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

T01 - ARADI Emily

Radiation damage suppression in AISI-316 steel nanoparticles: implications for the design of future nuclear materials

T02 - DWIVEDI Prashant

Classical molecular dynamics simulations of hypervelocity nanoparticle impacts on tungsten

T03 - LIN Yeping

Direct Transformation of Stacking Fault Tetrahedrons to Voids under Irradiation in Pure Ni and NiCoCr Medium-Entropy Alloys

T04 - NOCE Simone

Nuclear analysis and assessment of irradiation effects on the Divertor Plasma Facing Components of the DEMO fusion reactor

T05 - SAHU Pooja

Molecular Dynamics Simulations of Simplified Sodium Borosilicate Glasses for Nuclear Field Applications

T06 - SHAH Varun

A experimental-numerical study of microstructural evolution of tungsten under fusion conditions

T01

Radiation damage suppression in AISI-316 steel nanoparticles: implications for the design of future nuclear materials

Self-healing capability of point and extended defects that are introduced by energetic particle irradiation is a desired behaviour to be attained in the design and selection in potential materials for application in extreme environments. Nanoporous materials have potential for achieving higher radiation tolerance due to the presence of many active unsaturable surfaces to which defects may diffuse and thus be effectively annihilated. The effects of heavy ion collisions in the lattice of functional AISI-316 steel nanoparticles (NPs)-which serve as a model for the ligaments in a nanoporous–, are herein investigated in-situ within a transmission electron microscope. Comparisons are made directly with AISI-316 steel in the form of foils and the results show that the fewer radiation-induced defect clusters form in the NPs and that small NPs ($r < 50$ nm) were observed to accumulate fewer defects when compared to larger NPs. Post-irradiation analytical characterisation within a scanning transmission electron microscope (STEM) revealed that the AISI-316 steel NPs may develop a radiation-induced self-passivation (RISP) driven by a solute-drag mechanism: an effect that can potentially enhance their radiation corrosion resistance in the expected extreme conditions of a reactor. The capability of a NP to self-heal irradiation-induced point defects is investigated using the cellular model for active internal and surface sinks. The design of functional nanoscale materials for extreme environments is discussed.

T02

Classical molecular dynamics simulations of hypervelocity nanoparticle impacts on tungsten

P. Dwivedi[1], A. Fraile[2], G. Bonny[3], T. Polcar[1]
[1]*Department of Control Engineering, Faculty of Electrical Engineering, Czech Technical University in Prague, Karlovo náměstí 13, 121 35, Czech Republic*
[2]*Nuclear Futures Institute, Bangor University, Gwynedd, LL57 2DG, United Kingdom*
[3]*Nuclear Materials Science Institute, SCK CEN, Boeretang 200, B-2400 Mol, Belgium*

The presence of dust in the scrape-off layer (SOL) close to the chamber walls is an important issue for the development of fusion reactors [1,2]. Hypervelocity dust particles can be particularly harmful if they collide with tokamak material surfaces. Therefore, controlling plasma-wall interactions is critical to achieve high performance in present day tokamaks. Tungsten (W) is the main candidate as plasma facing components for fusion reactor and will be exclusively used in the ITER divertor [1]. The presence of high velocity impacts has been reported in several studies, with velocities being around 500 m/s to a few km/s [3,4].

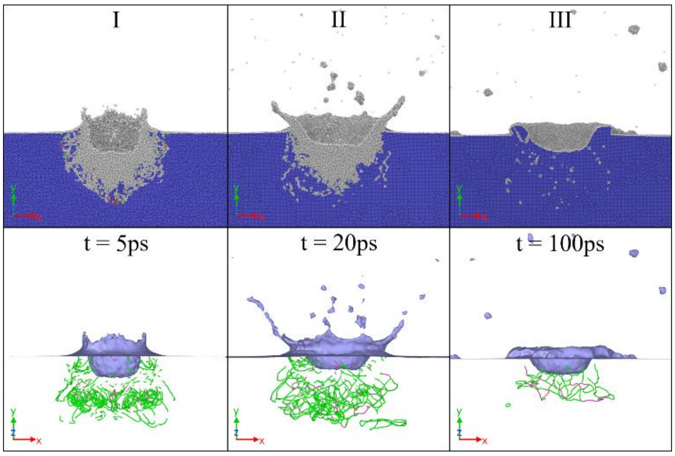

Fig. 1 High velocity impact (5 km/s) of a 40 nm-size W cluster on a W single crystal target, at times 5, 20 and 100 ps. Top row: Color code: Structural analysis. Bottom row: Same system, Blue surface indicate the sputtered atoms and Green curves corresponds to dislocations forest in the target.

In this work, the atomistic mechanisms of damage initiation during high velocity (v up to 9 km/s) impact of W projectiles on W has been investigated using molecular-dynamics simulations involving very large samples (up to 40 million atoms). Various aspects of the impact at high velocities where the projectile and part of the target materials undergo massive plastic deformation, breakup, melting, or vaporization are analyzed. Different stages of the penetration process are identified. Whether the damage occurring in the subsurface of the target is described by collision cascades or as the effect of shock waves will be discussed.

