MACHINE LEARNING ENABLED RATIONAL DESIGN OF HIGH ENTROPY ALLOYS

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ABSTRACT

High entropy alloys (HEAs) possess a vast compositional space, providing exciting prospects for tailoring material properties yet also presenting challenges in their rational design. Efficiently achieving a well-designed HEA often necessitates the aid of atomistic simulations, which rely on the availability of high-quality interatomic potentials. However, such potentials for most HEA systems are missing due to the complex interatomic interaction. To fundamentally resolve the challenge of the rational design of HEAs, we propose a strategy to build a machine learning (ML) interatomic potential for HEAs and demonstrate this strategy using CrFeCoNiPd as a model material. The fully trained ML model can achieve remarkable prediction precision (>0.92 R2) for atomic forces, comparable to the ab initio molecular dynamics (AIMD) simulations. To further validate the accuracy of the ML model, we implement the ML potential for CrFeCoNiPd in parallel molecular dynamics (MD) code. The MD simulations can predict the lattice constant (1% error) and stacking fault energy (10% error) of CrFeCoNiPd HEAs with high accuracy compared to experimental results. Through systematic MD simulations, for the first time, we reveal the atomic-scale deformation mechanisms associated with the stacking fault formation and dislocation cross-slips in CrFeCoNiPd HEAs under uniaxial compression, which are consistent with experimental observations. This study can help elucidate the underlying deformation mechanisms that govern the exceptional performance of CrFeCoNiPd HEAs. The strategy to establish ML interatomic potentials could accelerate the rational design of new HEAs with desirable properties.

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