science, v. 61, p. 1-1, 2014. DOI: 10.1109/TNS.2014.2322974

[2] Fukushima, Kikku; Rasyida, Amaliya; Yang, Ming-ChienYang. Characterization, degradation and biocompatibility of PBAT based nanocomposites**.** Applied Clay Science Vols 80–81, p. 291-298, 2013. DOI: https://doi.org/10.1016/j.clay.2013.04.015

[3] Schmitz, Daiane Cristina. Comportamento de Biocompatibilidade de Filmes de PBAT Previamente Tratados com UV na Presença de Fluidos Corporais. PT-UFRGS 2016. DOI: http://hdl.handle.net/10183/153304

CM05.18.03
Vertical Nanowires Enhanced X-Ray Radiation Damage of Cells Qingxuan Li, Liyuan Zheng and Ming Su; Northeastern University, Boston, Massachusetts, United States.

Cell behavior is affected by nanostructured surface, but it remains unknown how ionizing radiation affects cells on nanostructured surface. This abstract reports an experiment investigation of X-ray radiation induced damage of cells placed on an array of vertically aligned silicon nanowires. X-ray photoelectrons and secondary electrons produced from nanowire array are measured and compared to those from flat silicon substrate. The cell functions including morphology, viability, adhesion and proliferation have been examined and found to be drastically affected when cells are exposed to X-ray radiation, compared to those sitting on flat substrate and those only exposed to X-ray. The enhanced cell damage on nanowires upon X-ray exposure is attributed to nanowire enhanced production of photoelectrons including Auger electrons and secondary electrons, which have high escaping probability from sharp tips of nanowires. The escaped photoelectrons ionize water molecules and generate hydroxyl free radicals that can damage DNAs of cells. An inference of this work is that the contrast in scanning electron microscopy is useful in assessing the effects of nanomaterials for enhanced X-ray radiation therapy.

CM05.18.04
Study on H in Fe/W Interface by DFT Calculation Jingming Shi and Naoyuki Hashimoto; Hokkaido University, Sapporo, Japan.

In the development of fusion reactors, tungsten (W) and reduced activation ferritic /martensitic (RAFM) steel are strong candidates as divertor and structure materials of blanket. Many researches have devoted a lot of effort on the irradiation effect on W as well as on RAFM steel. Obviously, W component should be connected to RAFM steel in reactor, thus the cohesion properties between W and RAFM steel play an important role in their performance. In this study, a Fe(001)/W(001) interface configuration is built as a model for the cohesion between RAFM steel and W. The mono-vacancy and the dissolution behavior of H in the interface region are studied. This work is conducted by density functional theory (DFT) calculation. And all calculations are implemented by GPAW, a DFT calculation code.
Results show that, in the interface region, the lattice of Fe and W are different from in bulk materials. The vacancy formation energy (*E*v) in W side in interface region is smaller compared it in bulk W, while the *E*v in Fe side in interface is slightly higher than it in bulk Fe. From Fe side to W side, the dissolution energy of hydrogen in interface increases which indicates that the H prefers to stay in Fe side and the H in W side could diffuse to Fe side since no sink effect of the interface is found. And, the effect of vacancy and H atom on strength of the Fe/W interface is investigated. Vacancy in interface region make the strength of interface decrease. At most cases, H atom also make the strength of interface decrease.

CM05.18.05
Study of Nanopatterning Formation Dynamics by Ion Beam Bombardment on GaSb Angelica Hernandez, Rene Asomoza-Palacio, Miguel Avendaño and Yuriy Kudriavtsev; CINVESTAV, Mexico City, Mexico.

Abstract: In this work we have studied the formation of ordered nanostructures on the surface of gallium antimonide (GaSb) under ion irradiation. The substrate temperature was varied from room temperature (RT) up to 300 °C. The GaSb surfaces were bombarded by using a polyatomic bismuth ion beam (Bin+), from where Bi1+ and Bi3+ were selected as the incident ions, respectively. The energy beam utilized was 15 and 30 keV, whilst the angle of incidence was chosen to be 0° or 45°.
Different morphologies were observed for 45° angle of incidence and elevated substrate temperature depending on ion fluences. The morphological characteristics of nano dot patterns formed at normal incidence of the ion beam, were studied by atomic force microscopy (AFM). Also, the chemical and structural properties were characterized by micro Raman. We carried out a detailed study of the effects of substrate temperature, ion fluence, type of incident ion, energy beam and angle of incidence on the morphological characteristics of nano dot patterns.

