

MM 9: Hydrogen in metals II: Multiscale simulations

Time: Monday 11:45–13:15

Location: TC 006

Topical Talk

MM 9.1 Mon 11:45 TC 006

Multiscale modeling of hydrogen-dislocation interaction — ●GERARD PAUL LEYSON, BLAZEJ GRABOWSKI, and JÖRG NEUGEBAUER — Max-Planck-Straße 1, 40237 Düsseldorf, Germany

It has been well documented that hydrogen promotes embrittlement in a wide variety of materials. Despite the fact that the phenomenon is known for over a hundred years, the atomistic origin of hydrogen embrittlement is not well understood. One of the most promising models to explain hydrogen embrittlement is the Hydrogen Enhanced Local Plasticity (HELP) mechanism, which is based on the interaction between dislocations and hydrogen solutes. This mechanism has been well studied, but a quantitative connection between the hydrogen localization around dislocations and macroscopic embrittlement has yet to be achieved. To make this connection, we have developed a multi-scale model that can take into account the different length- and time-scale associated with the phenomenon, as well as takes into account the chemical interaction between hydrogen atoms. The hydrogen concentration profile generated by the model are in excellent agreement with direct atomistic simulations and predicts the correct relaxed dislocation core structure due to the formation of the nano-hydride, while being four orders of magnitudes faster. Direct connection with experiments was made by predicting the decrease in pop-in stress observed in hydrogen-charged nano-indentation experiments as a function of hydrogen chemical potential and temperature.

MM 9.2 Mon 12:15 TC 006

H-H interaction and critical temperature of hydride formation in palladium hydrogen thin films: Experiment and model — ●STEFAN WAGNER and ASTRID PUNDT — University of Göttingen, Institute of Materials Physics

Palladium hydrogen (PdH) thin films are used as a model system to investigate the impact of elastic and microstructural constraints on structural phase transitions. Hydrogen-induced mechanical stress arises both from palladium film clamping on an elastically hard substrate and at coherent interfaces in the two-phase-coexistence region. It strongly changes the chemical potential of hydrogen, modifying the stability of the hydride phase. Mechanical stress is superimposed by microstructural constraints, channeling stress relaxation processes such as the formation of misfit dislocations in the films. In this paper we investigate hydrogen absorption and hydride formation in PdH thin films with different microstructure and clamping conditions [1]. The attractive H-H interaction energy and the critical temperature of hydride formation are determined quantitatively from the analysis of the chemical potential in combination with in situ stress measurement [2]. They differ for films with coherent interfaces and films where stress relaxation is possible. [1] S. Wagner, A. Puntdt, *Acta Mat.* 59 (2011) 1862. [2] S. Wagner, M. Moser, A. Puntdt et al., *Int. J. Hydr. Energy* 38 (2013) 13822.

MM 9.3 Mon 12:30 TC 006

Scale bridging modelling of hydride formation — ●ROBERT SPATSCHEK, GEORGIA GOBBI, CLAAS HÜTER, AURAB CHAKRABARTY, UGUR AYDIN, and JÖRG NEUGEBAUER — Max-Planck Institut für Eisenforschung, Düsseldorf

We investigate phase separation in the bulk and at surfaces and find a reduction of the solubility limit near free surfaces due to elastic coherency effects. This mechanism favours nucleation from free surfaces even in the absence of external stresses. We apply the theory to hydride formation in nickel, iron and niobium and obtain a reduction of the solubility limit by up to two orders of magnitude at room tem-

perature at free surfaces. This leads to a blurring of the distinction between hydride-forming and non-hydride-forming metals. Near stiff substrates, in contrast, the solubility limit is increased, in agreement with experimental observations. These effects are concisely expressed through a solubility modification factor, which transparently expresses the long-ranged elastic effects in a terminology accessible e.g. to ab initio calculations and experiments. The predictions are confirmed by Cahn-Hilliard simulations on the continuum level.

MM 9.4 Mon 12:45 TC 006

The Role of Temperature on the Free Energy of Hydrogen in Iron. — ●ROBERT HORTON and MICHAEL FINNIS — Royal School of Mines, Imperial College, London

A key advance in the development of hydrogen resistant steels is the inclusion of defects (such as vacancies and carbides) within the steel matrix to act as traps for the hydrogen. The development of predictive mesoscopic models to aid in the design of these steels requires knowledge of the chemical potentials of hydrogen both in the bulk and within the traps as a function of temperature. The high concentrations and high mobility of hydrogen in these systems brings the validity of traditional atomistic approaches to the calculation of the free energy into question.

In recent years a number of Monte Carlo techniques have been developed [1,2] that allow the calculation of the full partition function and thus the free energy of the system. These techniques provide a promising route to calculating the free energy of systems containing high concentrations of defects [3]. Through the application of these techniques to a system containing hydrogen in iron we show that they indeed allow one to calculate the free energy of such systems. Free energies calculated in this manner can then be included in mesoscale simulations.

[1]Wang, Fugao and Landau, D. P. (Mar 2001). *Phys. Rev. Lett.* (American Physical Society) 86 (10): 2050*2053. [2]Skilling, J. *Bayesian Analysis* 1, 833*860 (2006). [3]Horton, R. M. et al. *Journal of Physics. Condensed matter* 25, 395001 (2013).

MM 9.5 Mon 13:00 TC 006

Multiscale modelling of hydrogen embrittlement in metals — ●PRATHEEK SHANTHRAJ, HAIMING ZHANG, GERARD LEYSON, FRANZ ROTERS, TILMANN HICKEL, DIERK RAABE, and JÖRG NEUGEBAUER — Max Planck Institut für Eisenforschung, Düsseldorf, Germany

A multiscale phase field damage model is developed and coupled to a finite-strain thermo-mechanical framework to investigate the evolution of damage in metals under hydrogen-loaded conditions. The evolution of damage is based on the nucleation and growth of voids driven by the conservative transport and coagulation of hydrogen-stabilized superabundant vacancies, as well as the propagation of cracks driven by the competition between stored elastic energy at the crack tip and the hydrogen-dependent material decohesion energy. The dynamics of the hydrogen-decorated-vacancy concentration field and the damage microstructure is expressed in the form of a coupled Cahn-Hilliard and Allen-Cahn system of equations, respectively, and the physically based model parameters, such as decohesion and vacancy formation energies under hydrogen-loaded conditions, are obtained from ab-initio calculations, thus rendering the approach a multiscale modeling framework. As a case study, a polycrystalline aggregate, whose elasto-plastic mechanical response is governed by a local crystal plasticity model, is deformed under a range of hydrogen-loaded conditions to investigate the role of grain boundaries in the damage evolution process as a potential source and sink for vacancies as well as a site for interface decohesion.