Joint ICTP-IAEA Virtual Workshop on Atomistic Modelling of Radiation Damage in Nuclear Systems | (SMR 3573)

04 Oct 2021 - 08 Oct 2021
Virtual, Virtual, Italy

P01 - ABID HUSSAIN Abid Hussain

Evaluation of damage in low energy ion irradiated NiCoCrFePd High Entropy Alloy

P02 - CHAKRAVORTY Anusmita

Damage recovery in Ar irradiated 4H-SiC by SHI

P03 - DARAMOLA Ayobami Daniel

Elementary dislocation properties influencing mechanical behaviour of austenitic High Entropy Alloys (HEAs)

P04 - DELUIGI Orlando

Simulations of primary damage in a High Entropy Alloy: probing enhanced radiation resistance

P05 - HANS Sukriti

ION-INDUCED TRIANGULAR FEATURES SUPERIMPOSED BY NANORIPPLES OF SILICON (001)

P06 - HENDY Mohamed

A multiscale and multiphysics framework to simulate radiation damage in nano-crystalline materials

P07 - IMANI Zeinab Sadat (not presenting)

Dependence of the defect introduction rate induced by MeV ions on the final degradation of the semiconductor detectors

P08 - KOREPANOVA Nadezda (not presenting)

Radiation Effects in 15-15Ti Steel

P09 - LASZYNSKA Ewa

Benchmark experiments with ITER materials irradiated in the JET tokamak – cross-check of the neutron-induced activity results obtained by Laboratories

P10 - NAIR Adithya

Modeling the primary damage in nickel and nickel-based alloys: influence of cascade energies and morphologies in displacement cascades

P11 - ORYEMA Bosco

Atomistic simulation of primary radiation displacements and damage in multi-atomic target using BCA-based SRIM code

P12 - PANDEY Dhanshree

Radiation and its effect on materials

P13 - REALI Luca

Macroscopic elastic stress and strain produced by irradiation

P14 - SHIN Younggak

Reduction of interstitial mobility by multicomponent alloying with transition metal elements in bcc W

P01

Evaluation of damage in low energy ion irradiated NiCoCrFePd High Entropy Alloy

High entropy alloys (HEA) are the proposed materials for the next generation nuclear reactors, because of their good mechanical properties and excellent radiation stability. Incorporation of large size element like palladium(Pd) further enhance the radiation tolerance due to accommodation of the defects locally because of large strain produced by the Pd in the base matrix [3,4]. Thus, a Pd based HEA NiCoCrFePd have been synthesized by Arc-melting technique. The as-prepared got ingot cuts into thin disc of thickness 2 mm and the cold-rolled to reduce the thickness up to 0.5 mm, subsequently homogenized at 1200 oC for more than 24 hrs afterward the samples were mechanically polished to obtain mirror like finish surface. X-ray diffraction technique is used to investigate the phase conformation and phase stability at lower temperature down to 40 K. Mechanically polished surface side were then irradiated using 1.05 MeV Xe+3 at ion fluences ranging from 1x1016 to 1x1017 ions/cm2. XRD studies exhibited an increase in the micro-strain along with reduction in crystallite size. Further, electric transport study is used to evaluate the damage accumulation produced by energetic ions. This study further explores the understanding the mechanism of response of HEA towards low energy ion irradiation.

P02

Damage recovery in Ar irradiated 4H-SiC by SHI

The atomistic features of damage recovery in 4H-SiC are studied utilizing an ultrafast thermal spike with a period of a few picoseconds created by intense ionizing energy deposited using 100 MeV Ag ions. To demonstrate swift heavy induced (SHI) recovery, sequential single ion irradiations with 300 keV Ar and 100 MeV Ag in 4H-SiC are performed in samples with varying degrees of pre-damage and Ag ion fluences (ions/cm2). The findings highlight the importance of various degrees of pre-damage i.e. initial physico-chemical conditions, and irradiation temperature in observing SHI-induced recrystallization, as determined by Rutherford Backscattering/Channeling and Raman spectroscopy. For samples with different initial disorders, the absence of significant crystalline surroundings, and the development of complex defects with homonuclear bonds are found to impede the recovery process. For samples having the same initial pre-damage, the SHI fluence is found to play a significant role in determining the extent of damage recovery. The results are interpreted within the framework of the SHI-induced inelastic thermal spike model.

