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Nanoindentation and Defect Behavior in Irradiated FCC NiFe Alloys: Experimental Insights and Atomistic Modeling

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Fcc NixFe1-x single-crystal alloys are key model systems for studying defect evolution under self-ion irradiation at room temperature, with fluences ranging from 4×10^{13} to 2×10^{15} ions/cm² [1,2]. This study investigates the effects of irradiation-induced defects on the nanomechanical response of NiFe alloys through a combination of experimentally guided nanoindentation and atomistic simulations. Defects in the irradiated materials were characterized using transmission electron microscopy (TEM), providing essential input for molecular dynamics simulations of overlapping collision cascades to prepare irradiated samples at various doses [3]. The simulations revealed mechanisms of defect formation and evolution, including the emergence of an A15 Frank-Kasper phase within the {111} plane in pure Ni, $Ni_{0.88}Fe_{0.12}$, and $Ni_{0.77}Fe_{0.23}$ at fluences up to 2×10^{14} ions/cm², serving as a precursor to Frank loop nucleation. The findings also highlight the critical role of Fe atoms in influencing dislocation nucleation and evolution. In $Ni_{0.77}Fe_{0.23}$, compact 3D precipitates heavily decorated with Fe atoms were observed. However, these precipitates remained too small to evolve into Frank loops, even at elevated fluences. Nanoindentation experiments and simulations demonstrated a notable increase in hardness in irradiated alloys compared to their pristine counterparts [4,5]. From the atomistic modeling, we provide detailed analyses of the irradiated samples revealed surface morphologies, dislocation densities, and strain mappings to discuss the mechanisms of dislocation pinning during mechanical loading due to irradiation-induced defects. These defects were found to obstruct dislocation motion, contributing to the enhanced hardness of the material. Overall, this study provides critical insights into the interplay between composition, irradiation-induced defect structures, and their mechanical consequences in NixFe1-x alloys. These findings enhance our understanding of the mechanisms underpinning radiation resistance in these materials, supporting their potential applications in radiation-intensive environments. [1] E. Wyszkowska et al. Nanoscale 15, 4870 (2023). [2] A. Ustrzycka et al. Int. J. Plasticity 182, 104118 (2024) [3] K. Mulewska et al. J. Nucl. Materials 586, 154690 (2023) [4] L. Kurpaska et al. Materials & Design 217, 110639 (2022). [5] F. Dominguez-Gutierrez et al. J. Appl. Phys. 135, 185101 (2024)

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