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# Multiscale modeling of dislocation-mediated plasticity of refractory high entropy alloys

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## Abstract

Refractory high entropy alloys (RHEAs) have drawn growing attention due to their remarkable strength retention at high temperatures. Understanding dislocation mobility is vital for optimizing high-temperature properties and ambient temperature ductility of RHEAs. Nevertheless, fundamental questions persist regarding the variability of dislocation motion in the rugged energy landscape and the effective activation barrier for specific mechanisms, such as kink-pair nucleation and kink migration. Here we perform systematic atomistic simulations and conduct statistical analysis to obtain the effective activation barrier for the mechanisms underlying various types of dislocation motion in a typical RHEA, NbMoTaW. Moreover, a stochastic line tension model is developed to calculate the activation barrier with substantially reduced computational costs. By incorporating the activation barrier into the crystal plasticity model, a multiscale simulation framework for predicting the mechanical properties of RHEAs is established. The ambient temperature yield strength of NbMoTaW is well-predicted by the kink-pair nucleation mechanism of screw dislocations, while the strengthening originating from screw dislocations does not predominate at high temperatures. Our work provides a robust foundation for atomistic studies of effective dislocation behaviors in random solution solids, elucidating the intricate relationship between microscopic mechanisms and macroscopic properties.

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