P03

Elementary dislocation properties influencing mechanical behaviour of austenitic High Entropy Alloys (HEAs)

In HEA, some specific features have been largely reported. Especially high solid solution and strain hardenings, unusual combinations of strength and ductility, slowed down phase transformation kinetics, as well as an improved irradiation resistance. Crystal defects such as dislocation’s structure are obviously at the origin of many observed features. This present work will search for better understanding of the impact of dislocations elementary properties on the plastic behaviour of single phased HEAs thanks to atomistic simulation techniques. In this framework molecular dynamics (MD) will be the main simulation technique used. Static properties (dislocation core structure, stacking fault energy, dissociation of dislocations) will be studied, as a function of local chemical environment and temperature. Then, using a specific MD protocol and dislocation dynamics formalism, dislocation behaviour under stress will be evaluated, with focus on effects of temperature and local chemical composition on lattice stress and dislocation mobility, related to the defect’s character (edge or screw segment). The so-obtained characteristics of dislocations will be used to describe the collective behaviour of defects which can be analysed on macroscopic scale (interaction coefficients and hardening) and compared with mechanical characterisation of the existing HEA, tested in the frame of the same research project (HERIA ANR PRCE).

P04

Simulations of primary damage in a High Entropy Alloy: probing enhanced radiation resistance

High Entropy Alloys attract attention as possible radiation resistant materials, a feature observed in some experiments that has been attributed to several unique properties of HEA, in particular to the disorder-induced reduced thermal conductivity and to the peculiar defect properties originating from the chemical complexity. To explore the origin of such behavior we study the early stages (less than 0.1 ns), of radiation damage response of a HEA using molecular dynamics simulations of collision cascades induced by primary knock-on atoms with 10, 20 and 40 keV, at room temperature, on an idealized model equiatomic quinary fcc FeNiCrCoCu alloy, the corresponding “Average Atom” material, and on pure Ni. We include accurate corrections to describe short-range atomic interactions during the cascade. In all cases the average number of defects in the HEA is lower than for pure Ni, which has been previously used to help claiming that HEA is radiation resistant. However, simulated defect evolution during primary damage, including the number of surviving Frenkel Pairs, and the defect cluster size distributions are nearly the same in all cases, within our statistical uncertainty. The number of surviving FP in the alloy is predicted fairly well by analytical models of defect production in pure materials. All of this indicates that the origin of radiation resistance in HEAs as observed in experiments may not be related to a reduction in primary damage due to chemical disorder, but is probably caused by longer-time defect evolution. [Deluigi2021] Deluigi, O., et al. Acta Materialia 213 (2021): 116951. https://doi.org/10.1016/j.actamat.2021.116951.

P05

ION-INDUCED TRIANGULAR FEATURES SUPERIMPOSED BY NANORIPPLES OF SILICON (001)

Irradiation of silicon surfaces with low energy ions with Argon ions at oblique incidence results in formation of triangular features with elevations and depressions superimposed by nanoripples [1, 2]. These triangular features depend on ion beam irradiation parameters such as ion species, ion energy, angle of incidence and fluence. In this work, we report on the investigation about the ion-induced triangular features on silicon surfaces varying the ion energy, angle of incidence and ion fluence. Triangular features start evolving after 200 eV energy leading to well enhanced features at 300eV and with increase in energy the lateral length of these features increases from 160 nm at 300 eV to 450 nm at 500 eV. These features don't appear when the energy exceeds 500 eV. Also they appear in two categories: elevations and depressions. It was found that there is more number of elevations than depressions when angle of incidence was varied and this number increases up to 67o and decreases after this. As reported by Loew et al. in 2019 [3], dispersion is the responsible mechanism for the formation of triangular features on ripple patterns which is confirmed in our experiments by varying the ion fluence. With increase in the ion fluence, the lateral length of the triangular features increases with the constant base angle. This is also found for all the ion energies studied here i.e. 200 - 500 eV. These triangular features can be described by modified AKS equation. Simulations are performed using this modified equation by Loew and

P06

A multiscale and multiphysics framework to simulate radiation damage in nano-crystalline materials

This work presents a multiscale and multiphysics framework to investigate the radiation-induced damage in nano-crystalline materials. The framework combines two methodologies, including molecular dynamics simulations with electronic effects and long-term atomistic diffusion simulations in nano-crystalline materials. Using this framework, we investigated nano-crystalline materials' self-healing behavior under radiation events. We found that the number of defects generated in nano-crystals during the cascade simulations was less than in single crystals. This behavior was due to the fast absorption of interstitial atoms in the grain boundary network during the cascade simulations, while vacancies migrated to the boundaries in a much longer time scale than interstitial atoms. Thus, nano-crystalline materials showed a self-healing behavior where the number and size of the defects are drastically reduced with time.

