MM 34: Hydrogen in Materials I

Time: Thursday 15:45–17:30 Location: SCH/A215

MM 34.1 Thu 15:45 SCH/A215

In-situ mechanical characterization of 316Ti hollow specimens in hydrogen environments - from ambient down to 20 K — •Elvina Gaisina, Simeon Eckerle, Camelia Schulz, Zahra Abbasi, Astrid Pundt, and Klaus-Peter Weiss — Karlsruhe Institute of Technology, Germany

The Application of Liquid Hydrogen (AppLHy) project explores the feasibility of a hybrid pipeline system transporting liquid hydrogen while simultaneously using the cold enables superconducting electrical energy transmission. Developing such a system requires a reliable understanding of material behavior under cryogenic conditions and exposure to hydrogen environments. However, conventional test setups that simulate these conditions are often large, complex, and require extensive safety measures to prevent hydrogen leakage. To provide a safer and more efficient testing method, this study presents an in-situ mechanical testing approach using hollow cylindrical specimens pressurized with gas. Austenitic stainless steel 316Ti, a widely applied cryogenic compatible material, was selected for testing. The hollow specimens were filled with hydrogen or helium at pressures up to 200 bar and subjected to tensile loading at temperatures ranging from ambient down to 20 K. The results show that some hydrogen-induced effects become noticeable primarily after substantial plastic deformation. Significant changes in mechanical properties and fracture behavior are observed only at 200 K.

MM 34.2 Thu 16:00 SCH/A215

In situ Micromechanical Investigation of Hydrogen Embrittlement Mechanisms in Fe3%Si — •Maral Sarebanzadeh[1], Svetlana Korneychuk[1,2], Rolf Rolli[1], Hans-Christian Schneider[1], Astrid Punt[1], Xufei Fang[1], and Christoph kirchlechner[1] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Insitute of Nanotechnology, Karlsruhe Institute Technology, Karlsruhe, Germany

Hydrogen embrittlement (HE) remains a critical limitation for the reliable use of hydrogen in structural applications. Among the proposed micromechanisms, hydrogen-enhanced localized plasticity (HELP) is widely discussed, suggesting that hydrogen facilitates dislocation motion and localizes deformation. However, its microstructural manifestation remains insufficiently understood and rarely observed directly. To address this, we investigate HE in Fe3%Si using in-situ micropillar compression combined with tritium charging, leveraging the advantage of probing a few dislocations in a well-defined geometry. Micropillar tests conducted before and after charging with a protium/tritium gas mixture show a strong increase in yield strength, indicating pronounced dislocation blocking rather than enhanced glide. We demonstrate that dislocations can lose mobility, with the activating stress increasing by a factor of 2-3. Transmission electron microscopy (TEM) and electron energy loss spectroscopy (EELS) investigations are being performed to identify hydrogen-containing features around dislocations and to clarify how hydrogen governs dislocation mobility in bcc materials such as Fe3%Si.

MM 34.3 Thu 16:15 SCH/A215

Theoretical study of temperature dependencies in HELP- and HEDE-based damage models on the fatigue behavior of ferritic steel by hydrogen — Alexandra Stark[1,2], Petra Sonnweber-Ribic[1], and •Christian Elsässer[2,3] — [1]Robert Bosch GmbH, CR, 71272 Renningen — [2]Fraunhofer IWM, 79108 Freiburg — [3]University of Freiburg, FMF, 79104 Freiburg

In this theoretical study, the influence of temperature dependencies in hydrogen embrittlement (HE) models on the fatigue damage of ferritic steel is investigated by using a coupled hydrogen-diffusion and crystal-plasticity finite-element simulation framework. We focus on the characteristic "bell-shaped" dependence of HE on temperature and examine its effects by means of HE models based on Hydrogen Enhanced Local Plasticity (HELP) and Hydrogen Enhanced Decohesion (HEDE) mechanisms. Hydrogen-induced fatigue damage is monitored by a fatigue indicator parameter (FIP): maximized damage occurs within a narrow temperature range consistent with experimental results reported in literature. Our results arise from an interplay of plastic strain localization and hydrogen trapping, combined with a sufficiently efficient supply of hydrogen. The findings of this study highlight how the interplay of hydrogen diffusivity, trap filling kinetics, and available diffusible hydrogen plays a critical role for the temperature dependence of HE. In addition, the influence of varying trap binding energies is explored, which has a substantial effect on both temperature behavior and induced fatigue damage.

