Multiscale QM/MM simulation of chemo-mechanical processes in materials: from crack propagation in silicon to dislocation motion in tungsten

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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. It is important to gain an understanding of dislocation mobility 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.

More geneerally, materials failure remains one of the most challenging multiscale modelling problems, requiring both an accurate description of the chemical processes occurring near crack tips or at dislocation cores and the inclusion of a much larger region in the model systems. 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 (*e.g.* with dislocation dipoles and quadrupoles with complex symmetry). On the other hand, classical interatomic potentials are much more computationally affordable allowing systems of required size to be studied, but the accuracy and transferability is often poor, especially for multi-element systems.

I will explain how these requirements can be met simultaneously by combining a quantum mechanical description of local chemical processes with a classical atomistic model that captures the long-range elastic behaviour of the surrounding crystal matrix, using a QM/MM (quantum mechanics/molecular mechanics) [1]. I will review recent developments in this area, along with applications to slow crack growth [2] and chemically activated fracture [3]. and a recently developed extension of the QM/MM scheme that uses the virtual work principle [4] to compute energy barriers. I will show how this can be used to investigate the effect of H atoms in tungsten on the dislocation core structure together with the energetics of dislocations and impurities.

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