Modeling Investigation of the Stability and Irradiation-Induced Evolution of Nanoscale Precipitates in Advanced Structural Materials

PI: Brian Wirth – University of California, Berkeley **Collaborators**: None

Program: MR-IIR

ABSTRACT

Materials used in extremely hostile environments such as nuclear reactors are subject to a high flux of neutron irradiation, and as a result vast concentrations of vacancy and interstitial point defects are produced because of collisions of energetic neutrons with host lattice atoms. The fate of these defects depends on various reaction mechanisms that occur immediately following the displacement cascade evolution and during the longer-time kinetically dominated evolution such as annihilation, recombination, clustering or trapping at sinks of vacancies, interstitials and their clusters. The long-range diffusional transport and evolution of point defects and self-defect clusters drive a microstructural and microchemical evolution that are known to produce degradation of mechanical properties including the creep rate, yield strength, ductility, or fracture toughness, thus significantly affecting material serviceability and lifetimes in nuclear applications. Therefore, a detailed understanding of microstructural evolution in materials at different time and length scales is of significant importance. The primary objective of this work is to utilize a hierarchical computational modeling approach (1) to evaluate the potential for nanoscale precipitates to enhance point defect recombination rates and thereby the self-healing ability of advanced structural materials, and (2) to evaluate the stability and irradiation-induced evolution of such nanoscale precipitates resulting from enhanced point defect transport to and annihilation at precipitate interfaces.

The hierarchical computational modeling approach primarily involves the use of molecular dynamics (MD), kinetic Monte Carlo (KMC) and spatially dependent cluster dynamics modeling and will be used to evaluate the structure of spherical nanometer-scale precipitates in model-body-centered cubic alloys and subsequently evaluate the ability of these precipitate structures to attract and accumulate vacancy and interstitial-type defects to promote mutual recombination. Furthermore, the resulting structural changes to the precipitate-matrix interfaces will be evaluated using atomistic modeling techniques. These parameters will then be utilized in a cluster dynamics evolution model to predict the irradiation-induced evolution of the nanoscale precipitates.