

MM 27: Hydrogen in Materials

Time: Wednesday 10:15–13:00

Location: SCH A 215

MM 27.1 Wed 10:15 SCH A 215

Strain-induced twins and martensite: Effects on hydrogen embrittlement of additive manufactured (AM) 316L

— ●STEFAN WAGNER¹, YUANJIAN HONG², CHENGSHUANG ZHOU², SABINE SCHLABACH^{1,3}, ASTRID PUNDT¹, LIN ZHANG⁴, and JINYANG ZHENG⁴ — ¹Karlsruhe Institute of Technology (KIT), Institute for Applied Materials - Materials Science and Engineering (IAM-WK), Karlsruhe, Germany — ²Institute of Material Forming and Control Engineering, Zhejiang University of Technology, Hangzhou, China — ³Karlsruhe Nano Micro Facility (KNMF), KIT-Campus North, Eggenstein-Leopoldshafen, Germany — ⁴Institute of Process Equipment, Zhejiang University, Hangzhou, China

Extending the use of hydrogen as a renewable energy carrier 316L is one of the most important structural materials. Additive manufacturing significantly enhances the steels' strength, allowing for weight reduction of construction parts. In this contribution [1] we investigate effects of strain-induced twins and martensite on hydrogen embrittlement of AM316L under tension in the temperature range from 80 K to 300 K. It is revealed that quasi-cleavage of twin boundaries is the major path of material failure. Strain-induced martensite has low impact on the H-embrittlement of AM316L, since it emerges only late in the deformation process.

[1]: Yuanjian Hong et al., 2022. Corrosion Science, 208; 110669-1-16.

MM 27.2 Wed 10:30 SCH A 215

Ab-initio insights into hydrogen-carbide interaction in bcc Fe

— SAURABH SAGAR and ●POULUMI DEY — Delft University of Technology, Delft, The Netherlands

Development of advanced high-strength steels is in high demand owing to its wide scale applications. The excellent mechanical properties of these steel grades are attributed to the underlying microstructure which comprises of finely dispersed nano-precipitates. However, one major factor restricting their application is their susceptibility to Hydrogen Embrittlement (HE). Experimental and theoretical work have been carried out to understand if the nano-sized carbides can aid in reducing the susceptibility to HE along with providing strengthening. Within this study, we investigated the effectiveness of finely dispersed nano-carbides (i.e., TiC, NbC and VC) to limit the diffusible hydrogen content in bcc Fe. Our study revealed that the interplay between hydrogen and carbon vacancies, local atomic environment at interface as well as interface geometry can lead to significantly increased hydrogen solubilities. Thus, the trapping at these sites leads to a reduction in concentration of diffusible hydrogen. However, the question remains whether hydrogen can populate the deepest traps (i.e., the carbon vacancies) in the bulk of these carbides. We, thus, extended our study to compute migration barriers of hydrogen across the coherent interface between bcc Fe and TiC, NbC and VC using climbing-image Nudged Elastic Band method. Furthermore, we evaluated whether a chain of interconnected carbon vacancies from the interface to the bulk of the carbides leads to a reduction in the migration barrier of hydrogen.

MM 27.3 Wed 10:45 SCH A 215

Role of diffusible hydrogen on the mechanical behavior of bcc alloys by in situ micromechanics during hydrogen charging —

●MARIA JAZMIN DUARTE CORREA, JING RAO, and GERHARD DEHM — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Hydrogen embrittlement represents a major challenge for the use of hydrogen (H) as energy carrier. Understanding individual hydrogen-microstructure interactions by targeting analyses at the nano-/microscale during H exposure is essential to prevent material degradation. We will present nanoindentation and micropillar compression tests during H charging of Fe-Cr alloys (8-20 wt.%Cr) using our novel "back-side" electrochemical H charging approach for nanoindentation related techniques. 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 as well analyzed in terms of the diffusion behavior and used to develop a nanohardness-based H diffusion coefficient approach. On the other hand, 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 which will be shown

using the example of the model alloys mentioned above.