References:

[1] Federici G. *et al* 2001 *Nucl. Fusion* **41** 1967.
[2] Tsytovich V.N. and Winter J. 1998 *Phys.—Usp.* **41** 815.
[3] Castaldo C, *et al*. 2007 *Nucl. Fusion* **47** L5-L9.
[4] Ratynskaia S, , *et al*. 2008 *Nucl. Fusion* **48** 015006.

T03

Direct Transformation of Stacking Fault Tetrahedrons to Voids under Irradiation in Pure Ni and NiCoCr Medium-Entropy Alloys

It is well known that vacancy clusters tend to agglomerate to stacking fault tetrahedrons (SFTs) rather than voids in most face-centered-cubic (fcc) metals. However, void swelling becomes one of the dominant effects of irradiation for materials when temperature is increasing. Recent researches observed that the SFTs coexisted with voids under irradiation in many fcc metals, which indicates an extraordinary relationship between SFTs and voids. In present study, molecular dynamics simulations have been performed to model void creation in pure Ni and NiCoCr Medium-Entropy Alloys (MEAs) with preexisting SFTs. It is observed that the void can be directly transformed from SFT under a single cascade simulation in pure Ni. However, in the NiCoCr MEA, the inhibited void transformation and the coexistence of SFTs and voids are both observed, as observed in experiments. The supersaturated vacancy atmosphere deriving from the collapse of SFTs, induced by displacement cascade simulations, could be the physical origin for void nucleation. The much lower stacking fault energy in NiCoCr MEA than that in pure Ni indicates that the SFT in NiCoCr MEA is more stable, which might be one of the major reasons for the inhibited transformation of SFT into voids in NiCoCr MEA.

T04

Nuclear analysis and assessment of irradiation effects on the Divertor Plasma Facing Components of the DEMO fusion reactor

The Plasma Facing Components (PFCs) of the divertor target contribute to the crucial functions of the divertor such as heat removal and particle exhaust during fusion operation. They are subjected to a very harsh and complex loading environment characterized by intense particle bombardment, high heat fluxes (HHF), fast neutron irradiation, varying stresses and impact loads. In particular way this study is fully devoted to the comprehension of the neutron irradiation impact on the DEMO divertor PFCs performance (lifetime, potential failures phenomena, main critical issues and concerns), which represents one of the main issues still with many pending questions. The achievement of this purpose has required the performing of a detailed neutronics and activation analyses carried out for the first time so thoroughly, followed by a thermo-structural integrity assessment based on the structural design rules defined in the Inelastic Analysis Procedure (IAP) methodology. A first element of novelty of this study, lies in the evaluation of the synergetic effects of high thermo-mechanical loads and intense neutron irradiation expected on the main plasma facing materials (W, Cu/CuCrZr). Three-dimensional neutronics analyses have been performed with the MCNP5 Monte Carlo code and the recommended JEFF 3.3 nuclear data libraries, activation analyses have been performed by means of FISPACT-II inventory code and TENDL 2015 nuclear data libraries. The thermo-structural analyses have been carried-out by means of ANSYS Mechanical. The main critical issues which affect the PFCs performance and lifetime are the strong embrittlement of Cu/CuCrZr and W, as well as the low cycle fatigue duration.

T05

Molecular Dynamics Simulations of Simplified Sodium Borosilicate Glasses for Nuclear Field Applications

Fusion of valuable material properties has lent the acceptance of sodium borosilicate (NBS) glasses for nuclear waste immobilization. In spite of popularity, the mechanisms associated to these properties are yet only partially discovered and need further exploration. Bearing this in mind, the combination of experiments, molecular dynamics (MD) simulations and Dell Yuan and Bray model has been used to understand the role of composition variation for structural and physical aspects of vitrified borosilicate glasses. Experiments have been conducted to evaluate the macroscopic glass parameters: density (ρ), glass transition temperature (Tg) and thermal expansion coefficient (TEC). Experimentally observed trends for ρ, Tg and TEC with composition have been found in good agreement with the MD results. In addition, MD study provides microscopic understanding of the glass structure and phenomena associated with the change in glass composition. A detailed view of local structure and medium range connectivity for the borosilicate glasses has been explored. Owing to large B4 population, the results showed abundant presence of BO4-BO4 connections, hereby omit the generally accepted “B[4] avoidance rule” for glass. The relative propensity for connecting SiO4/BO3/BO4 structural motifs has been found in line with the predictions made by Dell Yuan and Bray model. Furthermore, the effect of composition on the mechanical integrity of NBS glasses including elastic nature, plastic distortion, yielding, breaking stress, and brittle facture has been explored by MD simulations

T06

A experimental-numerical study of microstructural evolution of tungsten under fusion conditions

Tungsten is the candidate material for the plasma facing components of the fusion reactor. This talk will address the bulk microstructure evolution of these W plasma facing components by means of an experimental-numerical approach, where feasible experiments on bulk W under thermal loads are performed, while the influence of synergistic particle and heat loads on microstructural changes are numerically modelled. Under high cyclic thermal loads, significant recrystallization of the W monoblocks is observed, whilst superior thermal fatigue performance. To assess the microstructure-property changes, high temperature tensile and small punch test are performed, while the temporal evolution of the recrystallized fraction in presence of a cyclic temperature gradient is modelled numerically. Moreover, to capture the synergistic defect dynamics due to neutron and ion irradiation in presence of a temperature gradient, a spatially dependent cluster dynamics model applied to a W monoblock geomtery is developed.