

PROCEEDINGS

Hydrogen-Helium Synergistic Effects on Core-Shell Cavity Evolution and Cavity-Mediated Deformation in BCC-Fe Under Fusion Conditions

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ABSTRACT

In the fusion environment, understanding the synergistic effects of transmutation-produced hydrogen (H), helium (He), and irradiation-induced displacement damage in iron (Fe)-based alloys is crucial for the development of structural materials for fusion reactors. In particular, the formation of irradiation-induced cavities with core-shell structures, where He is confined in the cavity core and H accumulates at the cavity surface, represents a critical but insufficiently understood mechanism controlling swelling, plasticity, and damage initiation. In this work, we develop an integrated computational framework combining molecular dynamics (MD) simulations, statistical thermodynamics, density functional theory (DFT) calculations, and experimentally informed cavity statistics to elucidate the nucleation, evolution, and mechanical response of H-He decorated cavities in BCC-Fe. An efficient Fe-H-He ternary interatomic potential is established to describe the coupled atomic interactions among matrix atoms, transmutation gases, and irradiation-induced defects. Based on this model, the kinetic processes of H and He capture by cavities are systematically resolved under different temperatures and cavity configurations. Thermodynamic analyses, constrained by experimentally relevant cavity size distributions, He/V ratios, and atomistically derived H-cavity binding energetics, identify the most probable H uptake and confirm the stability of the core-shell cavity configuration from both kinetic and thermodynamic perspectives. The mechanical response of these cavities is further investigated under hydrostatic/triaxial tensile loading over fusion-relevant temperature and strain-rate ranges. The results show that deformation remains cavity-centered and proceeds through a common sequence of stress concentration, dislocation emission, defect multiplication, and secondary cavity nucleation. Temperature and strain rate regulate the activation thresholds and kinetics of these processes, while H and He synergistically modify the stress-strain response: He sustains internal pressurization in the cavity core, whereas H stabilizes at the cavity surface and promotes interfacial defect activation. A dimensionless degradation analysis enables quantitative comparison of the individual and coupled contributions of H and He across deformation stages. These findings provide mechanistic insight into H-He synergistic damage in fusion structural materials and establish a physically grounded basis for multiscale modeling, irradiation-damage assessment, and the design of irradiation-tolerant Fe-based alloys.

KEYWORDS

Fusion structural materials; H-He synergy; core-shell cavities; irradiation damage; dynamic tensile; multiscale modeling; thermodynamic theory; MD simulations; DFT calculations

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