MM 28: Computational Materials Modelling - Hydrogen in metals

Time: Tuesday 14:15–15:15 Location: IFW B

MM 28.1 Tue 14:15 IFW B

Understanding rate dependent hydrogen embrittlement in polycrystalline nickel — •Ali Tehranchi, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

Hydrogen embrittlement (HE) is a persistent mode of failure in metals. It is well known that hydrogen decreases the fracture energy of grain boundaries (GBs) and promotes intergranular fracture. Hydrogen also increases the critical stress for dislocation-GB reactions. As a consequence, more populated pile-ups of the dislocations will form near the GBs. The dislocations in these pile-ups can attract more hydrogen atoms due to their stress field and deliver them to the GB and facilitate the formation of intergranular crack nuclei. If the length of the crack nucleus is larger than a certain critical length it can propagate along the GB without any need for long-range diffusion of H atoms from the bulk, causing embrittlement. In this work, atomistic simulations of the dislocation-GB interactions are used to demonstrate the increase in the critical stress. The energetics and kinetics of the population of the hydrogen atoms around the dislocation pile-up are presented and discussed. A criterion for fast intergranular fracture is given. This criterion explains the rate dependent experimental observations of HE in nickel as a representative fcc metal. The proposed framework is general and can be used for the prediction of HE in other metallic polycrystals.

MM 28.2 Tue 14:30 IFW B

Hydrogen-Metal Surface Interactions Under Strong Electric Fields — •Michael Ashton, Christoph Freysoldt, and Jörg Neugebauer — Max Planck Institut für Eisenforschung, Düsseldorf, Deutschland

The way that hydrogen arrives at and interacts with charged metal surfaces has important implications for catalysis, corrosion, field evaporation, and energy storage. With a focus on the most ubiquitous hydrogen sources (atomic H, H2, and H2O) interacting with prototypical metal surfaces under strong (~10 V/nm) fields, we use ab initio calculations to investigate energetic pathways for forming some simple hydride molecules that have been observed during field evaporation of tungsten and magnesium. Our results shed light on the fundamental behavior of hydrogen under extreme fields, providing particular insight into the origin and role of hydrogen in atom probe tomography experiments where it is *unintentionally* detected from the environment.

MM 28.3 Tue 14:45 IFW B

A grand canonical approach for modelling hydrogen trapping at vacancies in α-Fe — •Michael W. Finnis[1], Erlend R. M. Davidson[1], Thomas Daff[2], and Gábor Csanyi[2] — [1]Thomas Young Centre, Imperial College London, UK — [2]Engineering Laboratory, University of Cambridge, UK

Vacancies in iron are a potential trap for hydrogen, of importance in the understanding of hydrogen embrittlement of steel. We present a grand canonical approach to computing the trap occupancy, which deals with the entire range of hydrogen concentration, from practically zero to super-saturation. Our method is demonstrated here for hydrogen in α-Fe as a function of both temperature and bulk concentration, using a machine-learned H-Fe potential that we develop for the purpose, which enables rapid sampling with near density-functional theory accuracy. The statistical mechanical calculation of the trap occupancy is enabled by the technique of nested sampling. The almost universally used conventional assumption based on Oriani theory is that at industrially relevant concentrations and ambient conditions vacancy traps are fully occupied. In contrast we find that vacancy traps are less than fully occupied under these conditions, necessitating a reevaluation of how we think about *mobile hydrogen* in iron and steel.

MM 28.4 Tue 15:00 IFW B

Atomistic simulations of hydrogen interactions with dislocations in bcc Fe — •Tapaswani Pradhan, Daria Smirnova, Sergei Starikov, Matous Mrovec, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Germany

The presence of hydrogen degrades the mechanical properties of many metallic materials - the phenomenon known as hydrogen embrittlement (HE). One of the possible reasons of HE is the interaction of H with dislocations that leads to changes in dislocation cores and hence affects their intrinsic glide behavior. Atomic scale details of these interactions and especially the interplay between hydrogen diffusion and dislocation motion is still not fully understood. In this work, we investigate the interaction of H with three types of dislocations, namely, edge, mixed and screw, in body-centred cubic Fe using atomistic simulations. The simulations were carried out using two interatomic interaction models, a tight-binding-based magnetic bond order potential (BOP) and an empirical angularly dependent potential (ADP). Our study shows that H prefers to segregate to all dislocation cores but impacts more the mobility of the glissile mixed and edge dislocations whose Peierls barriers are very low. We present a detailed comparison of simulation predictions and discuss their relation to the HE phenomenon.