MM 10: Topical Session: Hydrogen in Materials: from Storage to Embrittlement I

Time: Monday 15:45–18:00 Location: C 130

Topical Talk MM 10.1 Mon 15:45 C 130

Unraveling the impact of defect-induced phases on hydrogen embrittlement and storage — •Ali Tehranchi[1], Poulami Chakraborty[1,2], Marti Lopez Freixes[1], Jing Rao[1], Maria J Duarte Correa[1], Baptiste Gault[1,3], Tilmann Hickel[1,4], and Jörg Neugebauer[1] — [1]-Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany — [2]Basque Center for Applied Mathematics, Bilbao, 48009, Spain — [3]-Department of Materials, Imperial College, South Kensington,London, SW7 2AZ, UK — [4]Bundesanstalt für Materialforschung und -prüfung (BAM)

Establishing a hydrogen economy to reduce carbon emissions has sparked renewed interest in hydrogen embrittlement (HE) and hydrogen storage (HS) mechanisms. We examine the critical role of defect-induced hydride and metallic phases, highlighting associated challenges and opportunities. First, using ab initio thermodynamics the role of H on the relative stability of the fcc/bcc/hcp phases in steels is studied. These studies show the existence of a few atomic percent of H in retained austenite (RA) at experimentally relevant H chemical potentials. Therefore, a phase transformation of H-charged fcc to bcc will release the excess H. We discuss the interplay of H in grain/phase boundaries to assess the role of these excess H in HE. Second, the formation of nano-hydrides (NHs) in vicinity of various defects in ferritic FeCr and high-strength Al-based alloys is analyzed. NHs under indentors and around dislocations significantly alter the mechanical response of FeCr alloy. NHs in the vicinity of dislocations and micro-cracks in Al-based alloys provide new opportunities for enhancing HS.

MM 10.2 Mon 16:15 C 130

Strengths and Weaknesses of Classical Interatomic potentials for Hydrogen Embrittlement — •Ram Mohan Tirunelveli Vallinayagm[1,2], Elena Akhmatskaya[1,3], Iban Quintana[2], and Mauricio Rincon Bonilla[1] — [1]BCAM-Basque Center for Applied Mathematics, Alameda de Mazarredo 14, E-48009 Bilbao, Spain — [2]IK4-Tekniker, Surface Engineering and Materials Science Unit, Eibar, Spain — [3]IKERBASQUE, Basque Foundation for Science, Plaza Euskadi 5, 48009 Bilbao, Spain

Molecular Dynamics is a common computational approach to probe the Hydrogen Embrittlement (HE) of steels at the atomistic scale. The reliability of these simulations depends on the interatomic potentials (IPs) describing particle interactions. A large number of IPs have been developed for the H-Fe system, yet no systematic benchmarking has been reported to date. Here, seven widely used IPs were benchmarked on the basis of four metrics, each critical to predicting HE: H-distribution, H-Diffusivity, Mechanical properties and H/grain boundary interactions. We put forward a classification scheme that allows practitioners to quickly choose the best IP for a particular application. The EAM potential by Song et al (Nat. Mater, 12, 145) was found to be the most adequate across the board, leading to reasonable predictions in each metric. Interestingly, we observed that other EAM IPs produce unrealistic H agglomeration, leading to long equilibration times and consistent underestimation of the H diffusivity. Poor performance of examined Modified EAM and Bond Order IPs could be due to the lack of H transport data during training.