P07

Dependence of the defect introduction rate induced by MeV ions on the final degradation of the semiconductor detectors

Particles passing through matter lose energy by means of a variety of interactions and scattering processes, which results in two major effects: collision energy loss and atomic displacement. Displacement damage refers to the dislodging of atoms from their normal lattice sites in a target material by impinging energetic radiation. The resulting damage causes degradation of the electronic and optical properties of materials and devices. That degradation is generally due to the introduction of new energy levels in the semiconductor bandgap, which changes properties such as recombination lifetime. Due to the microscopic and macroscopic effects of ion radiation on semiconductor components, research in this regard is ongoing. The objective of this doctoral dissertation is to obtain the ability to model and simulate the interaction of ions with the matter, to experimentally determine the rate of damage caused by ion radiation on the performance of semiconductor components, and laboratory instrumentation to measure the induced current of ion beam using alpha source. In this study, in addition to C-V and I-V methods, the Ion Beam Induced Charge (IBIC) method will be used to measure the effects of vacancies. Complementary methods such as Positron Annihilation Spectroscopy (PAS) and X-Ray Diffraction (XRD) are used as needed for their unique ability to describe defect configurations and nanostructures in Si samples. To understand the response of Si crystals to ion beam radiation in different energy regimes and radiation conditions, simulation using existing codes will be used, which can create significant openings in the interpretation of experimental data.

P08

Radiation Effects in 15-15Ti Steel

The integrity of materials in reactors is associated with the safety and reliability of a nuclear power plant. The accurate evaluation of radiation effects in a material is one way of controlling the reliability of the material. The study presents an evaluation of radiation effects for 15-15Ti steel as a cladding material in irradiation conditions of the China Initiative Accelerator Driven System (CiADS). We compute displacement cross-section for 15-15Ti steel in NRT and BCA-arc-dpa models, using NJOY2016 and IOTA software suites. Then, based on obtained NRT displacement cross-section and empirical property-dpa correlations, we estimate degradation of the cladding material in the CiADS radiation environment, such as expected swelling and hardening of the steel and failure lifetime of the cladding due to swelling. We also simulate titanium carbide precipitations in the steel under irradiation using Cluster Dynamic. Where point defect production rate was estimated by the BCA-arc-dpa displacement cross-section.

P09

Benchmark experiments with ITER materials irradiated in the JET tokamak – cross-check of the neutron-induced activity results obtained by Laboratories

Due to the lack of the existing material irradiation facility with an intense neutron source characterized by a broad energy spectrum peaked at around 14 MeV, experiments performed at the JET tokamak provide a unique opportunity to check the activation behaviour of the materials used as construction materials of fusion reactors in the real fusion environment. The D-T campaign at JET is planned to take place in 2021 with a total neutron budget of 1.3E21. During the 2019 D-D campaign first irradiation experiments with samples of real ITER materials were performed to optimize procedures and check the level of the neutron-induced activity and capabilities of predicting it via calculations. The selected materials and dosimetry foils that were irradiated in the specially designed long-term irradiation sample holder assembly were installed in the redundant Be evaporator in octant 7. Over a 147-day period of irradiation, a total neutron yield of 3.151E19 neutrons was observed. Following irradiation, the ITER samples were distributed across the five EU gamma-spectrometry laboratories, a.o. to IFJ PAN and IPPLM, for analysis. The poster presents the results of the gamma spectrometry measurements performed at IPPLM.

P10

Modeling the primary damage in nickel and nickel-based alloys: influence of cascade energies and morphologies in displacement cascades

The interaction between high energetic particles and metals causing primary radiation damage has been studied for a long time using molecular dynamics. Five interatomic potentials for nickel differing either by their equilibrium part or by the hardening procedure have been included in this study. A characterization based on static non-equilibrium properties and threshold displacement energy (TDE) was done to look for correlations between the potential characteristics and the cascade properties. The dominating feature of this work is to explore extensive statistics of more than 7000 cascades for each interatomic potential with cascade energies ranging from 0.5 keV to 120 keV in pure nickel. The total number of defects, the number of SIA and vacancy clusters, and the size distributions are analyzed using multivariate multiple linear regression analysis based on seven primary damage descriptors and three morphology descriptors.

