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Multiscale Modeling of Irradiation Induced Hardening in Ferritic-Martensitic Steels HUSSEIN ZBIB, IOANNIS MASTORAKOS, Washington State University, MOHAMMAD KHALEEL, XIN SUN, Pacific Northwest National Laboratory — The development of structural materials for use in new generation nuclear reactors depends critically on predicting and understanding the underlying physical mechanisms responsible for microstructural evolution along with corresponding dimensional instabilities and mechanical property changes. As the phenomena involved are very complex and span in several length scales, a multiscale approach is necessary in order to fully understand the degradation of materials in irradiated environments. The purpose of this work is to study the mechanical behaviour of Fe systems (namely a-Fe, Fe-Cr and Fe-Ni) under irradiation using both Molecular Dynamics (MD) and Dislocation Dynamics (DD) simulations. Critical information is passed from the atomistic (MD) to the microscopic scale (DD) in order to study the degradation of the material under examination. In particular, information pertaining to the dislocation-defects (particularly voids, helium bubbles and prismatic loops) interaction is obtained from MD simulations. This information is used in large scale DD simulations to analyze systems with high dislocation and defect densities, predicting the dependence of strength and ductility on defect density.

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