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ABSTRACT:

Voids or Stacking-Fault Tetrahedra Induced by Diffusion and Local Chemical Variations in High Entropy Alloys

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Selecting materials for advanced fission and fusion reactors presents significant challenges due to their exposure to intense radiation and high temperatures. Such extreme conditions foster the development of extended defect clusters, which affect material performance. These clusters can manifest in various forms, with their formation dynamics strongly influenced by diffusion and interactions within the local elemental environment. Deciphering how elemental composition affects defect cluster formation remains a pivotal issue in materials science. By integrating long-timescale defect rate simulations, molecular dynamics modeling, and irradiation experiments, we reveal a distinctive cluster-mediated pathway—driven by element-specific interactions and diffusion—as the predominant mechanism regulating vacancy cluster evolution into voids or stacking fault tetrahedra (SFTs) in irradiated complex concentrated alloys, including NiCoCr, Fe50Mn30Co10Cr10, and Ni at high temperatures. In addition to traditional approaches that emphasize point defect diffusion behavior, our model introduces a critical two-step process: vacancy-tetrahedron formation and annihilation, which directs the divergence of vacancy clusters. Ni and Co promote void formation through favoring annihilation, resulting in their segregation, while larger atoms like Cr, Fe, and Mn impede annihilation, thereby favoring SFT formation. These insights enhance our understanding of the role of local chemistry and diffusion in defect evolution and inform the design of materials optimized for extreme environments.

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