

## MM 23: Topical Session: Hydrogen in Materials: from Storage to Embrittlement III

Time: Tuesday 11:45–13:15

Location: C 130

**Topical Talk**

MM 23.1 Tue 11:45 C 130

**Hydrogen trapping evaluation by thermal desorption spectroscopy coupled with advanced microstructural characterization: from BCC to FCC** — LIESE VANDEWALLE, MARGOT PINSON, SIMON VANDER VENNET, LISA CLAEYS, KIM VERBEKEN, and •TOM DEPOVER — Technologiepark 46, 9052 Zwijnaarde, Ghent University, Belgium

The most used technique to evaluate hydrogen trapping is thermal desorption spectroscopy (TDS). However, based on the TDS spectrum itself, one can find a variety of possible hydrogen trapping sites linked to specific microstructural features. Therefore, TDS should always be combined with advanced microstructural characterization to elucidate the hydrogen/metal interactions, where variations in defect density should be coupled with a corresponding increase/decrease in the TDS profile. In this work, the hydrogen trapping ability of a wide range of metals is considered, starting from ultra-low carbon steel (pure ferrite, BCC), over high carbon martensitic steels (BCT), towards the role retained austenite (FCC) can play in advanced high strength Q&P steels, ending with limitations of the technique in a pure austenitic microstructure. This is coupled with the characterization of the microstructure, studied by combined internal friction, positron annihilation spectroscopy, SEM-EBSD, XRD, DSC and TEM.

MM 23.2 Tue 12:15 C 130

**Hydrogen sorption kinetics in nanoporous palladium** — •SEOYUN SOHN<sup>1</sup>, JÜRGEN MARKMANN<sup>1,2</sup>, SHAN SHI<sup>3,1</sup>, and JÖRG WEISSMÜLLER<sup>2,1</sup> — <sup>1</sup>Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany — <sup>2</sup>Institute of Materials Physics and Technology, Hamburg University of Technology, 21073 Hamburg, Germany — <sup>3</sup>Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, 21073 Hamburg, Germany

Palladium is one of the most intensely studied model materials for hydrogen in metals. The fabrication of nanoporous Pd by dealloying results in a macroscopic sample with a nanoscale network structure, which can efficiently absorb hydrogen due to its large specific surface area and short diffusion paths. The material has been reported to undergo more than 1000 loading/unloading cycles through the  $\alpha/\alpha'$  phase transformation without degradation. In this work, the ligament size of nanoporous Pd is tuned from 20 to 500 nm with the aim of understanding the role of the geometry on the charging kinetics and ultimately on the phase transformation mechanism. The hydrogen ad/absorption and desorption kinetics are studied using electrochemical impedance spectroscopy and potential jump tests. The results suggest a controlling role of the interfacial injection process and an extremely small Damköhler number. This outcome will offer guidance to improve charging kinetics for functional performance.

MM 23.3 Tue 12:30 C 130

**Influence of Varying Conditions on Kinetics of Reactive Hydride Composites** — •OU JIN<sup>1,3</sup>, YUANYUAN SHANG<sup>2</sup>, XIAOHUI HUANG<sup>3</sup>, DOROTHÉE VINGA SZABÓ<sup>1,3,4</sup>, THI THU LE<sup>2</sup>, STEFAN WAGNER<sup>1</sup>, CHRISTIAN KÜBEL<sup>3,4,5</sup>, CLAUDIO PISTIDDA<sup>2</sup>, and ASTRID PUNDT<sup>1,3</sup> — <sup>1</sup>Institute for Applied Materials, KIT — <sup>2</sup>Institute of Hydrogen Technology, hereon — <sup>3</sup>Institute of Nanotechnology, KIT — <sup>4</sup>Karlsruhe Nano Micro Facility, KIT — <sup>5</sup>Joint Research Laboratory Nanomaterials, TUD