MM 27.4 Wed 11:00 SCH A 215

Hydrogen interstitials in iron oxides using ab-initio calculations —

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The steel making industry is responsible for more than 6% of CO₂ emissions. These emissions come from the dependency on carbon and carbon monoxide as reducing agents. Hydrogen, on the other hand, can reduce iron oxides with water released instead. The reduction route from Magnetite to Hematite, then Wüstite, and finally to pure iron requires hydrogen to diffuse into and react with the different solid structures as well as with the multiple solid-solid interfaces. To optimize the reduction process, the mechanistic details of this process requires understanding to the role of hydrogen interstitials in the bulk iron oxides. We therefore computed the diffusion paths of hydrogen through the different iron oxide phases employing density functional theory (DFT) calculations for all three iron oxides - Magnetite, Hematite, and Wüstite. Analyzing the electronic structure of the studied oxides, we examine the reliability of the used exchange correlation functionals and how the electronic structure is affected by the inclusion of hydrogen, both as a neutral and a charged point defect. Finally, we utilize symmetrized plane waves to map the full 3D potential energy surfaces (PESs) for hydrogen interstitials within these iron oxides using a modest number of DFT calculations. Based on these calculations we identify the hydrogen preferential interstitial sites, diffusion barriers, and diffusion paths.

MM 27.5 Wed 11:15 SCH A 215

Influence of impurity atoms on the hydrogen diffusion into ruthenium —

●JULIAN GEBHARDT and DANIEL URBAN — Fraunhofer IWM, 79108 Freiburg

Ruthenium is considered as a promising protection layer to prevent the penetration of small atoms such as hydrogen into the underlying material. However, hydrogen is known to be able to penetrate ruthenium films under certain conditions and it has been hypothesized that impurity atoms, such as Sn, could play a major role in this process, decreasing the barrier of diffusion into the material for incoming hydrogen. We demonstrate that this is not the case for low to medium coverages, i.e., as long as the adsorbed species can be treated individually without significant adsorbate-adsorbate interactions. Within this coverage regime, the hydrogenation is destabilized in the vicinity of impurity atoms, such as X=Mg, P, S, Si, or Zn, due to the strong bonding of the adsorbates with the free ruthenium surface. As a result, the diffusion barriers are not significantly reduced in the vicinity of any of the tested impurity atoms. The most likely and energetically favorable process occurs at a sufficiently large distance to the impurity, with an energy barrier that is almost identical to that of the free surface. Due to the chemical variety of the considered impurity atoms, this finding appears to be general. This means that impurities can be ruled out to enhance hydrogen uptake of ruthenium layers for the considered coverages and other structural properties such as grain boundaries and dislocations should be considered as pathway for the hydrogen penetration.

15 min. break

MM 27.6 Wed 11:45 SCH A 215

Metal Hydride Materials for Solid-State Hydrogen Storage Applications: Utilizing the Synergy of Experiment & Theory for Future Materials Design Challenges —

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Metal hydride materials present a safe, efficient and long-term storage option for hydrogen under mild conditions for many stationary and mobile applications and will play an important role in the transition towards an emission-free energy economy.

Deep understanding of (de)hydrogenation thermodynamics and kinetics of such materials is essential to enable targeted design of novel

storage materials and optimization of existing compositions tailored for specific applications. To obtain the necessary insights, computation and experiment need to work closely together to fully leverage theory-experiment feedback loops.

In this talk, an overview will be given of how experimental activities can be connected with computational multi-scale methodology (from atomistic to mesoscale), as currently performed in the joint efforts by the metal hydride materials research groups at Hereon and LLNL, with the goal being to develop virtual workflows linking Density Functional Theory methods, thermodynamic modeling and phase-field simulations together with experimental investigations for an integrated description of metal hydride (de)hydrogenation processes.

MM 27.7 Wed 12:00 SCH A 215

Ab Initio Simulations of Laves-phase high-entropy alloys for hydrogen storage — ●YUJI IKEDA¹, KAVEH EDALATI², and BLAZEJ GRABOWSKI¹ — ¹University of Stuttgart, Stuttgart, Germany — ²Kyushu University, Fukuoka, Japan

High-entropy alloys (HEAs), particularly those in the Laves phases, are promising candidates for hydrogen-storage alloys. Recent experiments have indeed revealed that the equiatomic TiZrCrMnFeNi Laves-phase HEA can work as a hydrogen-storage alloy at room temperature (i.e., without heating) under nearly atmospheric pressure [1,2]. Tuning the compositions of such Laves-phase HEAs should be possible to design hydrogen-storage alloys with more desirable properties. We have demonstrated that ab initio H adsorption energies in $Ti_xZr_{2-x}CrMnFeNi$ become more negative (thus energetically more favorable) on average with increasing the Ti content, consistent with experiments [3]. We will also show how the H adsorption energy depends on the local chemical environment in the Laves-phase HEAs.

