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# Fracture Mechanisms in Irradiated Fe–Ni–Cr Alloys: Atomic-Scale Insights and Energy-Based Modeling of the Ductile-to-Brittle Transition

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## Abstract

Neutron irradiation induces profound microstructural changes in structural materials, critically influencing their fracture behavior and posing significant challenges for nuclear reactor safety. This study employs molecular dynamics (MD) simulations to elucidate the mechanisms driving the radiation-induced ductile-to-brittle transition (DBT) in Fe–Ni–Cr alloys, a phenomenon distinct from classical temperature-driven DBT. While previous studies (1, 2) have focused on thermal effects, this work introduces a comprehensive analysis of how irradiation-induced defects, specifically voids and dislocation loops, govern fracture dynamics by altering dislocation mobility and energy dissipation pathways.

Crack propagation in irradiated Fe–Ni–Cr alloys was systematically investigated using MD simulations across a broad range of displacements per atom (dpa parameter) (3, 4). Radiation-induced voids reduce cohesive energy, accelerating crack growth through coalescence, while dislocation loops act as immobile barriers, redirecting cracks and promoting secondary crack formation. At higher dpa, dense defect networks suppress plasticity.

Crack propagation is driven by three competing mechanisms: (1) void coalescence weakens the lattice, lowering resistance and promoting crack growth along weakened zones, often leading to branching, (2) dislocation loops form stable structures, obstruct the motion of dislocations near the crack tip, which temporarily halts crack progression, (3) high defect densities, particularly dislocation loop clusters, induce crack branching and secondary crack formation due to stress concentration effects, increasing fracture complexity.

A key aspect of this study is the energy-based framework for quantifying irradiation-induced embrittlement. The critical energy release rate,  $G_c$ , is decomposed into two fundamental contributions: surface energy, which represents the energy required to create new fracture surfaces, and plastic work, associated with dislocation motion and other inelastic deformations. To isolate these components, we leverage a low-temperature reference state where plasticity is significantly suppressed, allowing  $G_c$  at this condition to approximate the surface energy. By comparing fracture energy at a higher temperature, where plasticity is active, to the near-brittle reference state, the plastic work contribution can be extracted. This approach enables a generalizable assessment of embrittlement, independent of specific temperature values, as long as the selected low-temperature condition captures near-brittle

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behavior and the high-temperature condition allows sufficient plasticity. Simulation results reveal that irradiation progressively reduces plastic work, directly linking irradiation hardening to suppressed dislocation activity.

This study advances the understanding of irradiation embrittlement through three key contributions. First, it establishes a direct link between defect density, crack morphology, and energy dissipation, demonstrating that voids weaken the material by reducing cohesive strength, while dislocation loops obstruct crack propagation by pinning dislocations, collectively driving the transition from ductile tearing to brittle cleavage. Second, it develops a microstructural-mechanical framework that bridges atomic-scale defect interactions with macroscopic fracture resistance, correlating defect-driven crack morphology with energy dissipation changes. Third, it refines the decomposition of  $G_c$  to quantify irradiation-induced plasticity suppression, distinguishing irradiation-driven embrittlement from thermal effects and providing a predictive framework for fracture behavior based on defect density.

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