CM05.18.06
The Effect of Radiation Fluence on the Performance of a High Voltage CMOS Monolithic Active Pixel Sensor Using TCAD Simulation Tuan A. Bui, Hiep Tran, Geoffrey Reeves, Patrick W. Leech and Anthony Holland; School of Engineering, RMIT University, Melbourne, Victoria, Australia.

Pixel semiconductor detectors with position sensitivity have played a critical role in the success of high energy physics experiments. Located only a few centimeters from the collision point of the beam at the innermost layer of the ATLAS detector system, the pixel detectors and their electronics have been

required to withstand a high fluence of radiation. This paper presents a simulation using computer aided design (TCAD) of the effect of variation in the fluence of the radiation on the performance of a high voltage complementary metal-oxide-semiconductor (HV-CMOS) monolithic active pixel sensor (MAPS). The simulation has been performed using an existing TCAD model of a single pixel HV-CMOS MAPS with an on-pixel source follower amplifier [1]. The model was based on the impact of a minimum ionization particle which generated ~28000 electron-hole pairs in a thickness of silicon of 300µm when fully depleted at 120V bias [1]. The present work has expanded the modeling of the behavior of the detector by examining the effect of variation in the fluence of the radiation in the range 10^{13} - 10^{16} n_{eq}/cm^2. The induced radiation damage has been simulated using a 3-level trap model for a p-Si detector [2] to investigate the degradation in the performance of the detector as a function of varying fluence. The simulations of single event upset have also been performed on the NMOS and PMOS transistors which were used to implement the on-pixel readout circuit.
[1] T. A. Bui, G. K. Reeves, P. W. Leech, A. S. Holland and G. Taylor, MRS Advances, pp. 1-7, (2018).
[2] F. Moscatelli, D. Passeri, A. Morozzi, R. Mendicino, G.-F. Dalla Betta, and G. Bilei, IEEE Trans Nucl Sci, 63, 2716 (2016).

CM05.18.07
Induced Order-Disorder Transformations in Fluorite Based Oxides Michelle R. Moore[1], Maulik K. Patel[1, 2], Susan Morgan[5], David Hambley[5], Kurt Sickafus[3], Gianguido Baldinozzi[4] and Karl R. Whittle[1]; [1]School of Engineering, University of Liverpool, Liverpool, United Kingdom; [2]Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, New Mexico, United States; [3]Materials Science and Engineering, The University of Tennessee, Knoxville, Knoxville, Tennessee, United States; [4]Laboratoire Structures, Propriétés et Modélisation des Solides, CentraleSupelec, Gif-sur-Yvette, France; [5]National Nuclear Laboratory, Seascale, United Kingdom.

Fluorites and fluorite-related materials are of interest within the nuclear context, primarily due to the use of UO_2 as the predominant fuel in reactors, along with pyrochlore/zirconolite/fluorite being a key waste form for actinide immobilisation. This study examines the radiation damage response of fluorite-derivative structures within the Sc_2O_3-HfO_2 system. Such oxides, for example δ-$Sc_4Hf_3O_{12}$, γ-$Sc_2Hf_5O_{13}$, and β-$Sc_2Hf_7O_{17}$ exhibit distortion away from the ideal fluorite crystal lattice undergoing an order-to-disorder transformation upon irradiation. Samples of γ-$Sc_2Hf_5O_{13}$, and β-$Sc_2Hf_7O_{17}$ were irradiated by 400 keV Ne and 600 keV Kr under cryogenic conditions with fluences between $1x10^{14}$-$4x10^{15}$ ions cm^{-2}. Irradiations by 400 keV He were undertaken on δ-$Sc_4Hf_3O_{12}$ and γ-$Sc_2Hf_5O_{13}$ samples at 500°C, at fluences of $1x10^{15}$ and $1x10^{16}$ ions cm^{-2}.

