MM 39: SYM Hydrogen in Materials: New Developments III

Time: Thursday 14:00–16:00 Location: H 1058

Invited Talk MM 39.1 Thu 14:00 H 1058

Hydrogen Chemisorption to Clusters — •Gerd Gantefoer — Department of Physics, University of Konstanz, Germany

The properties of nanoclusters consisting of up to 100 atoms are different from the ones of the corresponding bulk materials. Their geometric and electronic structures change with each additional atom. As a consequence chemical properties also vary dramatically with size. The interaction of such nanoparticles with hydrogen exhibits a broad variety of new and unexpected effects. E.g., single hydrogen atoms behave like gold atoms if attached to a small Au cluster. The interaction of small Al clusters with atomic hydrogen results in the formation of a new, previously unknown family of Aluminum hydrides. These examples demonstrate, that chemistry of nanoclusters is different and provides a new approach to the problem of hydrogen storage.

Invited Talk MM 39.2 Thu 14:30 H 1058

Hydrogen Storage in Light Weight Metal Hydrides: Mg-based Reactive Hydride Composites — •M. Dornheim, U. Bösenberg, C. Pistidda, G. Barkhordarian, J. Bellosta v. Colbe, and R. Bormann — GKSS-Research Centre Geesthacht, Institute of Materials Research, Max-Planck-Str. 1, 21502 Geesthacht, Germany

Compared to conventional room temperature hydrides light weight metal hydrides have much higher gravimetric hydrogen storage densities. However, kinetic and/or thermodynamic restrictions limit the potential use of such high capacity hydrides. There is still a large number of hydrides with high storage capacities which have to be considered as irreversible or at least require high pressures and/or very high temperatures for reversible hydrogenation / dehydrogenation as well as very long absorption and desorption times. Prominent examples are borohydrides like $LiBH_4$. Another crucial parameter is the reaction enthalpy. Most of the past attempts to alter and tailor the hydrogen reaction enthalpy of light weight metal hydrides like Mg either failed or led to dramatically reduced gravimetric hydrogen storage capacities. An exciting and promising novel approach is the concept of the Reactive Hydride Composites (RHC). RHC consisting of MgH_2 and borohydrides show significantly reduced total reaction enthalpies as well as improved ab- and desorption kinetics compared to the pure borohydrides while a high hydrogen storage capacity is maintained [1]. In this talk, an overview on the sorption behaviour of the doped nanocrystalline RHCs $2LiBH_4+MgH_2$, $2NaBH_4+MgH_2$ and $Ca(BH_4)_2+MgH_2$ will be given.

[1] Scripta Materialia 56 (2007) 841-846.

MM 39.3 Thu 15:00 H 1058

Direct synthesis of $LiBH_4$ monitored by in-situ neutron diffraction — •Arndt Remhof[1], Oliver Friedrichs[1], Florian Buchter[1], Andreas Züttel[1], and Dirk Wallacher[2] — [1]EMPA, Swiss Federal Laboratories for Materials Resaerch, Dübendorf, Switzerland — [2]Hahn Meitner Institut, Berlin Neutron Scattering Facility, Berlin, Germany

Due to its large hydrogen content, $LiBH_4$ is a promising candidate for a hydrogen storage material. Recently, we discovered a way to synthesize LiBH4 directly from the respective elements, by exposing Li and B to hydrogen gas at high temperatures 700°C and at high pressures (150 bar) [1]. The synthesis can be facilitated by using intermetallic Li-B compounds as starting material. We have shown by in-situ neutron powder diffraction that starting from an intermetallic Li-B compound $LiBD_4$ can be synthesized at 180bar at a temperature of 350°C, which is about 350°C lower than the temperature required for the direct synthesis [1,2]. The experiment was carried out at the powder diffraction instrument E6 of the Hahn Meitner Institut. Support by A. Hoser and N. Stüsser is gratefully acknowledged. Financial support from the 6^{th} Framework Program of the European Commission (NESSHY Contract No.: 518271) and the Swiss Federal Office of Energy is acknowledged.

[1] O. Friedrichs et al., Acta Materialia, in press
[2] D. Goerrig, Deutsches Patent; Auslegungsschrift (1960)

MM 39.4 Thu 15:20 H 1058

Refinement of the phonon analysis in the complex hydride systems $LiBH_4$ and $LiBD_4$ — •Ana Maria Racu[1], Joachim Schoenes[1], Zbigniev Lodziana[2], Andreas Borgschulte[2], and Andreas Züttel[2] — [1]Institut für Physik der Kondensierten Materie, Technische Universität Braunschweig, Germany — [2]EMPA Materials Sciences and Technology, Div. Hydrogen and Energy, Dübendorf, Switzerland

In the present study we have performed low temperature micro Raman measurements on small $LiBH_4$ and $LiBD_4$ crystals. At the lowest temperature, the spectra compare very well with the calculated phonons for the orthorombic structure. The spectra are dominated by three separated bands: the external modes, the internal bending and the internal stretching vibrations. Internal refers to vibrations within the BH_4^- tetrahedra while external modes imply motions of Li^+ and BH_4^-. The temperature dependence of the observed phonons corroborates the strong anharmonicity of the system. Due to the anharmonicity, Fermi resonances occur between the first order stretching modes and the second order bending modes of $LiBH_4$. Moreover, the linewidths have an Arrhenius-like component, with an activation energy of 40 meV. This value corresponds to the energy of the librational mode determined by inelastic neutron scattering [1] and is strongly related to the reorientation motions of the BH_4^- tetrahedra.

[1] J. Tomkinson, T. C. Waddington, J. Chem. Soc. Faraday Trans 2 **72**, 528 (1976).

MM 39.5 Thu 15:40 H 1058

Hydrogen release of $Mg(BH_4)_2$ under helium and hydrogen backpressure — •Wiebke Lohstroh, Nobuko Hanada, Christoph Frommen, and Maximilian Fichtner — Institut für Nanotechnologie, Forschungszentrum Karlsruhe GmbH, Postfach 3640, 76021 Karlsruhe

$Mg(BH_4)_2$ is one of the potential materials to be used in solid state hydrogen storage systems due to its high capacity of 14.9 wt% H_2 and a favourable reaction enthalpy. However, experimentally, hydrogen is only released at temperatures above 300 °C. Depending on the surrounding gas atmosphere (helium or hydrogen) and the applied backpressure several decomposition steps are observed. We will present thermal analysis and structural investigations at various stages of the decomposition and the hydrogen release mechanism will be discussed.