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Simulation of Irradiation Properties and Damage Evolution of High Entropy Alloys

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ABSTRACT

High entropy alloys (HEA) are considered as the candidate materials for the next generation of nuclear systems due to the excellent high temperature properties and radiation resistance. However, for the lack of atomic lattice distortion information from the micromechanical description, the existing simulation methods are difficult to capture the microstructure and damage evolution of the HEA at submicron scale. To address this, we develop the random field theory informed discrete dislocation dynamics simulations based on the results of high-resolution transmission electron microscopy to systematically clarify the role of heterogeneous lattice strain on the complex interactions between the dislocation loop and dislocation in three-dimensional space [1]. At the same time, we studied the effect of lattice distortion on the defect-free channels in irradiated alloys. The severe lattice distortion makes the defect-free channels more narrow and evenly distributed, and reduce the irradiation hardening of the alloys. In addition, we study the dislocation behavior and damage evolution in oxide dispersion strengthening HEA considering the influence of severe lattice distortion and nanoscale oxide particles. An abnormal trend of the damage decreasing first and then increasing during loading is captured [2]. These studies can deeply understand atomic-scale damage mechanism and guide the design of HEA with high radiation resistance.

KEYWORDS

Steel; corrosion mechanism; creep; multiscale simulation

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