Analysis of the induced changes has been undertaken using grazing incidence X-ray diffraction (GIXRD), Raman spectroscopy and electron imaging/diffraction, to elucidate the order to disorder transformation. The results will then be compared with similar transitions in other nuclear-related oxides, such as the pyrochlore-disordered fluorite transformation.

CM05.18.08
Irradiation Behavior of Multi-Layer Coatings on ZIRLO for Accident Tolerant Fuel Cladding Jamie K. Nanson[1], Maulik K. Patel[1], Yongqiang Wang[2] and Karl R. Whittle[1]; [1]School of Engineering, University of Liverpool, Liverpool, United Kingdom; [2]Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, New Mexico, United States.

The continued development of accident tolerant fuels/coatings is a key driver in the continuing nuclear renaissance, in a bid to minimize the chances of an event similar to Fukushima Daiichi repeating. As a consequence of this we have examined a range of multi-layer coatings based on Nb, Al, and C, focusing in particular on how they behave under ion irradiation as a proxy for neutron damage expected within a core. Once irradiated these coated samples underwent oxidation testing at 360 ºC, modelling the conditions expected within a PWR.The coatings were irradiated with 400 keV Kr and 150 keV C, both at 300 ºC , across a range of fluences, up to 9 x 10^{16} ions cm^{-2}.The damaged materials were subsequently analysed using electron microscopy (SEM, EDX, and TEM) coupled with grazing incidence X-ray diffraction (GIXRD) and Raman spectroscopy. Results indicate there is significant improvement over uncoated ZIRLO under the same conditions, suggesting the possibility of use within a reactor core.

CM05.18.09
Broad-Beam Simulations of Si^+ Ions in Stacked Si/SiO_2 Heterostructures for Meta-Stable SiO_x Formation Christoffer Fridlund[1], Kai Nordlund[1] and Flyura Djurabekova[1, 2]; [1]University of Helsinki, Department of Physics, Helsinki, Finland; [2]Helsinki Institute of Physics, Helsinki, Finland.

There is no easy way to commercially manufacture Single Electron Transistors (SET) at large scale. A method for creating the nanostructures needed for operating SETs at room temperature (RT), is to use low energetic broad-beam irradiation (25 to 60 keV) inducing atom-mixing over the interfaces in a stacked Si/SiO_2/Si semiconductor structure. An excessive amount of Si atoms are transfered into the SiO_2 matrix from the surrounding Si layers. By controlling the fluence of the broad beam, it is possible to control the atomic density profile of the Si atoms along the axis of the irradiation.

The excessive Si in the SiO_2 layer, give rise to a difference in the atomic density profile around the interfaces, and meta-stable SiO_x is formed in these regions. When the system is annealed, Si nanoclusters form through self-assembly towards the center of the SiO_2 slab. Both the size and the location of the nanocluster is crucial for flawless operation of the SET at RT. The diameter of the SET should be around 2 nm, and the tunneling distances should be in the range of 1.5 nm to 2.5 nm both above and below the nanocluster. A 7 nm thick SiO_2 slab with 25 nm c-Si on top and 20 nm c-Si below, are cut into pillars for the simulations. We use Molecular Dynamics (MD) to simulate the 25 keV Si^+ broad-beam conditions in various Si/SiO_2systems. The annealing process is simulated with Kinetic Monte Carlo (KMC) based on the density profiles from the MD simulations. The Stillinger-Weber-like Watanabe potential was used to simulate Si-Si, Si-O, and O-O interactions. The interactions of the kinetic ions were handled by the universal repulsive ZBL potential. To speed up the MD simulations, we allowed 10 ion cascades to develop consecutively (1.5 ps each), all ending with a temperature quench back to RT, alternated by a longer relaxation run (5.0 ps). Repeating the steps until the desired fluence of 1.5e16 cm^{-2} was acheived.