MM 34.4 Thu 16:30 SCH/A215

Atomistically Informed Grain-Boundary Thermodynamics for Phase-Field Modelling of Hydrogen-Driven Microstructural Evolution in Aluminium — •Bharathi Ganesh Ganesan Sekar[1], Ali Tehranchi[1], Tilmann Hickel[1], and Nils Warnken[2] — [1]Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany — [2]University of Birmingham, Birmingham, United Kingdom

Hydrogen-driven microstructural evolution in polycrystalline aluminium (Al) is strongly influenced by grain-boundary (GB) structure and hydrogen (H) segregation. We aim to develop an atomistically informed phase-field framework to describe these effects, with relevance to hydride formation. Molecular-statics simulations were performed for representative FCC Al symmetric-tilt boundaries $\Sigma5(310)$, $\Sigma5(210)$, and $\Sigma3(111)$ to assess whether H segregation can initiate hydride formation. Instead, H induces defect-mediated structural transitions and shows distinct relaxation pathways during ingress and discharge. At high H content, the GB cleaves and free surfaces form. To generalise these insights, a library of 250 microstates was generated for each GB plane normal within the $\Sigma5$ family by sampling rigid-body translations and boundary-plane atomic fractions. This enables construction of GB energies as a function of plane normal, with temperature dependence introduced through Boltzmann weighting. H effects are included by evaluating segregation energies for the minimum-energy microstate of each plane normal, yielding H-chemical-potential-dependent GB energies. These results provide essential GB energetics for phase-field modelling of H-driven microstructural evolution in Al.

MM 34.5 Thu 16:45 SCH/A215

Understanding of hydrogenation induced planar defects in a proton-based battery material — •Yujun Zhao, Stefan Zaefferer, Yug Joshi, and Dierk Raabe — Max-Planck-Institut für Nachhaltige Materialien, Max-Planck-Straße 1, 40237 Düsseldorf, Deutschland

Research on nickel-metal hydride batteries provides valuable insights for advancing hydrogen storage systems. However, the battery cycle stability is limited by crystalline defects generated during hydrogenation. Therefore, an in-depth understanding of these defects is critical for improving the long-term cyclic performance of electrode materials. In this work, electrochemically charged hydrogen induces the formation of planar defects and dislocation bands in LaNi5 intermetallic compound. The correlations among crystallographic orientations, defect characteristics, and local hydrogen concentration were explored by multiscale characterization techniques, including electron backscattered diffraction (EBSD), electron channeling contrast imaging (ECCI), transmission electron microscopy (TEM), and atom probe tomography (APT). In particular, the atom probe evaporation behavior of LaNi5 along different orientations are revealed, clarifying the local magnification effect and the loss of spatial resolution. The influences of the planar defects on the evaporation behaviors of metallic elements and hydrogen atoms are also discussed.

MM 34.6 Thu 17:00 SCH/A215

Hydrogen Solution Energies at Microstructural Defects in Ferritic Steels — •Onur Can Şen[1,2,3], Santiago Benito[2], Sebastian Weber[2], and Rebecca Janisch[3] — [1]Max Planck Institute for Sustainable Materials, Germany — [2]Institute for Materials, Chair of Materials Technology, Ruhr-University Bochum, Germany — [3]ICAMS, Ruhr-University Bochum, Germany

Hydrogen is essential for sustainable industries but can also cause severe degradation through hydrogen embrittlement (HE). Trapping H at microstructural defects helps mitigate HE, though its efficiency depends on how each defect affects H solution energy.

This study combines experiments and DFT calculations to examine how microstructural defects in ferritic steels influence H trapping, focusing on different grain boundary (GB) types with and without segregants.

DFT was used to calculate solution energies at several special GBs in ferrite, both clean and with alloying elements (Cr, Cu, Ti) or vacancies, and these energies were linked to structural and electronic GB parameters.

Ferritic model alloys with varied compositions were produced and characterised. By optimizing processing, we increased the fraction of special GBs in the microstructure (Şen et al., JMRT (2025)).

The calculated solution energies serve as input for Oriani's model to predict thermal desorption spectra of these alloys.

Overall, this work shows how combining simulations and experiments clarifies the role of microstructural heterogeneities in HE.

MM 34.7 Thu 17:15 SCH/A215

Investigation of phase stability and defects in FeTi for H2 storage application — •Shankha Nag[1], Ali Tehranchi[1], Ruben Bueno Villoro[2], Christian Liebscher[2], Yuanyuan Shang[3], Claudio Pistidda[3], and Tilmann Hickel[1] — [1]Bundesanstalt für Materialforschung und -Prüfung, Berlin, Germany — [2]Fakultät für Physik und Astronomie, Ruhr Universität Bochum, Bochum, Germany — [3]Helmholtz-Zentrum Hereon, Geesthacht, Germany

Safe, durable, and efficient storage remains a central hurdle in hydrogen economy, where metal hydrides offer a promising route, particularly for stationary applications. Among these materials, FeTi stands out as a cost-effective system capable of reversible hydrogen uptake and release under near-ambient conditions. As part of BMBF-funded collaborative project GreenH2Metals, we performed atomistic simulations aimed at elucidating experimentally observed microstructural transformations such as formation of secondary phases and hydrides. We analyzed the thermodynamic stability of competing phases using ab initio calculations and examined chemical segregation as well as heterogeneous precipitation at dislocations and planar defects. Defect phase diagrams, along with the roles of vacancies and antisite defects in bulk diffusion, are explored in detail. The impact of various tramp elements on these processes is assessed through high-throughput calculations enabled by workflow frameworks such as pyiron. Together, these computational insights support a data-driven alloy design strategy for optimizing FeTi-based materials for sustainable hydrogen storage.