Atomistics of hydrogen at defects towards a multi-scale, bottom-up theory of hydrogen embrittlement

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The quest for cleaner alternative sources is all time high and hydrogen (H) has the potential to lead this transition owing to its clean and sustainable make-up. However, the realisation of H as an energy source requires resolving the embrittling phenomenon of H in metals. Over the past decades, several different embrittlement mechanisms have been proposed following experimental and numerical investigations [1]. Nevertheless, the operating conditions of these mechanisms are not completely understood yet, especially with respect to the role of local H concentration and the interplay of H with defects such as dislocations and cracks, which dictate the overall fracture toughness.

In this work, we primarily investigate the nano/micro-scale interaction of H with dislocations and cracks in iron (Fe). We first develop a novel machine-learning interatomic potential, based on an extensive database of Density Functional Theory (DFT) configurations. We implement an active learning technique [3] in order to simulate crack propagation mechanisms and (screw) dislocation glide with DFT accuracy. We then perform molecular static and dynamics simulations using the open-source code LAMMPS [2]. The simulations reveal the interplay between crack propagation and local hydrogen trapping. Dislocation plasticity in presence of H is investigated by modelling edge dislocations and using an empirical EAM potential [4], which captures the correct lattice parameter, elastic constant, Fe-H interaction and core structure. The influence of dislocation line length, varying distribution, and concentration of H atoms around the dislocation core is systematically investigated.

A significant increase in the Peierls stress is observed at low temperatures due to the dislocation pinning originating from the strong interaction (~ 0.4 eV) of H atoms at the dislocation core. This interaction energy leads to dislocation core saturation up to room temperature for lattice concentrations greater than 0.1 at.%. At finite temperatures up to T=300K, three different regimes, i.e., pinning, solute drag, and unpinning governed by the applied stress and temperature are observed. In the solute drag regime at T=300K, nearly three orders of magnitude reduction in dislocation mobility is observed as compared to the pure Fe case.

This observation of lower dislocation mobility in presence of H contradicts the existing notion that H enhances plasticity by increasing dislocation mobility. Instead, the reduced mobility of dislocations around pre-existing cracks can favour embrittlement over ductile fracture.

References

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