P11

Atomistic simulation of primary radiation displacements and damage in multi-atomic target using BCA-based SRIM code

In this study, the vacancy and damage production behaviors for H, He, C and O incident ions on fluorine-doped tin oxide (FTO) thin films were examined by using the full cascade (FC) option of SRIM-2013 code. The quick option was not deployed in this study because many authors have critiqued its applicability in multi-atomic targets. The ion energies were varied from 10 KeV to 10 MeV and the target thickness was adjusted at each ion energy until all the ions are absorbed within the target. The numbers of atomic displacements were evaluated using both the direct computation using the "vacancy.txt" SRIM output file, and the damage energy-based manual manipulation of the Norgett-Robinson-Torrens (NRT) defect production model. We compared the SRIM vacancy.txt results with the ion range and damage in nanostructures" (iradina) code in order to validate the SRIM results. Depth-dependent damage production profile, in unit of displacement per atom (dpa) was calculated using the damage energy approach only. It's observed that the "FC vacancy.txt" method overestimated vacancy production compared to values calculated using the "FC damage energy" method. Also, good agreements were observed between the SRIM and iradina vacancy productions. The dpa rate for O and C ions were found to be higher than that of He and H.

Radiation and its effect on materials

The influence of radiation on the characteristics of solids is of great interest, particularly in nuclear reactors, where the nuclear reactions produce energetic radiations of the neutron, which further cause radiation damage and deteriorate materials with time. Radiation damage happens when an energetic incoming neutron collides with a lattice atom in a material. The interaction or collision allows a significant amount of kinetic energy to be transferred to the lattice atom, which then is dislocated from its lattice position. Such an atom is called the primary knock-on atom (PKA). Because of the presence of PKA in the vicinity of the other atoms, its movement through the lattice causes numerous successive collisions and the formation of secondary knock-on atoms. This results in the collision cascade, which can cause point defects and dislocations in the material. The generation of defects and dislocations constitutes a major reason for structural alterations in materials, which further causes materials to become embrittled at high neutron irradiation. This can have a substantial influence on the functioning of materials and hence reducing their longevity. It is also possible that nuclear transformation of the elements within the material takes place, causing the material to swell. To comprehend the effects of radiation, a thorough understanding of the radiations and their interaction mechanisms with the material, as well as the characteristics of the irradiated material, is required. Atomistic modelling is crucial in this regard, as it provides insight into the fundamental physics governing the radiation damage processes.

P13

Macroscopic elastic stress and strain produced by irradiation

We present a method for computing macroscopic elastic stress and strain arising in components of a fusion power plant during operation. In a microstructurally isotropic material, the primary cause of macroscopic elastic stress and strain fields is the spatial variation of neutron exposure. Under traction-free boundary conditions the volume-average elastic stress always vanishes, signifying the formation of a spatially heterogeneous stress state, combining compressive and tensile elastic deformations at different locations in the same component, and resulting solely from the spatial variation of radiation exposure. Several case studies pertinent to the design of a fusion power plant are analysed analytically and numerically, showing that a spatially varying distribution of defects produces significant elastic stresses in ion-irradiated thin films, pressurised cylindrical tubes and breeding blanket modules.

P14

Reduction of interstitial mobility by multicomponent alloying with transition metal elements in bcc W

We present the first-principles calculations of the defect energetics in W ternary alloys. Two different kinds of solute atoms make a pair and tend to strongly attract a W self-interstitial atoms, forming a solute -interstitial triple complex. The attractive interaction between a solute atom and a self-interstitial atom in W-based binary systems has been reported over the years, however, the calculation results presented here suggest that it can be even stronger in ternary systems. The attractive interaction works as the primary dissociation barrier for the triple defect complex, reducing the interstitial mobility. The dissociation energy needed to break the triple complex can be higher than the mono vacancy migration energy, and it changes the irradiated damage mechanism under the fusion environment where a number of point defects are created due to cascade collisions.