MM 10.3 Mon 16:30 C 130

Effect of mechanical stress, chemical potential, and coverage on hydrogen solubility during decohesion of ferritic steel grain boundaries — Abril Azocar Guzman[1] and •Rebecca Janisch[2] — [1]IAS-9, Forschungszentrum Jülich, 52425 Jülich, DE — [2]ICAMS, Ruhr-Universität Bochum, 44801 Bochum, DE

Hydrogen embrittlement (HE) mechanisms in structural materials such as iron and iron alloys present a complex scenario, in which the interaction of H with different crystal defects and the solubility of H in the system depends on the concentration, chemical potential and applied mechanical stress. Therefore, understanding these processes at the atomic level is fundamental for developing methods that can mitigate the detrimental effects of H. Grain boundaries (GBs) play a critical role in hydrogen enhanced decohesion mechanism, where H weakens the interatomic bonds causing intergranular fracture. In this work, we carry out DFT calculations to investigate the decohesion of the $\Sigma5(310)[001]$ and $\Sigma3(112)[1\bar{1}0]$ symmetrical tilt GBs in bcc Fe. To address the aforementioned open questions regarding the solubility of H, both thermodynamic limits of the separation of segregated interfaces are analysed. The results indicate that at higher local concentrations, H leads to a significant reduction of the cohesive strength of the GB planes, more pronounced at the $\Sigma5$ GB due to a more open local atomic environment. However, at higher applied mechanical stress and chemical potential, the solubility becomes higher at the $\Sigma3$ GB. To proceed from Fe to ferritic steel, also the effects of the alloying elements C, V, Cr and Mn at the GB are studied.

MM 10.4 Mon 16:45 C 130

The effect of solute atoms on the bulk and grain boundary cohesion in Fe: Implications for hydrogen embrittlement — •Poulami Chakraborty, Mauricio Rincon Bonilla, and Elena Akhmatskaya — Basque Centre for Applied Mathematics, Bilbao, Spain

Hydrogen embrittlement includes the mechanisms by which hydrogen diffuses in a system and causes mechanical degradation by loss of ductility. Therefore, in structural metals including Fe, selective alloying is used for strengthening and reducing the diffusivity of hydrogen by formation of precipitates or intermetallic phases which act as potential trapping sites. We have performed ab initio calculations focusing on the interactions of several alloying elements Cr, Ni, Mn commonly used in austenitic steels with grain boundaries. Our calculations helped us to identify alloying elements with the highest stabilising power. This is quantified by the calculation of thermodynamic parameters such as segregation and embrittlement energy. We have then compared these parameters in presence of hydrogen. Our systematic investigation enables us to understand the basic mechanism of hydrogen interaction with defects in alloys. Identification of such trends in presence of hydrogen can guide experimentalists in the choice of alloying elements and ultimately advance materials design.

MM 10.5 Mon 17:00 C 130

Hydrogen-driven surface segregation in Pd-alloys from atomic scale simulations — •Pernilla Ekborg-Tanner and Paul Erhart — Department of Physics, Chalmers University of Technology, Gothenburg, Sweden

Pd-based nanoalloys show great promise as plasmonic hydrogen sensors. Nanoalloys are, however, subject to issues related to the chemical order such as surface segregation. The surface composition is directly related to the kinetic properties necessary for H sensing and as such, understanding the surface segregation during fabrication, operation and storage is crucial to ensure long-term stable sensors. In this work, we employ cluster expansions of PdAu and PdCu surface alloys with variable H coverage, trained using DFT calculations and sampled in Monte-Carlo simulations. This approach allows us to study the H coverage and the layer-by-layer composition of the near-surface region as a function of bulk composition, temperature and H pressure. We find that in the case of AuPd, Au segregates to the surface in vacuum while Pd segregates to the surface at full H coverage, and the transition between these regimes occurs over a narrow H pressure interval. In the case of CuPd, on the other hand, the H coverage varies much more gradually with H pressure and and is coupled to a non-monotonic variation of the Cu concentration in the topmost surface layer. The results demonstrate the rich behavior that can result from the coupling of metal-metal and metal-hydrogen interactions at surfaces, even in apparently simple but concentrated systems.

