MULTISCALE MODELING OF RADIATION DAMAGE IN FE-BASED ALLOYS IN THE FUSION ENVIRONMENT—B. D. Wirth (Department of Nuclear Engineering, University of California Berkeley), G. R. Odette (University of California, Santa Barbara), J. Marian (California Institute of Technology), L. Ventelon (University of California, Berkeley), J. A. Young and L. A. Zepeda-Ruiz (Lawrence Livermore National Laboratory)

EXTENDED ABSTRACT

Ferritic alloys represent a technologically important class of candidate materials for plasma-facing first wall structures in future fusion energy facilities. Predicting their in-service performance requires a detailed understanding of the mechanisms of defect accumulation and microstructure evolution. The physical processes involved in radiation damage are inherently multiscale and hierarchical, spanning length and timescales from the atomic nucleus to meters and picosecond to decades. In this paper, we present a multiscale modeling methodology to describe the accumulation of radiation damage and the corresponding effects on material microstructure and property degradation within the fusion energy environment. Selected results from atomic scale investigation are presented in the paper, focusing on (i) the mechanisms of self-interstitial dislocation loop formation with Burgers vector of a <100> in Fe relative to Vanadium, (ii) He transport, (iii) the interaction between He and small self-interstitial clusters in Fe, and (iv) dislocation – helium bubble interactions in fcc Al.

The results illustrate a range of phenomena occurring during irradiation in the fusion environment that require further investigation and incorporation into evolution models.

1. MS simulations in Fe and V show that dislocation loop clusters of SIA are lowest energy with **b**=a/2<111>. However, loops with **b**=a<100> in Fe are closer in energy than anticipated by dislocation theory, allowing for the possibility of a<100> metastable loops.
2. a<100> junctions can form between intersecting a/2<111>-type dislocation loops in both V and Fe. In V, the junctions are thermally unstable and rapidly dissolve as the loops rotate to form a single a/2<111> dislocation loop. In Fe, the junction is stable over an intermediate temperature regime and can propagate, leading to a single a<100> dislocation loop.
3. Atomistic simulations of substitutional He diffusion in Fe within the framework of the multiple frequency diffusion analysis of Le Claire [27] reveals an activation energy of 0.65 eV. The simulations reveal that He is strongly delocalized in a di-vacancy – He complex and that substitutional He can jump into a second nearest neighbor vacancy with an activation energy of 0.66 eV.
4. MD simulations of the interactions between substitutional He and SIA in Fe, reveal strong interactions leading to SIA-V recombination and the kick-out of He to an interstitial position. The simulations indicate strong trapping and apparent immobility of a interstitial He – substitutional He complex, as well as the strong trapping of relatively small a/2<111> SIA clusters by both substitutional and interstitial He, with a calculated binding energy of 1.5 eV between a 6-SIA and interstitial He.
5. MD simulations of the interaction between an edge dislocation and under-pressurized He bubble in Al reveal a critical shear stress of about 35 MPa, with a bypass mechanism that involves the local annihilation and re-nucleation of dislocation segments, producing a shear step in the bubble.

Reference

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