Displacement Cascade Simulations in FCC Ni-Fe Solid Solutions

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Tungsten alloys and composites are actively researched in the fusion materials community to improve the fracture toughness and the ductile-to-brittle transition temperature of tungsten for use as plasma-facing materials. Among these materials, ductile-phase-toughened composites are particularly promising. W-Ni-Fe composites, consisting of tungsten particles embedded in a ductile face-centered cubic (fcc) Ni-Fe random solid solution with a Ni:Fe weight ratio of 7 :3, have been shown to exhibit a significantly higher fracture toughness (30-60 MPa√m) compared to pure tungsten (8 MPa√m) at room temperature [1]. However, the irradiation effects against fusion neutrons remain largely unknown. In this study, molecular dynamics (MD) is employed to simulate the displacement cascades in an fcc Ni-Fe solid solution. The cascades simulations are performed with a random Fe or Ni primary-knock-on atom (PKA) as a function of PKA energy to build a database of primary defects for future kinetic Monte Carlo simulations of damage accumulation. Irradiation-induced phase separation will be studied. Furthermore, the defect distribution will be compared to the data of pure Ni to elucidate the effect of Fe solute atoms on the cascades.

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