Atomistic Investigation of Anisotropic Radiation-Induced Embrittlement

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Abstract

Radiation-induced degradation in structural alloys originates from defect formation and evolution at the atomic scale, which significantly alters mechanical behavior and fracture mechanisms. In this study, we present an atomistic investigation of anisotropic radiation-induced embrittlement in Fe–Ni–Cr alloys using molecular dynamics (MD) simulations [1, 2].

Neutron irradiation generates complex defect populations, including vacancy clusters, stacking fault tetrahedra (SFTs), and dislocation structures, which emerge from displacement cascades and govern subsequent microstructural evolution [3]. To accurately represent the alloy system, simulations are performed using a validated Fe–Ni–Cr interatomic potential capable of capturing radiation-induced defect behavior [4]. Radiation-induced defect structures are systematically created, and their influence on crack-tip behavior and fracture mechanisms is analyzed under controlled loading conditions.

Crack propagation is analyzed under Mode-I loading for different crystallographic orientations, namely (001), (011), and (111). The results reveal strong orientation-dependent fracture behavior governed by defect–dislocation interactions and slip system activity. The (001) orientation exhibits pronounced embrittlement characterized by limited plasticity and rapid crack propagation. The (011) orientation shows intermediate behavior with partial stress redistribution through dislocation emission, while the (111) orientation demonstrates enhanced ductility due to multiple active slip systems. These findings are consistent with atomistic studies highlighting the critical role of dislocation mechanisms and microstructural interactions in deformation processes [5].

Furthermore, the results provide clear evidence of irradiation-assisted ductile-to-brittle transition (DBT), where increasing defect density suppresses plastic deformation and accelerates crack propagation [6]. The transition is quantified using atomistic energy-based fracture metrics, where the critical energy release rate is evaluated directly from MD simulations, providing a consistent description of fracture energetics at the nanoscale [7]. The observed anisotropic fracture response is closely linked to crystallographic orientation, in agreement with recent atomistic studies of orientation-dependent crack propagation [8].

This work provides a comprehensive atomistic framework for understanding the interplay between irradiation-induced defects, crystallographic anisotropy, and fracture behavior in Fe–Ni–Cr alloys, offering insights into the fundamental mechanisms governing embrittlement at the nanoscale.

Keywords: Crack propagation, Radiation defects, MD simulations, Cr-rich alloy, T–S law, Atomic-scale fracture energy, ductile-to-brittle transition

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