During irradiation, the systems are shrinking along the beam direction. This is in good agreement with experiments done on similar pillars at RT. However, while the dynamics in the experiment most likely come from sputtering effects, the dynamics of the simulations are a combination of both sputtering and the hammering effect, caused by short simulation times, not allowing the system to recrystallize inbetween the ion cascades. Coordination analysis indicate some overcoordination of the O, but this is expected due to the meta-stable SiO_x. Reference simulations of pure Si pillars generate the same general shape change.

The work has been funded by Svenska Kulturfonden and the European Union's Horizon 2020 research and innovation program under grant agreement No 688072.

CM05.18.10
Influence of Temperature on Nanofabrication Using Swift Heavy Silver (Ag^{+7}) Ion Irradiation on GaSb Satish Kumar[1, 2], Ajit K. Mahapatro[2] and Puspashree Mishra[1]; [1]DRDO, Solid State Physics Laboratory, Delhi, India; [2]University of Delhi, Delhi, India.

Gallium antimonide (GaSb) nanostructures have stimulated interest because of unique quantum confined nanoscale properties. GaSb has low band gap and

high hole mobility, which makes it a suitable candidate for various potential applications such as high frequency electronics, low power consumption electronics, near to mid infrared optoelectronics, and gas/chemical/bio-sensing devices etc. Ion irradiation technique has been effectively used to fabricate several kinds of nanostructures such as nanofibers or nanodots etc. The growth of semiconductor nanostructures in a controlled manner is the key for the development of future optoelectronic devices. This technique is versatile, cost effective, well controlled and reproducible for the spontaneous fabrication of different shapes of semiconductor nanostructures.
This work presents the fabrication of GaSb nanodots using swift heavy silver (Ag^{+7}) ion irradiation with ion fluence range from $1x10^{12}$ to $1x10^{14}$ ions/cm^2 under normal incidence at two different temperature (300K and 77K). The GaSb epitaxial layers were grown on semi-insulating gallium arsenide (GaAs) (001) substrates using molecular beam epitaxy (MBE). The surface morphology and crystalline quality of pristine and silver ion irradiated GaSb samples were characterized using atomic force microscopy (AFM) and Raman spectroscopy techniques respectively. The AFM micrograph of pristine GaSb sample shows that the surface is featureless and smooth with minimum rms (root mean square) surface roughness of 1.51 nm. Room temperature ion irradiation on GaSb samples clearly indicates the formation of well defined nanodots. The nanodots seem to be uniformly distributed over the surface and they coalesce with each other give rise to bigger dots for increasing ion fluences. Over a certain ion fluence ($1x10^{14}$ ions/cm^2) a smooth surface is observed. The presence of nanodots was also observed on irradiated GaSb samples using similar parameters at low temperature (77K) ion irradiation. However, the nanodots at 77 K are not well developed and are irregularly shaped as compared to the 300 K ion irradiation. The smoothening of irradiated surface starts at earlier ion fluence ($6x10^{13}$ ions/cm^2) for 77K compared to 300K samples ($1x10^{14}$ ions/cm^2). The dot morphology at the two different temperatures are analyzed by considering the different rates of surface diffusion of adatoms. Raman spectrum for pristine GaSb sample indicates good crystalline quality of epitaxial layer. The LO and TO phonon modes are found to shift to lower wave numbers with increasing ion fluence for irradiated GaSb surfaces at both temperature (77 and 300K). This is due to the presence of tensile strain in irradiated GaSb samples. Raman analysis reveals higher disorder in silver irradiated GaSb samples at 77K compared to 300K samples.

CM05.18.11
Defect Formation on Ultrathin Films with Highly Charged Ions Ardak Ainabayev[3], Masahito Niibe[4], Mititaka Terasawa[4] and Zinetula Z. Insepov[1, 2, 3]; [1]School of Nuclear Engineering, Purdue University, West Lafayette, Indiana, United States; [2]Condensed Matter Physics, National Research Nuclear University MEPhI, Moscow, Russian Federation; [3]Nazarbayev University, Astana, Kazakhstan; [4]Laboratory of Advanced Science and Technology for Industry, Kouto, Japan.

