Hybrid QM/ML study of carbon induced screw dislocation pinning in tungsten

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Screw dislocation glide by nucleation and propagation of kink pairs controls plasticity at low temperatures in BCC metals like tungsten. Interaction of solute impurities such as carbon with dislocations is one of the main mechanisms of solid solution strengthening. Atomistic simulations are essential to understand local effects of impurities on dislocation core, however application of ab initio methods is hindered by system size limitations. Recent developments in hybrid quantum mechanics/machine learning (QM/ML) simulation methods overcome these limitations by placing ab initio region at the impurity while the rest the large cell containing dislocation in bulk material is described by a highly adaptive ML potential [1].

In this work we investigate the dilute limit of solute-dislocation interaction, focusing on the interaction of a screw dislocation with an individual C atom in tungsten. We first look at the dislocation core reconstruction induced by a C atom and compare it to previous ab initio results [2]. Then we employ Nudge Elastic Band (NEB) calculations to obtain detailed dislocation unpinning mechanism and associated energy barriers. Finally, we analyse the effect of C atom on kink pair formation and single kink migration. Our results reveal that C atoms attractively interact with kinks, facilitating kink pair formation while simultaneously impeding single kink migration. This dual behaviour highlights the complex role of solute-dislocation interactions in solid solution strengthening in BCC metals.

References:

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