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Strengthening Mechanism and Deformation Behavior of Multi-Principal Element Alloys Using Multiscale Modelling and Simulation

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ABSTRACT

The multi-principal elemental alloys (MPEAs) exhibit excellent combinations of mechanical properties and radiation-resistant, are considered potential candidates for aerospace industries and advanced reactors. However, the quantitative contribution of microstructure on the strengthening mechanism remains challenging at the micro-scale, which greatly limits the long-term application. To address this, we developed a hierarchical multiscale simulation framework that covers potential physical mechanisms to explore the hardening effects of chemical short-range order (CSRO) and irradiation defects in MPEA. Firstly, by combining atomic simulation, discrete dislocation dynamics, and crystal plasticity finite element method, a hierarchical cross-scale model covering heterostructure lattice distortion and dislocation hardening effects is developed, which demonstrated high accuracy and universal applicability for MPEAs [1]. Secondly, the strain field caused by short-range ordered structures is captured based on random field theory and introduced into the multi-scale simulation framework. The CSRO structure greatly improves the dislocation-based strength and suppresses dislocation slip, resulting in a significant increase in flow stress [2,3]. The irradiation mechanism and damage evolution of oxide dispersion strengthening (ODS) MPEAs are studied through discrete dislocation dynamics, and the abnormal trend of damage decreasing first and then increasing is captured, demonstrating the excellent radiation resistance of ODS MPEAs [4]. The present work not only provides a general approach to physically predict the mesoscopic mechanical response in MPEAs, but also gives guidance for the design of MPEAs with desired mechanical properties.

KEYWORDS

Multi-principal element alloy; multiscale simulation; deformation mechanism; irradiation damage

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