# Mechanisms of Stability and Defect Trapping in Doped Iron Grain Boundaries

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Tailored microstructures incorporating grain and interphase boundaries provide energetically favorable sites for combating displacement damage from irradiation. This effect will be heightened in nanocrystalline materials due to their intrinsically large interfacial area per unit volume. Unfortunately, many of these materials also occupy a thermodynamically unfavorable state due to their excess interfacial free energy. Targeted doping of the grain boundaries has shown to stabilize nanocrystalline materials by offsetting the interfacial free energy and in turn, reducing the intrinsic driving force for grain growth. In this presentation, we explore the implications of nanocrystalline grain boundary doping for interface stability and defect sink behavior during displacement cascade events. Using a hybrid simulation technique combining transmutation Monte Carlo simulations with molecular dynamics calculations, we first map the segregation behavior of four dopant species in the nanocrystalline state – Cr, Al, Ni, and Cu – which were selected based on their importance for cladding materials and structural ferritic alloys. These simulations show that Cu offers the widest range of segregation states as a function of alloy concentration and equilibration temperature. On this basis, a library of 16 energy-minimized coincident site lattice (CSL) boundary configurations was constructed for displacement cascade simulations including both pure Fe and Cu-doped grain boundaries. By initiating cascade events within the different CSL boundaries, we show that structural reconfigurations from direct overlap of the cascade's peak damage region with the pure Fe grain boundaries are suppressed upon the addition of Cu. The degree of stability is shown to be a function of interfacial structure and concentration with a general dependence on the grain boundary energy. Cascade initiation instead at distances where the peak damage region did not directly interact with the boundaries revealed that the defect trapping propensity scales with the product of the interstitial segregation energy and probability for defect chain events to reach the grain boundary. Collectively, our simulations indicate that targeted doping of grain boundaries in the nanocrystalline state enhances stability while having a limited impact on sink efficiency, thus representing a new direction for radiation tolerant alloy design.