A sustainable energy future necessitates the incorporation of hydrogen as a critical energy vector. However, its widespread use is restricted by available storage techniques. The LiBH<sub>4</sub>-MgH<sub>2</sub> composite, among the reactive hydride composites, possesses an exceptional storage capacity of about 12 wt% H<sub>2</sub> while using milder operating conditions compared to current commercial solutions. However, the material's practical

application is hindered by sluggish kinetics due to the slow formation of MgB<sub>2</sub> during dehydrogenation. Facilitation of MgB<sub>2</sub> formation was proposed through transition metal-based additives to expedite the LiBH<sub>4</sub>-MgH<sub>2</sub> dehydrogenation. Despite of this, the mechanism underpinning these improvements was not fully explored at the time. This research investigates the effect of variables such as the kind of additive, annealing temperature, and cycling on the MgB<sub>2</sub> formation during the decomposition of LiBH<sub>4</sub>-MgH<sub>2</sub> using various transmission electron microscopy (TEM) techniques. The analysis reveals that the improved kinetics in the material results from the tuned nucleation and growth behavior of MgB<sub>2</sub>, due to different MgB<sub>2</sub> nucleation behaviors.

MM 23.4 Tue 12:45 C 130

**The role of manganese and aluminium on hydrogen trapping and diffusion in Mn/Al rich steel alloys** — BIKRAM KUMAR DAS<sup>1</sup>, •MAURICIO BONILLA<sup>1</sup>, POULAMI CHAKRABORTY<sup>1</sup>, and ELENA AKHMATSKAYA<sup>1,2</sup> — <sup>1</sup>BCAM - Basque Center for Applied Mathematics, Bilbao, Spain — <sup>2</sup>IKERBASQUE, Basque Foundation for Science, Bilbao, Spain

Hydrogen-induced embrittlement (HIE) remains a serious bottleneck for using steel in infrastructure for H<sub>2</sub> storage and transport. Small amounts of Al and Mn have been shown to mitigate HIE, but the proposed mechanisms are often contradictory. To address this problem, we present a systematic approach to model the local environments (LEs) around the H-binding sites in FCC Fe-Mn-Al alloys up to the 3<sup>rd</sup> nearest neighbor (NN) shell. First, the most favorable LEs are determined using Density Functional Theory (DFT). Then, the local impact of Al/Mn content and distribution on the binding and diffusion of H is examined through the nudge elastic band method and crystal orbital Hamilton population analysis. We found that H-binding correlates most strongly with Al content, and is weakly influenced by Mn up to 5 wt%. Moreover, direct H-Al bonding destabilizes H binding, but the presence of Al in the 2<sup>nd</sup> NN shell of the H-binding site leads to a strong stabilizing effect by promoting H-Fe bonding. The presence of Al and Mn in grain boundaries and precipitates is known to play a prominent role in HIE. Here, we show that Al ability to indirectly trap H in bulk austenite could mitigate HIE. The analysis approach in this work could readily be adapted to study similar alloy systems.

MM 23.5 Tue 13:00 C 130

**Unprecedented switchable rigidity in a nanoporous Pd alloy-hydrogen solid solution near critical point** — •SAMBIT BAPARI<sup>1</sup> and JÖRG WEISSMÜLLER<sup>1,2</sup> — <sup>1</sup>Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — <sup>2</sup>Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, Geesthacht, Germany

A remarkable prediction due to Larché and Cahn is deformation at no cost of energy at the critical point for open systems with miscibility gaps. Bulk nanoporous palladium is an ideal system for studying open system elasticity as palladium with randomly oriented nanometer size ligaments affords rapid equilibration of hydrogen between an environment and the materials bulk. In this work, nanoporous Pd-Pt (5 at%) alloy with residual Cu (13 at%) was prepared by electrochemical dealloying to experimentally verify the prediction for a wide solute-concentration range. The average ligament size of the as dealloyed nanoporous alloy is  $\sim 4$  nm, facilitating fast equilibration with the acidic electrolyte present in the open pores under applied potential. Hydrogen solubility isotherms show near critical point behavior in the Pd-Cu-Pt-H solid solution at room temperature. Solute susceptibility and concentration-strain coefficient were determined to estimate the difference in stiffness between open and closed systems. In-situ dynamic mechanical tests show an unprecedented 50% drop in the storage modulus owing to simultaneous mechanical and chemical equilibration near critical point.