MM 47: SYM Hydrogen in Materials: New Developments V

Time: Friday 10:15–11:55 Location: H 1058

MM 47.1 Fri 10:15 H 1058

Mechanisms and thermodynamics of hydrogen embrittlement in metals — •Reiner Kirchheim — Institute for Materials Physics, University of Goettingen, Germany

Depending on temperature, hydrogen concentration, its diffusion coefficient and its terminal solubility different mechanisms of hydrogen embrittlement are relevant. Some of them are dealing with the ease of generating new surfaces (cracks) or dislocations in the presence of hydrogen. The formation energy of these defects as well as their mobility depends on the chemical potential of hydrogen. This relationship is discussed in the framework of a generalized Gibbs adsorption theory.

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Hydrogen embrittlement revisited by in-situ electrochemical nanoindentation — •Afrooz Barnoush and Horst Vehoff — Saarland University Bldg. D22 P.O. Box 151150, Postcode D-66041, Saarbruecken, Germany

Electrochemical NI-AFM was used to examine the effect of hydrogen on dislocation nucleation. It was shown that hydrogen reduces the pop-in load in all of the tested materials except Cu. The reduced pop-in load can be interpreted as the HELP mechanism. Classical dislocation theory was used to model the homogeneous dislocation nucleation and it was shown that H reduces the activation energy for dislocation nucleation. The activation energy for dislocation nucleation is related to the material specific parameters; shear modulus, dislocation core radius and in the case of partial dislocation nucleation, stacking fault energy. These material properties can be influenced by H resulting in a reduced activation energy for dislocation nucleation. The universality of cohesion in metals relates the reduction of the shear modulus to the reduction of the cohesion, meaning HEDE mechanism. The increase in the core radius of a dislocation due to H is a direct evidence of decrease in dislocation line energy and H segregation on the dislocation line. In the case of partial dislocations, the H can segregate on to the stacking fault ribbon and decrease stacking fault energy.

Thus, depending on the experimental approach utilized to probe the H effect, either HELP or HEDE can be observed. In this study by utilizing a proper experimental approach, it was possible to resolve the interconnected nature of the HE.

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Hydrogen enhanced local plasticity: An atomistic study — •Johann von Pezold and Jörg Neugebauer — Max Planck Institut fuer Eisenforschung, Duesseldorf, Deutschland

The degradation of metals by H-embrittlement is a long-standing problem of huge economic impact, whose underlying mechanisms are still largely unclear, despite extensive research activities. Based on continuum elasticity theory as well as on experimental evidence, various mechanisms for the observed H-induced embrittlement of metals have been proposed, including stress-induced hydride formation, the HELP (hydrogen enhanced local plasticity) and the HEDE (hydrogen enhanced decohesion) mechanisms. However, the atomistic understanding of these mechanisms is still rudimentary.

In this study we consider the atomistic basis for the HELP mechanism, which is based on the assertion that H enhances the mobility of dislocations by shielding the elastic dislocation-dislocation and dislocation-solute interactions. In order to investigate the underlying atomistic mechanisms, the interaction of edge dislocations in Ni with dissolved H atoms has been studied using molecular dynamics simulations in conjunction with the embedded atom method (EAM).

In particular, the stability of isolated H atoms in the stress field of an edge dislocation, as well as the effect of H atoms on the elastic dislocation-dislocation interaction has been considered. In addition, the effect of H atoms on the velocity of an edge dislocation under the influence of an external stress will be presented.

MM 47.4 Fri 11:15 H 1058

Hydrogen-induced plastic deformation of rare earth metal thin films — •Mathias Getzlaff[1] and Astrid Pundt[2] — [1]Inst. of Applied Physics, University of Düsseldorf, D-40225 Düsseldorf — [2]Inst. of Material Physics, University of Göttingen, D-37077 Göttingen

Surface modification of thin Gd films during hydrogen adsorption and absorption has been investigated on the nanometer scale by STM.

The adsorption occurs in two steps. It is initiated by surface imperfections. Starting from these nucleation centers a domain-like spreading is present which is strongly hindered at surface steps.

The measurements have shown that during hydrogen loading two different types of surface pattern develop above a particular concentration: disc-like islands and ramps. These surface patterns can be well described by two plastic deformation processes in the films that lead to glide steps on the film surface: the emission of dislocation loops during hydride precipitation occurs and misfit dislocations near the film-substrate interface. Since plastic deformation leads to stress release we suggest that a lot of thin metal films that are clamped to a substrate relax plastically after reaching a certain hydrogen-induced stress that corresponds to a critical hydrogen concentration. This conclusion is corroborated by the observation that free-standing Gd islands are deformed without structural deformation. Overall, combining the ability of preparing high-quality epitaxial thin films with the detailed analysis of the mechanical properties during hydrogen absorption may lead to a deeper fundamental understanding of hydrogen switchable thin films. It may also improve their industrial applications.

MM 47.5 Fri 11:35 H 1058

Hydrogen interaction with vacancies studied by positron annihilation — •Jakub Cizek — Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

Vacancies as open-volume defects provide an additional space in lattice which makes them attractive for hydrogen. Trapping of multiple hydrogen atoms in vacancies was observed in metals. Hydrogen is not only trapped at vacancies existing already in the material, but new vacancies may also be created by hydrogen loading. Positron annihilation spectroscopy (PAS) is a well-developed non-destructive technique with very high sensitivity to open-volume defects, in particular vacancies. Type of defects and defect densities can be determined using PAS. Thus, PAS is an ideal tool for investigations of hydrogen interactions with vacancies. This contribution reports about defect studies of bulk Nb and Pd specimens step-by-step loaded to various hydrogen concentrations. PAS studies were combined with X-ray diffraction and TEM investigations. The experimental data were compared with theoretical calculations of energetic stability and positron characteristics of various defect-hydrogen configurations. We have found that vacancy-hydrogen complexes are introduced into the specimens by hydrogen loading. Density of these vacancy-hydrogen complexes increases with increasing concentration of hydrogen in the specimens. Additional defects are introduced at higher hydrogen concentrations due to precipitation of hydrides. Another type of vacancy-hydrogen complexes can be introduced by electron irradiation. Configuration, stability, and mechanism of formation of the hydrogen-induced defects are discussed.