Contribution ID: **48** Type: **invited**

Investigating the Influence of Helium on Screw Dislocation Mobility in Tungsten

Wednesday 28 May 2025 11:10 (30 minutes)

Tungsten, a candidate for nuclear fusion reactor armour, is susceptible to helium contamination. Such impurities are believed to interfere with the movement of screw dislocations, which typically propagate by nucleation and migration of kink pairs. Modelling this requires large simulations cells that are well beyond the limits of density functional theory, with a few heroic exceptions [1]. Therefore, we have built upon an existing machine learning interatomic potential for tungsten [2], with the aim of accurately modelling extended defects such as dislocation kinks and dislocation-helium interactions.

As has been previously reported in QM/MM studies [3], we observe a reconstruction to the split-core local to helium in the dilute regime. We then investigate the influence of helium on the kink pair mechanism, finding that the nucleation energy is reduced from 1.6eV (in the pure metal) to 0.5eV, caused by the preference for helium atoms to bind to the vacancy-like kink [4]. This preference is so large, that when bound to He_2/He_3 clusters, the kinked dislocation line becomes more stable than the straight one.

Using our potential, we have also run large-scale molecular dynamics simulations to obtain dislocation velocities. To accelerate these simulations, we are testing the new LAMMPS plugin: ML-MIX [5], where potentials of different complexities (and costs) can be spatially mixed, in the hope that our complex potential is only required at the dislocation core.

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Session Classification: invited