MM 26: Topical Session: Hydrogen in Materials: from Storage to Embrittlement IV

Time: Tuesday 14:00–14:45 Location: C 130

MM 26.1 Tue 14:00 C 130

Accurate representation of hydrogen in metals by machine-learning enhanced modelling of nuclear quantum effects — •Kai Sellschopp[1], Thomas Klassen[1,2], Paul Jerabek[1], and Claudio Pistidda[1] — [1]Institute of Hydrogen Technology, Helmholtz-Zentrum hereon, Geesthacht, Germany — [2]Helmut-Schmidt-University, Hamburg, Germany

In a sustainable economy built on renewable energy, hydrogen plays a key role for storing energy and replacing fossil fuels. An efficient way to store hydrogen is to keep it in the solid state by binding it chemically in a metal hydride, which is particularly useful for seasonal energy storage or for applications where safety is a concern. Despite the fact that hydrogen is known to show nuclear quantum effects (NQE) even at higher temperatures, these have been neglected in computational studies of metal hydrides so far due to the high cost of path-integral molecular dynamics (PIMD) calculations. In this work, a machine-learned potential (MLP) is trained for the Mg-H system, a well-known hydrogen storage material, in order to speed up the simulations and bring down the cost. At the same time, the sample collection is accelerated by training the potential "on-the-fly" during classical molecular dynamics runs, where ab-initio calculations are replaced by the MLP whenever the estimated errors are low enough. In this contribution, I present the training and validation of this MLP and evaluate the speed-up that allows to perform computationally expensive PIMD calculations. First insights obtained from these calculations enhance our understanding of metal-hydrogen systems.

MM 26.2 Tue 14:15 C 130

Revised reaction-diffusion model of hydrogen trapping in cavities in metals — •Mikhail Zibrov and Klaus Schmid — Max Planck Institute for Plasma Physics, 85748 Garching, Germany

A reaction-diffusion model of hydrogen (H) trapping and release from a metal containing spherical cavities has been developed. The model uses a kinetic description of H atom trapping at the cavity surface and H_2 gas precipitation in the cavity volume. We show that the common assumption of a local thermodynamic equilibrium between H_2 gas in the cavity and the solute H is inadequate in several instances. We discuss the importance of correlated H retrapping by the same cavity and inhomogeneous H potential energy landscape in the vicinity of the cavity surface. H thermal desorption spectra from cavities have features that are difficult to describe with conventional models but are readily observed in experiments: Sharp rising edges of desorption peaks and constant desorption at a fixed temperature. The kinetics of H transport and trapping in the material containing cavities differs from that for point defects, especially at low temperatures.

MM 26.3 Tue 14:30 C 130

Hydrogen redistribution during electrochemical charging and mechanical testing: insights from a combined ab initio and finite element method — Christian Posch-Peperkorn[1], Philipp Hammer[1], Vsevolod Razumovskiy[1], Werner Ecker[1], Klemens Mraczek[2], Ali Tehranchi[3], and •Tilmann Hickel[4] — [1]Materials Centre Leoben Forschung GmbH, Austria — [2]voestalpine Stahl GmbH, Linz, Austria — [3]MPI für Eisenforschung Düsseldorf, Germany — [4]Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany

In advanced high strength steels the mechanisms of hydrogen embrittlement are expected to be strongly connected to the amount of retained austenite (RA) contained in the microstructure and its transformation upon deformation. We have developed a multi-scale model for the H redistribution during H charging and tensile loading within a martensitic/austenitic microstructure. Ab initio simulations have been used to resolve the complex energy profile of H in the phase boundaries. Representative microstructures with different amounts of RA have been converted form experimental SEM-EBSD measurements. Simulations with the finite element method (FEM) have been used to analyse H concentration profiles. The simulations confirm an accumulation of H within the austenitic phase during charging, which undergoes a phase transformation under mechanical load and releases accumulated H into the martensite matrix. The latter segregates to the microstructure regions subjected to high hydrostatic tensile stresses and plastic strains, driving H embrittlement.