MM 10.6 Mon 17:15 C 130

Unveiling Synergies between Theory and Experiment for an Enhanced Understanding of Solid-State Hydrogen Storage — •Paul Jerabek[1], Thomas Klassen[1,2], and Claudio Pistidda[1] — [1]Abteilung für Materialdesign, Institut für Wasserstofftechnologie, Helmholtz-Zentrum Hereon, 21502 Geesthacht — [2]Helmut-Schmidt-Universität, Holstenhofweg 85, 22043 Hamburg

Metal hydride materials are a cornerstone for the secure and efficient storage of hydrogen in a versatile manner and play a pivotal role in realizing a carbon-emission-free transition energy. This underscores the need for a profound understanding of their material properties like stability against outside influences, (de)hydrogenation thermodynamics and kinetics across various length scales.

This contribution provides an overview of our journey to comprehend the fundamental principles of hydrogen storage within metal hydride materials, employing a combination of experimental and theoretical methods. The focus is on the intricate challenges inherent in this approach.

The collaborative synergy between theoretical frameworks, spanning from the atomistic to the mesoscopic scale, and experimental endeavors at our research center is highlighted. Concrete examples illustrate how DFT contributes to exploring interface properties of different hydrides and enable predictions of material stability against cosmic radiation. Additionally, this talk offers insights into how machine-learning techniques can drive progress toward a better understanding of solid-state hydrogen storage in various application scenarios.

MM 10.7 Mon 17:30 C 130

LaNi5 intermetallic compound for hydrogen storage in space applications; Theoretical investigation of material stability and dynamics — •Archa Santhosh[1], Thomas Klassen[1,2], Paul Jerabek[1], and Claudio Pistidda[1] — [1]Helmholtz-Zentrum Hereon GmbH, Max-Planck Strasse 1, 21502 Geesthacht — [2]Helmut-Schmidt-Universität, Holstenhofweg 85, 22043 Hamburg

LaNi5 intermetallic compound is a well studied hydrogen storage material owing to the good kinetics, high volumetric storage capacity and safety aspects. However, application in a space environment presents unique challenges concerning radiation exposure and subsequent material stability that needs to be understood further. In this work, we employed a combination of density functional theory (DFT) and molecular dynamics (MD) calculations to study the long-term stability of LaNi5 and its hydride phases when exposed to low-energy ionizing radiation. Valuable insights on primary damage events were obtained with MD calculations and the mechanism of defect formations, energetics, and the impact of defects on the electronic structure and stability were studied. The complexity and computational cost of the calculations were reduced by training a machine-learned (ML) interatomic potential and thereby coupling large-scale MD with ab-initio methods. This work further contributes a fundamental understanding of radiation tolerance and the subsequent suitability of LaNi5 alloys for hydrogen storage under the harsh conditions in space.

MM 10.8 Mon 17:45 C 130

Multiscale Modeling Metal-Hydride Interphases: Deconvoluted Chemo-Mechanical Energy for Phase-Field Simulations. — •Ebert Alvares[1], Kai Sellschopp[1], Bo Wang[2], Shinyoung Kang[2], Thomas Klassen[3], Tae Wook Heo[2], Paul Jerabek[1], and Claudio Pistidda[1] — [1]Institute of Hydrogen Technology, Helmholtz-Zentrum hereon GmbH, Max-Planck-Straße 1, D-21502 Geesthacht, Germany — [2]Materials Science Division, Lawrence Livermore National Laboratory, Livermore, California 94550, USA — [3]Helmut Schmidt University, Holstenhofweg 85, 22043 Hamburg, Germany

Understanding the multiscale factors of the interphase boundary properties between metal-hydrides is crucial for simulating the hydrogenation process. It influences the hydride's stability, its rate of precipitation, and its morphology, thereby affecting the kinetics of transformation.

In this study, based on first-principles, thermodynamic models and micromechanical analysis were employed to deconvolute the interconnected chemo-mechanical components of the interphase boundary energy in the FeTi-H system, showing its application within an under-development quantitative-based phase-field model.

This generalizable approach offers valuable insights into the interplay between chemical and elastic contributions to any interstitial hydride formation, holding significant implications for the integration of micromechanics into phase field simulations of FeTi alloy hydrogenation, an ongoing research focus in our group.