BOR4STORE: Fast, Reliable and Cost effective Boron Hydride based high capacity Solid state Hydrogen Storage Materials

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General

- **Project funded by the European "Fuel Cells and Hydrogen Joint Undertaking"**

→Total Budget 4.07 Mio.€, total funding 2.3 Mio. €.
→Runtime April 2012 to March 2015
→3 Industry partners, 6 Research Institutes

→ Integrated approach for development and testing of novel, optimised and cost-efficient boron hydride based hydrogen storage materials with superior performance (materials capacity more than 8 wt.% and 80 kg H_2/m^3) for specific fuel cell applications.

Approach

BOR4STORE aspires to tackle the S&T challenges that still hinder the practical use of the extremely attractive boron hydrides. The technical objectives of the project reflect an innovative and carefully designed strategy involving

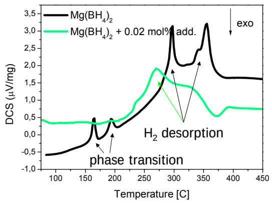
(a) new methods for the synthesis and modification of stable and unstable boron hydrides, as well as their combinations resulting in Reactive Hydride Composites and eutectic mixtures,
(b) systematic and rationalised investigation of the effect of special catalysts and additives, and
(c) adaptation of scaffolding concepts.

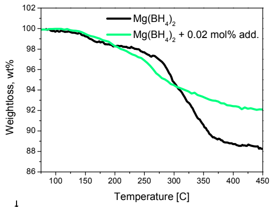
Examples of current work

γ-$Mg(BH_4)_2$: study of additives

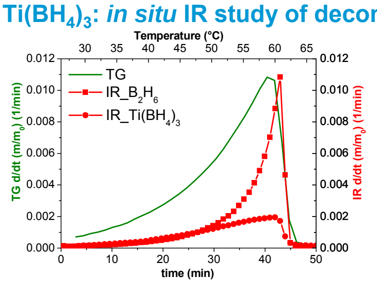
NbF_5 additive
→H_2 release temperature decreased by ca. 30°C
→Different desorption scheme
  →No phase transition below 200°C
  →Just one broad desorption peak
→rather high gravimetric H_2 content of 8 wt.%

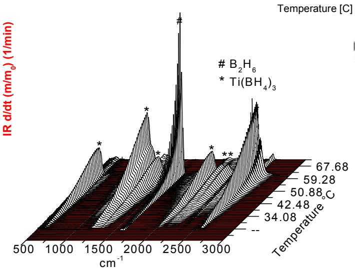
More:
→ TuOC01 Invited (F4): B.C. Hauback: Synthesis, Crystal Structure and Properties of Novel Borohydrides





$Ti(BH_4)_3$: *in situ* IR study of decomposition

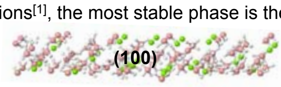




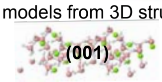
$Ti(BH_4)_3$ decomposes by release of B_2H_6
E. Callini, et al., manuscript in preparation
More:
→ ThOC02 F1: A. Borgschulte: From Mobile Bulk Species to Hydrogen Release in Borohydrides

$Mg(BH_4)_2$: *ab initio* calculations

First results on the study of phase stability
→ Comparison among six different phases: experimental (α, γ and δ) and theoretically predicted ones
→ In agreement with experiment and previous calculations[1], the most stable phase is the α-phase (correct order of stability: α > γ > δ)
Next steps:
→ Surface stability of different faces of the α-phase
→ Role of the additives (e.g. TM):
  → in the bulk (supercells with point defects)
  → at the surface (slab models with point defects)



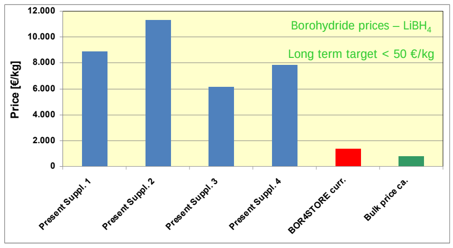
Slab models from 3D structure



More
→ TuOB07 M2: M. Baricco: Theoretical And Experimental Study On Mg(BH4)2-Zn(BH4)2 Mixed Borohydrides

[1] A. Bil, B. Kolb, R. Atkinson, D. G. Pettifor, T. Thonhauser and A. N. Kolmogorov, Phys. Rev., B 83, 224103 (2011)

Decrease of materials cost ⇒ Economics

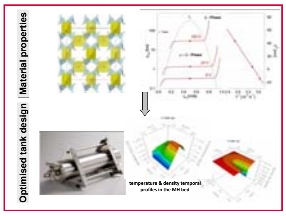


c.f. J. Jepsen et. al: Economic potential of complex hydrides compared to conventional hydrogen storage systems, Int. J. Hydrogen Energy. Vol. 37 (2012) 5, 4204 - 4214. (DOI: 10.1016/j.ijhydene.2011.11.141)

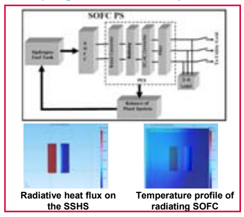
Simulation of combined SOFC – solid state hydrogen storage (SSHS) system

including thermo-chemical model of the storage material

Simulation of stand-alone SSHS system



Coupling of SOFC- SSHS systems



dynamic process simulation and optimization software: COMSOL, gPROMS

Prototype construction and testing

1st generation prototype tank
$LiBH_4 – MgH_2$ Reactive Hydride Composite
→ Ca. 250 g of storage material ⇒ ca. 22g / 250Nl H_2
→ External heating by heating jacket (front) or oil bath (back) possible
→ Operation at ca. 350°C with heating jacket
→ Loading time app. 1 h at 50 bar of hydrogen
→ 2nd generation tank constructed and under testing (500 g storage material)

More:
→ MoOA02 Invited (A1): M. Dornheim: Hydrogen Storage based on Complex Hydrides and Reactive Hydride Composites
→ MoP-59 M1 O. Metz: In-Situ Neutron radiography of Hydrogen Storage Test Tank based on $NaAlH_4$
→ TuP-59 M2 J. Jepsen: Scaled up LiBH4 / MgH2 Composite Storage System as new Promising Hydrogen Storage

Main anticipated progress

Novel solid state hydrogen storage prototype system based on boron hydrides
→ System capacity > 40 kg H_2/m^3 , > 4 wt.% with priority on volumetric cap.
⇒ > 80 kg H_2/m^3, > 8 wt.% on materials level
→ Materials reaction enthalpies and kinetics of hydrogen loading and discharge suitable for typical load cycles of SOFC in net independent power supply
→ Cycling stability >98% of retained capacity over at least 500 loading-unloading cycles

Cost effective production route of the hydrogen storage material
→ Use of low purity raw materials, if possible
→ Cost effective materials processing by combination of wet chemical and high energy milling routes
→ Demonstration of potential for scale-up of production and system cost of 500 €/kg of stored H_2

Laboratory prototype of SOFC integrated with hydrogen storage system
→ Model for a continuous power supply for specific applications like net independent telephone or weather stations, backup power for lighting and control, CHP, potentially being also a model for APU's for trains or ships and other "quasi portable" applications.
→ Power in the range 0.1 – 1 kW ⇒ tank system ca. 100 - 1000 Nl
Compared to compressed gas storage and other fuel cell technologies, respectively
→Improved storage capacity
→Improved overall energy efficiency
→Decreased total cost of ownership
→ Indicator of allowable hydrogen purity for stable storage properties
Demonstration of
Techno-economical readiness of solid state hydrogen storage technology

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