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Anisotropic effects on radiation-induced embrittlement in Fe-Ni-Cr alloys: a molecular dynamics study

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Abstract

In this research, we comprehensively investigate the mechanical behavior and fracture mechanisms of Fe-Ni-Cr alloys subjected to neutron irradiation, emphasizing the influence of anisotropy on radiation-induced embrittlement. Considering the crucial application of these alloys in nuclear reactor components [1], we aim to enhance our understanding of how irradiation defects impact material integrity under different crystallographic orientations, specifically (001), (011), and (111). Initially, Molecular Dynamic (MD) simulations were performed using ternary interatomic potential [2] to evaluate the radiation-induce defects impact on elastic properties through the Born matrix method [3].

Further analysis focuses on the detailed physical mechanisms which impact crack propagation under Mode-I loading conditions by using MD simulation. Particular attention was given to the role of irradiation-induced defects, including stacking fault tetrahedra (SFTs), voids, and entangled dislocations, on crack-tip behavior and crack propagation [4]. The (001) orientation exhibited severe embrittlement, with significantly restricted dislocation activity and rapid cleavage fracture. Conversely, the (011) orientation showed moderate embrittlement, maintaining some ability to redistribute stress through symmetric dislocation emissions. Remarkably, the (111) orientation demonstrated the highest fracture resistance, preserving notable ductility even after irradiation, attributed primarily to its multiple active slip systems that mitigate stress concentrations.

To quantify local fracture responses and assess the ductile-to-brittle transition behavior [5], we employed the cohesive zone model (CZM) based on Traction-Separation (T-S) law framework [6]. Critical energy release rates (G_{cr}) derived from the integration of T-S curves clearly illustrated orientation-dependent trends according to the different level of irradiation. Specifically, the (001) orientation possessed the lowest G_{cr}, which indicate a pronounced brittleness, whereas the (111) orientation consistently retained the highest G_{cr}, reflecting sustained ductility and efficient stress dissipation.

By integrating these atomic-scale insights, our study contributes significantly toward comprehending the anisotropic fracture behavior of Fe-Ni-Cr alloys under irradiation conditions.

Scientific field: computational mechanics

Keywords: radiation-induced defects, crack propagation, MD simulations, critical energy release rate, ductile to brittle transition

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