

## MM 33: Topical Session: Interface-dominated phenomena - Hydrogen at Interfaces

Time: Wednesday 10:15–11:30

Location: IFW A

MM 33.1 Wed 10:15 IFW A

**Effect of grain boundaries on self-diffusion and hydrogen diffusion in bcc iron** — ●DARIA SMIRNOVA, SERGEI STARIKOV, MATOUS MROVEC, and RALF DRAUTZ — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum, Bochum, Germany

Grain boundaries (GBs) are known to affect diffusion processes in most materials. In this work, we employed atomistic simulations to investigate how both self-diffusion and hydrogen diffusion processes are altered in the vicinity of various GBs in body-centered cubic (bcc) iron. The investigations were performed using accurate ab initio calculations based on density functional theory and large-scale molecular dynamics simulations with various interatomic potentials. We found that for symmetric tilt GBs the self-diffusion is mostly driven by interstitial atoms while in general GBs Fe atoms diffuse predominantly via an exchange mechanism that does not involve a particular defect and is similar to liquid diffusion. In most investigated cases, the self-diffusion along GBs is significantly enhanced compared to that in bulk. In contrast, the motion of H atoms along GBs is at ambient temperatures several orders of magnitude slower than the H bulk diffusion. This outcome is related to larger migration barriers in the distorted crystal structure of GBs, compared to a very low H migration barrier in bulk bcc Fe. We present temperature variations of diffusion coefficients for different GBs and compare the simulation predictions with available experimental data.

MM 33.2 Wed 10:30 IFW A

**Ab initio analysis of hydrogen segregation and embrittlement at cleavage plains and at a grain boundary in bcc Fe** — ●ABRIL AZÓCAR GUZMÁN, JEONGWOOK JEON, ALEXANDER HARTMAIER, and REBECCA JANISCH — ICAMS, Ruhr-Universität Bochum

Grain boundaries in ferritic microstructures play a dual role in the context of hydrogen embrittlement: on the one hand, they act as H traps and thus reduce the amount of mobile H in the system. On the other hand, exactly this trapping is expected to promote hydrogen enhanced decohesion at the grain boundaries. In order to influence the segregation process as well as the cohesive properties of interfaces in ferrite, one needs to understand in detail the relationship between strain, hydrogen solubility, and cohesive strength.

We present the results of ab-initio studies of H segregation in Fe single crystal {001} and {111} cleavage planes, as well as at a  $\Sigma 5$  symmetrical tilt grain boundary. We determine the solution energy as a function of tractions normal to the interface for different loading and relaxation schemes. While the chosen method clearly affects the quantitative results, the qualitative findings are the same: In relaxed as well as strained microstructures, H tends to accumulate at the grain boundary. While it reduces the surface energies, and hence the work of separation, there is no significant impact of H on the transgranular or intergranular fracture stress.

MM 33.3 Wed 10:45 IFW A

**Solute - hydrogen interactions at Al grain boundaries: A first principle study** — ●POULAMI CHAKRABORTY, TILMANN HICKEL, BAPTISTE GAULT, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH

The deleterious effect of hydrogen on the mechanical properties of metallic alloys is known to reduce strongly limits the applicability of

high strength metallic materials. Therefore, the characterization and simulation of hydrogen in such alloys is decisive. In this work, the interaction of hydrogen with GBs in aluminium in terms of decohesion effect has been investigated by means of density functional theory simulations. Two distinct types of GBs have been considered: the  $\Sigma 11(113)$  [011] with a close-packed interface structure and the  $\Sigma 5(210)$  [001] with a more open interface structure. We first identify the potential interstitial sites of H adsorption at GBs and then the mechanisms governing the H segregation energetics. A thermodynamic assessment of the impact of solutes onto H chemisorption in the interfacial vicinity is provided by performing a high-throughput analysis for potential alloying candidates. The identified trends of the solute-H interactions are comparable in the two representative cases studied, which motivated us to extend the work towards a more generalized approach.

MM 33.4 Wed 11:00 IFW A

**Niobium Hydrogen Thin Films: Mechanical Stress, Interface Coherency and Phase Equilibria** — ●STEFAN WAGNER<sup>1</sup>, PHILIPP KLOSE<sup>1</sup>, VLADIMIR BURLAKA<sup>2</sup>, KAI NÖRTHEMANN<sup>2</sup>, MAGNUS HAMM<sup>2</sup>, and ASTRID PUNDT<sup>1</sup> — <sup>1</sup>Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — <sup>2</sup>Göttingen University, Institute of Applied Materials, Göttingen, Germany

Metal-hydrogen systems offer grand opportunities for studies on fundamental aspects of alloy thermodynamics and kinetics. When the system size is reduced to the nanoscale, interface effects related to microstructural defects as well as mechanical stress affect the systems' properties [1]. In thin films the lattice expansion linked to hydrogen absorption is hindered by the substrate. Resulting stresses are usually compensated by plastic deformation, lowering the film's coherency state. Here we show for the model case of niobium-hydrogen (Nb-H) thin films on sapphire substrates that plastic deformation is suppressed below critical values of film thickness. This yields ultra-high stresses of up to -10 GPa, changing the film's phase stabilities, phase diagrams as well as the phases' nucleation and growth dynamics. [1] S. Wagner et al., Chem. Phys. Chem. 20 (2019) 1890.

MM 33.5 Wed 11:15 IFW A

**ETEM studies on hydride precipitation and growth in Mg films** — MAGNUS HAMM<sup>1</sup>, MARIAN DAVID BONGERS<sup>1</sup>, VLADIMIR RODDASIS<sup>1</sup>, STEFAN DIETRICH<sup>2</sup>, KARL-HEINZ LANG<sup>2</sup>, and ●ASTRID PUNDT<sup>2</sup> — <sup>1</sup>Göttingen University, Institute of Materials Physics (IMP), Göttingen, Germany — <sup>2</sup>Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Understanding solute-induced phase transformations is crucial in a variety of research fields such as catalysis, memory switching or energy storage. We present solute-induced phase transformations studied on the model system magnesium-hydrogen (MgH) which provides high lattice expansion during the phase transformation. In situ precipitation and growth of MgH<sub>2</sub> is studied in an environmental transmission electron microscope (ETEM), combining electron energy loss spectroscopy (EELS) and various imaging techniques. We observe that the Mg-hydride (MgH<sub>2</sub>) formation proceeds through the formation of nanocrystals that are separated by low-angle grain boundaries. We attribute this microstructural change to large strains and stresses between the matrix and the MgH<sub>2</sub> created during the transformation. [1] M. Hamm et al., Int. J. Hydr. Energy 44 (2019) 32112.