

MM 17: Hydrogen in Materials: Hydrogen Storage

Time: Tuesday 14:00–15:15

Location: H46

MM 17.1 Tue 14:00 H46

Open system mechanical behavior of nanoporous palladium-platinum-hydrogen solid solution near critical point —

•SAMBIT BAPARI and JÖRG WEISSMÜLLER — Werkstoffphysik und technologie, Technische Universität Hamburg

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 [1]. In this work, nanoporous palladium-platinum (5 at%) alloy was prepared by electrochemical dealloying. Transmission electron microscopy, oxygen adsorption*desorption methods were used to characterize the morphology and structure of the nanoporous alloy. The average ligament size of the as dealloyed nanoporous palladium-platinum alloy is 4 nm compared to 20 nm for nanoporous palladium. Hydrogen solubility isotherms show near critical point behavior in palladium-platinum-hydrogen solid solution at room temperature. Solute susceptibility and concentration-strain coefficient were determined to estimate the difference in compliance between open and closed systems. In situ quasistatic mechanical tests and strain rate jump tests were conducted to analyze the open system elastic and plastic deformations at near critical point. [1] S Shi, J Markmann, J Weissmüller. Verifying Larché-Cahn elasticity, a milestone of 20th-century thermodynamics, PNAS, 2018,115 (43) 10914-10919

MM 17.2 Tue 14:15 H46

Metal-organic frameworks for hydrogen isotope separation —

•MICHAEL HIRSCHER — Max-Planck-Institut für Intelligent Systeme, Stuttgart, Germany

One of the important operations in chemical industry is separation and purification of gaseous products. Especially H_2/D_2 isotope separation is a difficult task since its size, shape and thermodynamic properties resemble each other. Porous materials offer two different mechanisms for separating hydrogen isotopes, either confinement in small pores, i.e., *kinetic quantum sieving*, or adsorption on strong binding sites, i.e., *chemical affinity quantum sieving*. The new class of metal-organic frameworks (MOFs) allows the exact tailoring of pore size and aperture as well as including open metal sites into the framework. Furthermore, if MOFs consist not of a static, but flexible framework, they can reversibly respond to external stimuli, which may even enhance the separation selectivity.

Experimentally, the measurement of the selectivity for hydrogen isotope separation is very challenging, since it requires low temperatures near the boiling point of the gases. Using low-temperature thermal desorption spectroscopy (TDS), we have developed a method for measuring directly the isotope selectivity after exposure to H_2/D_2 mixtures.

Exemplarily, this talk will present experimental results on hydrogen isotope separation in MOFs.

MM 17.3 Tue 14:30 H46

Microstructural study of MgB_2 in the $LiBH_4$ - MgH_2 composite by TEM —•OU JIN¹, YUANYUAN SHANG², XIAOHUI HUANG¹, XIAOKE MU¹, DOROTHÉE VINGA SZABÓ¹, THI THU LE², STEFAN WAGNER¹, CHRISTIAN KÜBEL³, CLAUDIO PISTIDDA², and ASTRID PUNDT¹ — ¹Karlsruhe Institute of Technology, Karlsruhe, Germany — ²Helmholtz-Zentrum hereon GmbH, Geesthacht, Germany — ³Technical University of Darmstadt, Darmstadt, Germany

The $LiBH_4$ - MgH_2 composite is known as Reactive Hydride Composite for hydrogen storage that has an exceptional hydrogen storage capacity (up to ~ 12 wt% H_2) and enhanced thermodynamic properties (down to ~ 45 kJ/mol H_2). The main challenge that limits the extensive

application of this material is its sluggish kinetic performance, which is primarily ascribed to the hampered nucleation of MgB_2 during decomposition. It was found that transition metal-based additives could facilitate the formation of MgB_2 and accelerate the decomposition of $LiBH_4$ - MgH_2 . However, the additive effect on the kinetic improvement had not been fully understood until now. To unravel the uncertainties, the formation of MgB_2 in the decomposed $LiBH_4$ - MgH_2 with and without the additive $3TiCl_3$ - $AlCl_3$ was studied using manifold transmission electron microscopy techniques. Varied MgB_2 morphologies have been determined, originating from different nucleation centers. Given the heterogeneous nucleation, the crystallographic orientation relationship of the relevant phases is in depth discussed. It turns out that atomic misfit plays a dominant role and directly affects the in-plane strain energy density, leading to varied kinetic performance.

MM 17.4 Tue 14:45 H46

ETEM studies on hydride precipitation and growth in Mg films —MAGNUS HAMM¹, MARIAN DAVID BONGERS¹, VLADIMIR RODATIS¹, STEFAN DIETRICH², KARL-HEINZ LANG², and •ASTRID PUNDT² — ¹Göttingen University, Institute of Materials Physics (IMP), Göttingen, Germany — ²Karlsruhe Institute of Technology (KIT), Institute for Applied Materials - Materials Science and Engineering (IAM-WK), 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_2 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_2) 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_2 created during the transformation. [1] M. Hamm et al., Int. J. Hydr. Energy 44 (2019) 32112.

MM 17.5 Tue 15:00 H46

Recycling as the key for developing sustainable hydrogen storage materials —•CLAUDIO PISTIDDA¹, YUANYUAN SHANG¹, THI THU LE¹, GOKHAN GIZER¹, HUJUN CAO¹, NILS BERGEMANN¹, RIFAN HARDIAN¹, MARTIN DORNHEIM¹, and THOMAS KLASSEN^{1,2} — ¹Department of Materials Design, Institute of Hydrogen Technology, Helmholtz-Zentrum hereon GmbH, 21502, Geesthacht, Germany — ²Helmut Schmidt University, Holstenhofweg 85, 22043, Hamburg, Germany

Metals play a crucial role in supporting the global economy and the wellbeing of humankind. Supported by the constantly increasing demand for metal-based products, the extraction of mineral resources has increased, over the last decades, at a faster rate than economic growth. This trend is forecasted to steadily increase in the near future, thus leading to concerns over the exploitation of the Earth's natural resources and the environmental impact that the extraction of metals will have. In this scenario, finding new ways to recycle metals and metal alloys, even those of low purity, is mandatory.

To reduce the carbon footprint and environmental impact that the mining of metals for hydrogen storage purposes entails and to reduce their cost, at the Helmholtz-Zentrum Hereon we pursue the possibility of obtaining high-quality hydride-based materials from industrial metal waste. A complete overview of recent scientific breakthroughs in the synthesis and characterization of hydrogen storage materials made from recovered metal wastes will be presented.