Microstructure-based Multiscale Modeling of Mechanical Behaviors in Metals

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Abstract

We proposed a multiscale model to predict the thermo-mechanical properties of structural materials and high-entropy alloys, specifically involving the impacts of microstructure, interfaces, and size effects, through a combination of experiments, simulations, and theoretical modeling. Additionally, a probabilistic model was established that integrates with the constitutive model to elucidate the competition between cleavage and ductile void failure in structural materials. We also developed a machine learning-based nonlinear micromechanics framework for materials with complex interfacial behaviors. Moreover, we explored the coupled size effects and microstructural effects on strength, toughness, and creep, providing theoretical fundamentals for understanding the mechanical properties of small-scale samples.

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