

MM 16: Topical session (Symposium MM): Hydrogen in Materials

Hydrogen storage materials

Time: Monday 17:30–19:00

Location: H 0107

Topical Talk MM 16.1 Mon 17:30 H 0107**Development of Hydrogen Storage Materials and Systems** — ●MARTIN DORNHEIM — Helmholtz-Zentrum Geesthacht, Geesthacht, Germany

In recent years a huge number of novel light weight hydrides has been discovered with many of them showing a rather promising prospect for the use in hydrogen storage. Results attained by different characterisation techniques such as in-situ XRD, small angle X-ray scattering, EXAFS and XANES, volumetric Sieverts* type measurements, in-situ neutron radiography etc. on different hydrides and hydride composites will be presented. Insights about reaction mechanisms, sorption behaviour, cycling stability of light weight hydrides and Reactive Hydride Composites, the influence and optimisation of compaction on such materials to pellets and the behaviour of such pellets under in-situ conditions are given. The possibility for scale-up of the synthesis as well as the kinetic and cycle behaviour of larger sample batches considering for example the effect of temperature inhomogeneities on the performance and cycle life time of the storage materials will be discussed. An overview about methods and achieved results on the scale-up of synthesis and testing of different hydrides will be given.

MM 16.2 Mon 18:00 H 0107

Understanding the effect of nanostructured additives on hydride systems by means of electron transmission microscopy

— ●JULIÁN PUSZKIEL^{1,2}, MARÍA VICTORIA CASTRO RIGLOS³, CALUDIO PISTIDDA¹, HUIJUN CAO¹, THI-THU LE¹, ANTONIO SANTORU¹, THOMAS KLASSEN^{1,4}, and MARTIN DORNHEIM¹ — ¹Helmholtz Zentrum Geesthacht (HZG), Department of Nanotechnology, Geesthacht, Germany. — ²Department of Physicochemistry of Materials, Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET) and Centro Atómico Bariloche, S.C. de Bariloche, Argentina — ³Department of Metalphysics, Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET) and Centro Atómico Bariloche, S.C. de Bariloche, Argentina — ⁴Helmut Schmidt University, Hamburg, Germany

One of the main limitations for the implementation of hydrogen as energy carrier is the lack of an efficient and safe hydrogen storage system. Hydrogen storage in solid state through the formation of hydride compounds is a potential alternative to address this problem. In recent years, much effort has been devoted to improve the kinetic behavior of promising Li-Mg-B-H and Li-Mg-B-N-H destabilized hydride systems. In this work, nanosized additives added to 2LiBH₄+MgH₂ and 6Mg(NH₂)₂+9LiH+LiBH₄ are characterized via transmission electron microscopy (TEM). The aim is to understand the role of in situ formed nanostructured additives on the kinetic behavior of the investigated hydride systems. The information gained by TEM is helpful to optimize solid state hydrogen storage system for practical applications.

MM 16.3 Mon 18:15 H 0107

Grain Boundary Diffusion in the Magnesium-Hydrogen system - Harrison regimes C in action — ●MAGNUS HAMM and ASTRID PUNDT — Institute for Material Physics, Georg-August University, Göttingen, Germany

Magnesium acts as storage material for hydrogen in a future hydrogen energy based economy because of its high reversible hydrogen capacity of up to 7.6 wt% [1]. However the slow kinetics its high desorption temperature provide a significant barrier to its commercial use [2]. This kinetic limitation may be improved by the presence of grain

boundaries. Grain boundary (GB) diffusion differs from bulk diffusion in crystals. For interstitial diffusion it can be either slower or faster, depending on the solvent concentration [4][5]. Magnesium seems to offer an ideal model system to study the dominant influence of the GBs in diffusion measurements as discussed in a recent publication [6]. The knowledge gained from finite-element-(FEM) simulations [6] will be used to evaluate diffusion coefficients of hydrogen in magnesium. The diffusion coefficients were measured by gasvolumetry and resistivity measurements. Combining experimental with FEM and analytical models results allows to show how grain boundaries can influence the kinetics in the Mg-H system.

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[1] Dornheim, R. et al., Scr. Mat. 56 (2007) [2] Bogdanović, B. et al., J. Alloys Compd. 282 (1999) [3] [4] T. Muetschele and R. Kirchheim, Scr. Metall. 21, (1987) [5] M. Hamm and A. Pundt, IJHE 42(2017)

MM 16.4 Mon 18:30 H 0107

Development of the atomistic model for study of hydrogen behavior in magnesium — ●DARIA SMIRNOVA^{1,2} and SERGEI STARIKOV^{1,2} — ¹Joint institute for high temperatures, Moscow, Russia — ²ICAMS Ruhr University Bochum, Bochum, Germany

We report a new attempt to simulation of binary Mg-H system. For this purpose, we constructed a new angular-dependent many-body interatomic potential. The potential functions were fitted towards the ab initio data computed for a large set of reference structures representing various phases of magnesium and its hydrides. We performed molecular dynamic simulations illustrating that the structure and properties (i.e. melting temperatures, defects and stacking faults energies, elastic properties) of magnesium are reproduced with a good accuracy. In addition, the potential describes hcp-bcc phase transition occurring in magnesium at high pressures. The interatomic potential is also appropriate for study of magnesium hydrides existing at different pressures: alpha-MgH₂ and gamma-MgH₂. We also estimated characteristics of the hydrogen diffusion in magnesium. The results are proven to correlate with the existing experimental and theoretical data. We assume that the created interatomic potential can be applied for predictions dealing with hydrogen diffusivity and magnesium and magnesium hydrides. Also, it can provide an insight in mechanisms of phase transitions and characteristics of dislocations in magnesium.

MM 16.5 Mon 18:45 H 0107

Hydrogenation, dehydrogenation of α -tetragonal boron and its transition to δ -orthorhombic boron — NAOKI UEMURA¹, KOUN SHIRAI¹, ●JENS KUNSTMANN², EVGENY A. EKIMOV³, and YULIYA B. LEBED⁴ — ¹Osaka University, Japan — ²TU Dresden, Germany — ³HPPI RAS, Troitsk, Russia — ⁴NR RAS, Troitsk, Russia

α -tetragonal boron (α -T) was recently added to the list of known boron allotropes. Experiments show that upon annealing of hydrogenated α -T boron (B_nH_m) the H release occurs non-continuous, in two steps, where the second one is associated with a structural change from α -T to δ -orthorhombic boron (δ -O) and full H release [1]. Our free energy calculations based on density functional theory reproduce the experimental trends well, explain the origin of the two-step transition, and show that the difference between α -T and δ -O boron lies in the ordering of interstitial boron atoms occupying 4c sites of the crystal structure. The latter implies an order-disorder transition. [1] Ekimov et al., J. Mater. Res. 31, 2773 (2016).