MM 31: Topical Session: Hydrogen in Materials: from Storage to Embrittlement V

Time: Wednesday 10:15–11:30 Location: C 130

Topical Talk MM 31.1 Wed 10:15 C 130

Compositional effects on the hydrogen sorption in refractory high entropy alloys — •Claudia Zlotea and Nayely Pineda-Romero — ICMPE CNRS Thiais France

High entropy alloys represent a novel alloying strategy that can yield exceptional performance properties needed across a variety of technology applications, including hydrogen storage. Examples include high volumetric capacity materials (BCC alloys forming FCC dihydrides) with improved thermodynamics relative to conventional high-capacity metal hydrides (like MgH2), but still further destabilization is needed to reduce operating temperature and increase materials-level capacity. In this presentation, we will show a strategy to effectively destabilize TiVNb-based hydrides by adding small amounts of Al/Mo/Cr. We specifically evaluate the effect of Al/Mo/Cr addition on the phase structure, microstructure, hydrogen absorption and desorption properties. The experiments demonstrate that increasing Al/Mo/Cr content results in a significant hydride destabilization. The change of the local structure as function of chemical composition and hydrogen concentration will be emphasized by total X-ray scattering at synchrotron and related pair distribution function analysis. Moreover, the phase transition during reaction with hydrogen will be highlighted by in situ neutron and synchrotron X-ray diffraction. Finally, hydrogen absorption/desorption cycling properties will be addressed with an emphasis on the structure/microstructure cycle-life stability. The presentation will conclude about possible strategies for the design of high-entropy hydrides targeted for specific hydrogen use cases.

MM 31.2 Wed 10:45 C 130

Revealing hydrogen-rich phases in NiTi shape memory alloys — •David Holec[1], Anna M. Paulik[1], Adam Weiser[2], Juraj Todt[1], Jitka Holcova[1], Jozef Keckes[1], and Antonin Dlouhy[2] — [1]Department of Materials Science, Montanuniversität Leoben, Franz-Josef-Strasse 18, 8700 Leoben, Austria — [2]Institute of Physics of Materials ASCR, Zizkova 22, 616 62 Brno, Czech Republic

The shape memory alloy NiTi is particularly popular for medical applications and implants due to its excellent biocompatibility and corrosion resistance. Specifically, the interaction with hydrogen is critical due to its natural prevalence in living tissues.

The focus of this work is the characterization of NiTi hydrides using the density functional. Based on experimental observations, structural models have been created for different hydrogen concentrations and distributions. The formation energy has been calculated and compared between the models to find the most stable hydride structure. This is further complemented using Monte Carlo optimization of interstitial H distributions, using DFT-derived ML interatomic potential. The thus obtained compositional dependence of structural parameters is used to rationalize observed variations in the B2 and B19* lattice parameters and associated volumetric changes obtained from the in-situ X-ray synchrotron diffraction measurement during the H uptake experiment.

MM 31.3 Wed 11:00 C 130

Mixed Metal Solid Solutions in Amide-Hydride Systems — •Thi Thu Le[1], Michele Chierotti[2], Stefan Walders[3], Denis Kramer[3], Alexander Schoekel[4], Thomas Klassen[1,3], and Claudio Pistidda[1] — [1]Helmholtz-Zentrum hereon GmbH, Geesthacht, Germany — [2]University of Torino, Torino, Italy — [3]Helmut Schmidt University, Hamburg, Germany — [4]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Metal amide-hydride materials have been extensively studied for use in energy applications. In particular, the solid solution formation in metal-amide hydride system promotes fast hydrogen sorption kinetics and tunes the thermodynamics, which allow hydrogen absorption/desorption below 150 *C in hydrogen storage systems. In addition, these intermediates are potentially ionic conductors for solid-state batteries. In this work, a series of M-N-H solid solution structures based on mixed MNH2-MH materials of Group 1 elements (M = K, Rb, Cs and their combinations) is reported. The results obtained by ex-situ / in-situ XRD, and MAS NMR confirm the formation of mixed solid solution associated with an exchange between both anionic (NH2- and H-) and cationic species (K+, Rb+ and Cs+). Moreover, MD calculations show that the NH2 rotation barrier is lowest in the Cs system, which has the lowest phase transition temperature, indicating a positive correlation of two variables, where a higher anion rotation barrier is associated with a higher phase transition temperature, in agreement with experimetal data. This work provides the basis for further studies on the ionic conductivity of solid electrolytes or dopants.

MM 31.4 Wed 11:15 C 130

Hydrogen storage in porous FeTi nanofoams — •Lukas Schweiger[1], Florian Spieckermann[1], Nikolaos Kostoglou[1], Sebastian Stock[2], Peter Cengeri[3], Michael Zehetbauer[3], Oskar Paris[2], Daniel Kiener[1], and Jürgen Eckert[1,4] — [1]Montanuniversität Leoben, Department Materials Science, Austria — [2]Montanuniversität Leoben, Chair of Physics, Austria — [3]University of Vienna, Faculty of Physics, Austria — [4]Austrian Academy of Sciences, Erich Schmid Institute, Austria

While metal hydrides are promising for hydrogen storage, challenges persist due to slow kinetics, inadequate stability, and unfavorable pressure-temperature conditions. A well-studied material is the intermetallic FeTi, qualifying as a good candidate to overcome these limitations. We intend to achieve this by prototyping a FeTi-based nanoporous metallic foam. Therefore, FeTi and Cu powders were blended, whereby Cu is removed after high-pressure torsion (HPT) processing. Detailed exploration of the FeTi-Cu system, including varying deformation temperature and Cu content, reveals optimal conditions for obtaining a homogeneous nanocrystalline composite. The process retains flexibility, providing tunability through temperature adjustments during HPT or subsequent heat treatments. Removing the Cu transforms the nanocomposite into a metallic nanofoam. Characterization via nitrogen ad-/desorption highlights a specific surface area of 17 m2/g and a well-defined mesoporous structure. Hydrogen absorption measurements reveal rapid and reversible hydrogen uptake, with the nanoporous FeTi maintaining mechanical stability.