Hybrid QM/MM study of dislocation glide in tungsten in the presence of plasma components

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Tungsten has been chosen as the divertor armour material in ITER and is the main candidate material for plasma-facing components for future fusion reactors. Interaction of plasma components with the material is unavoidable and will lead to degradation of the performance and the lifetime of the in-vessel components. From this point of view it is important to gain an understanding of dislocation mobility as one of the fundamental mechanisms of a plasticity of the material as well as the influence of fusion plasma components (H and He) on the mechanism.

Dislocation glide is governed by the localised rearrangement of atoms inside the dislocation core but is tightly coupled to the stress and strain fields on larger length scale. Thus, a correct description of the process requires chemically accurate treatment of the dislocation core atoms together with the use of the systems large enough to accommodate the corresponding stress fields. On the one hand, Density Functional Theory (DFT) provides an accurate description of the interatomic bonding, however the computational cost of the method does not allow one to study large enough systems and requires usage of periodic cells (*i. e.* with dislocation dipoles and quadrupoles with complex symmetry). On the other hand, classical interatomic potentials are much more computationally affordable allowing to study systems of required size, but the accuracy and transferability of the description of dislocation core is poor, especially for multi-element systems.

In this study we use a hybrid musltiscale approach, namely quantum mechanics/molecular mechanics (QM/MM) [1], combining an accurate local QM description of the dislocation core atoms with a classical model for the rest of the system. We apply a recently developed QM/MM implementation of the virtual work principle [2] to compute energy barriers. The effect of H and He atoms in the material on the dislocation core structure together with the energetics of dislocations and impurities are investigated. The obtained results are analysed by comparison with pure DFT studies from literature [3, 4, 5] together with machine learning based Gaussian Approximation Potential (GAP) model [5].

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