MM 15: Hydrogen in Materials: Hydrogen Effects

Time: Tuesday 11:45–13:00 Location: H46

MM 15.1 Tue 11:45 H46

Atomistic study of hydrogen behavior in bcc and fcc Fe in presence of crystal defects — •Daria Smirnova[1], Sergei Starikov[2], Tapaswani Pradhan[2], Ralf Drautz[2], and Matous Mrovec[2] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Ruhr University Bochum, ICAMS, Bochum, Germany

We apply atomistic simulations to consider hydrogen behavior in Fe in presence of the given lattice distortions, namely, crystal defects or lattice expansion/compression due to applied stresses. Simulations are based on a new interatomic potential developed by the authors of current work. Firstly, we consider segregation of hydrogen on typical defects of different complexity: from vacancies to grain boundaries (GBs). Estimated segregation energies obtained for different types of GBs generally agree with the existing DFT data. Moreover, performed classical atomistic simulations give information on several types of GBs, which, due to their complex structure and considerable model size, are inaccessible for ab initio modeling. High-temperature simulations of H diffusion in the presence of GBs also show that for bcc Fe hydrogen diffusion coefficient in the GB is much lower than in bulk. The same type of study is carried out for fcc Fe. Also, we discuss variations in zero-temperature hydrogen migration barriers in bulk bcc Fe with applied stress and compare them with the results of the finite-temperature H diffusion simulations. We see that while the variations in the lattice parameter change hydrogen migration barrier, they give no significant impact on the finite-temperature hydrogen diffusion.

MM 15.2 Tue 12:00 H46

Interplay of hydrogen with defects in Al alloys — •Poulami Chakraborty[1], Huan Zhao[1], Baptiste Gault[1,2], Tilmann Hickel[1,3], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]Department of Materials, Royal School of Mines, Imperial College London, United Kingdom — [3]BAM Federal Institute for Materials Research and Testing, Berlin, Germany

Al alloys are used as major structural material in the aviation and more recently, automobile industries. This demands detail research of microstructural defects generated while usage. We have performed density functional theory calculations to study the competition of microstructural features including grain boundaries and second phase particles. The results reveal second phases as better trapping sites since H has a higher solubility compared to the GBs. However, it is seen that certain solutes such as Mg enhances the chance of HE at the forming surface during crack initiation. This is further supported by experimental data where a high strength 7xxx Al alloy is charged by deuterium using atom probe tomography (APT). Subsequently, we have extended our study to several other alloying elements such as Sc, Sn and Zr, at the GB which are inevitably present as impurities in technical alloys. Interestingly, it is seen that Sn strongly binds with H at the GB without increasing the embrittling tendency. Based on these insights, effective alloying strategies can be developed to improve the resistance to hydrogen embrittlement.

MM 15.3 Tue 12:15 H46

Impact of H on Fe and Cr diffusion in pure Fe and FeCr alloy — •Olga Lukianova[1], Anton Chyrkin[2], Vladislav Kulitckii[1], Jan Froitzheim[2], Sergei Starikov[3], Gerhard Wilde[1], Ralf Drautz[3], and Sergiy Divinski[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Chalmers University of Technology, Department of Chemistry and Chemical Engineering, Division of Energy and Materials, Gothenburg, Sweden — [3]ICAMS, Ruhr-Universität Bochum, Bochum, Germany

The impact of hydrogen on the tracer diffusion of the Fe and Cr in pure iron and Fe-18wt.%Cr alloy was measured at 873 K. The annealing treatments were performed in purified argon (H-free) and Ar+H2 atmospheres. Volume diffusion of Cr was found not to be affected by the presence of H in both alpha-Fe and the FeCr alloy whereas volume diffusion of Fe was enhanced by an order of magnitude. On the contrary, grain boundary diffusion of Cr in the FeCr alloy was retarded, while it was not affected by hydrogen in pure iron. Grain boundary diffusion of Fe remains practically unchanged in both materials. The tracer data are compared with the predictions from atomistic simulations.

MM 15.4 Tue 12:30 H46

Correlation of hydrogen diffusion behavior and in situ micromechanics during hydrogen charging of bcc Fe-Cr alloys — •Maria Jazmin Duarte Correa, Jing Rao, and Gerhard Dehm — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Hydrogen (H) is a strong candidate as energy carrier but it might cause material degradation through hydrogen embrittlement. Individual hydrogen-microstructure interactions, can be studied by targeting analyses at the nano-/microscale during H exposure. We will present our novel *back-side* electrochemical H charging approach for nanoindentation related techniques. Hydrogen diffusion from the charged back-side towards the testing (front) surface is quantified by Kelvin probe permeation tests and unwanted corrosion is avoided. Our unique method allows differentiating between the effects of trapped and mobile H, and performing well controlled measurements with different H levels monitored over time to consider H absorption, diffusion and release through the metal. These aspects will be presented by nanoindentation and micropillar compression tests during H charging of Fe-Cr alloys (8-20 wt.%Cr). An enhanced dislocation nucleation is shown consistent with the defactant theory, and a hardening effect while increasing the Cr content and the H entry. The mechanical data is finally analyzed in terms of the diffusion behavior and used to develop a nanohardness-based H diffusion coefficient approach.

MM 15.5 Tue 12:45 H46

Role of hydrogen on the relative stability of the phases in steels — •Ali Tehranchi, Tilmann Hickel, and Jörg Neugebauer — Max Planck institute for Iron research, Max Planck Straße 1, 40237 Düsseldorf

Hydrogen embrittlement (HE) is a persistent mode of failure in high-strength steels. During the service life of these steels phase transformations occur and are a key element that determines their response to the service loads. Thus the investigation of the role of H atoms in the relative stability of the phases present and forming in steels is of great interest. In this work, we studied the role of H on the relative stability of the fcc/bcc/hcp phases using the ab initio thermodynamics. The results indicate that at low hydrogen chemical potentials the stability of the fcc phase, which can be representative of retained austenite (RA) in steels, is slightly enhanced by the presence of H atoms. In contrast, at high hydrogen chemical potentials the bcc phase is stabilized by H. Moreover, since the excess volume of the hydrogen-rich bcc phase is significantly larger than that of the fcc phase, the presence of a stress field can change the relative stability of these phases in the coexistence regions of the phase diagram. This feature is particularly important for cyclic loading conditions: during loading cycles forward and reverse phase transformations occur and the H released by these transformations can damage the material.