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Machine Learning-Driven Rational Design and Cross-Scale Simulation in Multi-Principal Element Alloys

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ABSTRACT

Multi-principal element alloys have aroused extensive attention due to their outstanding mechanical, physical, and chemical performances. To achieve performance-orientated design with high efficiency and low cost and further predict the deformation mechanism, new design approaches and cross-simulation methods need to be developed. Here, we propose i) the approach combining with high-throughput atomic simulations, mechanical models as well as machine learning, to efficiently search optimal composition and microstructure [1,2]; (ii) a multistage design framework integrating physical laws, mechanical models and machine learning, to solve the two key problems--the forward problem (composition to performance) and the inverse problem avenue (performance to composition) [3]; (iii) a universal automatic cross-scale simulation framework that combines machine learning, dislocation dynamics, and constitutive model, to investigate the effects of chemical heterogeneity on strengthening behavior. The present work indicates that the target composition, microstructure and corresponding deformation mechanism are accurately predicted based on the proposed approaches, which is extended to other alloy systems.

KEYWORDS

Multi-principal element alloys; composition design; machine learning; cross-scale simulation

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