Irradiation of ultrathin films by highly charged ions (HCI) offers a very shallow modification of the surfaces by easily controlling of the density and the size of defects by changing fluence of ions (ion current and irradiation time) and the potential energies of bombarding ions.
Defect formation in the samples of ultrathin films such as graphene, graphene oxide, and MoS_2 by HCI irradiations were studied. Highly-charged ions (HCI) Xeq+ (q = 22, *E*kin=400 keV), were used to irradiate ultrathin films at National Nuclear Center, Astana, Kazakhstan, using a DC-60 cyclotron accelerator. Since the mechanisms of defect formation, charge neutralization and screening during HCI interaction with graphene are not clear and require further investigations [1], the study of the irradiated samples was conducted using Raman spectroscopy, atomic force microscopy (AFM), and NEXAFS (Near-Edge X-ray Absorption Fine Structure). The Raman spectroscopy (Horiba) study of the irradiated samples was conducted by a 632 nm laser wavelengths and 100x objective with a laser spot size of ~1 μm, 2 mW power and atomic force microscopy (AIST NT) measurements were carried out in a tapping mode by SUPERSHARPSILICON™ AFM probes for high resolution. NEXAFS spectroscopy measurements were carried out at the NewSUBARU BL09A beamline of the New SUBARU SRing8 LASTI facility at the University of Hyogo, using total-electron yield (TEY) method and without uncompleted correction of energy.

[1]. E. Gruber, R.A. Wilhelm, R. Pétuya, et al, Ultrafast electronic response of graphene to a strong and localized electric field. Nat. Commun. 384 (2016) 13948.

CM05.18.12
Influence of Temperature, Humidity and Light-Intensity on the Conductivity of Solution-Processed Zinc Oxide Thin Films José B. Cantuária[2], Giovani Gozzi[1] and Lucas Fugikawa Santos[1, 2]; [1]São Paulo State University, Rio Claro, Brazil; [2]IBILCE, São Paulo State University, São José do Rio Preto, Brazil.

Zinc oxide (ZnO) is a n-type transparent semiconductor which can be processed by low cost techniques, as spray-pyrolysis and spin-coating, and can be applied as active layer in a variety of electronic devices, including photodetectors and thin films transistors (TFTs). Electrical properties of ZnO TFTs, as threshold voltage, charge carrier mobility and on/off ratio, are strongly affected when the device it is exposed to room conditions. The current explanation to these effects considers the adsorption of atmospheric oxygen molecules, which acts as traps of charge carriers (electrons). In the current work, we studied the influence of environmental parameters, as temperature, humidity and light irradiance, on the electrical conductivity of spin-coated ZnO thin films. The experiments were performed using ZnO thin films with aluminum electrodes in a planar structure. The electrical current with the device biased at a fixed d.c. voltage was measured as a function of the exposure time to light from a filament/discharge lamp which simulates the solar spectrum (visible and UVA and UVB ranges). Variations on the film conductivity were interpreted as a consequence of adsorption-like and desorption-like processes of charge carrier traps, as atmospheric oxygen. As standard, we considered that desorption-like (adsorption-like) processes improves (reduces) the electrical conductivity and, as consequence, the device electrical current. We obtained that a desorption-like process dominates at the beginning of device irradiation (increasing the electrical conductivity) and, after a maximum current is reached, an adsorption-like process dominates, decreasing the electrical current until to a steady state is achieved. The concentration of carrier traps was determined from the current vs. time curves using the Henry model of adsorption and we verified that adsorption/desorption rates are exponentially dependent on time. The initial adsorption/desorption rate and the time constant of each exponential process were determined and used to evaluate the influence of the environmental parameters. This evaluation was performed using a Plackett-Burman experimental design analysis. The factorial analysis shows that the irradiance is the main factor which influences the adsorption/desorption rates. Environmental factors as the temperature and the humidity influence the overall device conductivity, however, do not presented significant influence on the adsorption/desorption rate, which is basically dependent on the irradiance in the observed range.