[1] P. Edalati, A. Mohammadi, Y. Li, H.-W. Li, R. Floriano, M. Fuji, and K. Edalati, *Scr. Mater.* 209, 114387 (2022).

[2] P. Edalati, R. Floriano, A. Mohammadi, Y. Li, G. Zepon, H.-W. Li, and K. Edalati, *Scr. Mater.* 178, 387 (2020).

[3] A. Mohammadi, Y. Ikeda, P. Edalati, M. Mito, B. Grabowski, H.-W. Li, and K. Edalati, *Acta Mater.* 236, 118117 (2022).

MM 27.8 Wed 12:15 SCH A 215

Visualizing radiation-induced damage by Hydrogen/Deuterium — ●APARNA SAKSENA, BINHAN SUN, HEENA KHANCHANDANI, and BAPTISTE GAULT — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf 40237, Germany

Atom probe tomography (APT) is now extensively used to measure the local chemistry of materials. APT proceeds by field evaporating a sharp, needle-shaped specimen with a radius ~ 50 nm, often prepared by focused ion beam (FIB) milling. The interaction of the ion beam at high currents is known to amorphize crystalline materials by changing the lattice and creating vacancies. Therefore, a platinum protective layer and a low-energy ion shower are routinely used to avoid or remove the damaged layer from the specimen. Additionally, for investigating the local chemistry of defects such as interfaces via APT, transmission Kikuchi diffraction (TKD) can be performed during milling steps. The damage resulting from these techniques is considered negligible. Here, we use deuterium charging to probe the

damage associated with specimen preparation as vacancies are known to be strong trapping sites for hydrogen/deuterium. We analyzed a medium Mn steel containing austenite (fcc) and ferrite (bcc). APT specimens were charged in a deuterium gas atmosphere, and the distribution of deuterium shows clusters of point defects after Pt deposition, conventional Ga-FIB preparation, and TKD. These deuterium-rich clusters are sequentially minimized by systematically eliminating these preparation-induced damages.

MM 27.9 Wed 12:30 SCH A 215

Mechanism-based Lifetime Assessment under the Influence of Hydrogen — ●FABIEN EBLING^{1,2}, HEINER OESTERLIN², ASTRID PUNDT¹, and KEN WACKERMANN² — ¹Karlsruhe Institute of Technology (KIT) Institute for Applied Materials - Materials Science and Engineering (IAM-WK), Karlsruhe, Germany — ²Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany

Components see a variety of mechanical and thermal loads during service. Increased damage can occur when used in a hydrogen atmosphere. The experimental investigation of all states is very time-consuming and expensive, especially for testing under hydrogen influence. Mechanism-based lifetime assessments can be used to model crack growth and predict service life. This can significantly reduce the need of experimental investigations for a safe design of components. This work discusses different approaches of modeling hydrogen assisted cracking and presents an adaptation of the ZD parameter according to Heitmann (1983) for the influence of hydrogen at different temperatures.

MM 27.10 Wed 12:45 SCH A 215

Validation of continuum simulations of materials at the mesoscopic level with X-ray and neutron diffraction with a focus on hydrogen storage materials — ●ARNAB MAJUMDAR¹, MARTIN MÜLLER², and SEBASTIAN BUSCH¹ — ¹GEMS at MLZ, Helmholtz-Zentrum hereon GmbH, Lichtenbergstr. 1, 85748 Garching, Germany — ²Institute of Materials Physics, Helmholtz-Zentrum hereon GmbH, Max-Planck-Str. 1, 21502 Geesthacht, Germany

With the advent of new technologies, it has been possible to design new materials through theoretical analysis and simulation. However, these simulations have to be validated by experiments. In this work, we develop a method to validate the structural features in continuum simulations directly on the mesoscopic level with X-ray and neutron scattering experiments. The workflow to compare atomistic computer simulations to scattering patterns is well established: the scattering amplitude of individual atoms is summed, whose positions are obtained from the simulation. This approach fails for larger mesoscopic structures due to the unrealistic computation time required to generate the simulations and scattering pattern on a mesoscopic scale with atomic resolution. We developed a methodology that calculates scattering patterns from a continuum simulation like phase-field modeling, where the material description is continuous instead of a collection of atoms. The approach is validated with simple structures and gradually applied to more complex structures. The long term goal is to use this technique for the simulation of hydrogen storage materials and validation of the simulations with scattering data.