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PROCEEDINGS

Modelling and Simulation on Deformation Behaviour and Strengthening Mechanism of Multi-Principal Element Alloys

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ABSTRACT

In order to accurately predict and evaluate the mechanical properties of multi-principal element alloys (MPEAs), some new models and simulation methods need to be developed to solve the problems caused by its unique natural characteristics, such as severe lattice distortion. The existing models are based on the development of low concentration alloys, and cannot be well applied to MPEAs. Here, we develop i) the random field theory informed discrete dislocation dynamics simulations based on 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 [1,2]; ii) a general framework by combining the atomic simulation, discrete dislocation dynamics, and crystal plasticity finite element method, to study the strain-hardening behavior for MPEAs, which achieves the influence of the complex cross-scale factors, including the lattice distortion at the nanoscale and the dislocation hardening at the microscale, on the plastic deformation [3]; iii) a multistage-design approach integrating machine learning, physical laws and a mathematical model for developing the desired-property MPEAs in a very time-efficient way [4]. The present work suggests that the property-guided composition and microstructure are precisely tailored through the newly built approach, which is readily extendable to other multi-principal element materials.

KEYWORDS

Multi-principal element alloy; mechanical properties; machine learning; multiscale simulation

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