

Development of Multiscale Materials Modeling Techniques and Coarse-Graining Strategies for Predicting Materials Degradation in Extreme Irradiation Environments

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ABSTRACT:

Fe-Cr based ferritic/martensitic steels, and their advanced oxide dispersion strengthened (ODS) and nanostructured ferritic alloy variants, are candidate fuel cladding, pressure vessel and structural materials for Generation IV reactors. These alloys share the characteristic of a body-centered cubic (or martensitic tetragonal) lattice that is known to have significantly improved swelling resistance when compared to face centered cubic austenitic alloys. It is now well established that fundamental understanding of microstructural evolution in these alloys under long-term and elevated temperature irradiation conditions is important, since microstructural and microchemical changes under irradiation control mechanical behavior and ultimately, performance. However, we do not yet have a complete understanding and predictive modeling capability to describe the basic mechanisms of radiation damage formation (cascade structure, defect formation) and kinetically-driven accumulation (defect cluster interactions, dislocation loop evolution, radiation-induced segregation and precipitation processes, formation or dissolution of second phases, sub-grain formation), and to address critical questions related to whether microstructural changes indeed saturate during long-term irradiation exposures.

The objective of this proposal is to further develop and evaluate mesoscale modeling techniques, including kinetic Monte Carlo and spatially dependent cluster dynamics, and develop strategies for coarse-graining, or up-scaling, these micro- and mesoscale models into constitutive level modeling approaches of materials degradation in nuclear environments. More specifically, this proposal will focus on i) modeling microstructural and microchemical evolutions in body centered cubic alloy systems, including molybdenum and ferritic/martensitic alloys, across a number of different micro-mesoscale modeling techniques (KMC, phase field and spatially-dependent cluster dynamics) to evaluate the optimal approach(es) to simulate the different aspects of high dose irradiation effects, namely defect cluster/dislocation loop saturation, radiation-induced segregation and nanoscale precipitate evolution and the onset of void nucleation leading to breakaway swelling; and 2) to identify and further develop the most promising strategies for information passing, or up-scaling, between the different multiscale modeling length and time scale modeling techniques.