Schweizerische Eidgenossenschaft
Confédération suisse
Confederazione Svizzera
Confederaziun svizra

Eidgenössisches Departement für
Umwelt, Verkehr, Energie und Kommunikation UVEK

Bundesamt für Energie BFE

RELEVANT PHYSICAL ASPECTS OF HYDRIDES FOR SYSTEM INTEGRATION AND SAFETY (SAFSYST)

Jahresbericht 2007

Autor und Koautoren	Andreas Züttel, Michael Bielmann
beauftragte Institution	EMPA Dübendorf, Abt. 138 Hydrogen & Energy
Adresse	Überlandstrasse 129, CH-8600 Dübendorf
Telefon, E-mail, Internetadresse	+41 44 823 4038, andreas.zuettel@empa.ch, www.empa.ch/h2e
BFE Projekt-/Vertrag-Nummer	Projekt Nr.: 102316, Verfügung Nr.: 152922
BFE-Projektleiter	Andreas Züttel
Dauer des Projekts (von – bis)	01.08.2007 – 31.07.2010
Datum	20.12.2007

ABSTRACT

Hydrogen as a potential energy carrier poses new opportunities and challenges towards safety. Solid hydrogen storage (metal- of complex hydrides) offers high volumetric and gravimetric hydrogen densities and therefore a very high energy density. This requires profound knowledge of the material properties. Complex hydrides are highly reactive materials and can be potentially hazardous. Assessment of surface reactivity with impurities and air, passivation mechanisms and decomposition by-products are issues currently not addressed. We will investigate these issues by means of ESCA (Electron Spectroscopy for Chemical Analysis) along with MS (Massspectroscopy) as a function of temperature. Temperature and therefore heat management are the essential parameters in solid hydrogen sorption and can be seen as inherent safety to uncontrolled release. Desorption and adsorption are endo-/exothermal processes and therefore thermal management is a key issue. Thermal conductivity, from phononic contributions over inter-grain conductivity has to be understood to implement these materials in a system in the future. Especially, on complex hydrides these questions are not yet understood. In this project, we will assess the thermal conductivity of solid hydrogen storage materials in a “bottom-up” approach. We plan to contribute to IEA Task 18 (Demonstrations) and IEA Task 19 (Safety). Furthermore, a close collaboration with SwissRe in order to elaborate a safety report as a basis for the definition of safety standards (Activities of Task 19) is planed.

Projektziele

The project is divided in four work packages:

Work Package 1:

Investigation of the surface reactivity of complex hydrides with oxygen, water and hydrogen impurities by means of X-ray photoelectron spectroscopy and mass spectroscopy.

Work Package 2:

Investigation of the thermal desorption products and description of the desorption mechanism on an atomistic level.

Work Package 3:

Thermal transport in complex hydrides, i.e. in the lattice, in grain boundaries and between particles, and in the hydrogen gas phase.

Work Package 4:

Dissemination of the results in IEA task 19 (Safety) and IEA task 18 (Demonstration). Collaboration with industry (e.g. SwissRe). Search for funding of the second part of the project

Durchgeführte Arbeiten und erreichte Ergebnisse

The main tasks during Q3/Q4 of 2007 where the finalizing of required setups and installations at EMPA necessary for the fullfillment of our workplans.

Experimental Setups:

In the second half of 2007 the ESCA Surface Analytical System was installed and completely updated at the new facilities of Hydrogen and Energy. The elaboration, modification and installation were completed in December. Currently, the system is going into the testing and commissioning is underway and first results are expected for Q1/2008. As this system is unique and a key point of the work described in WP1 and WP2, it has been the main focus of activities.

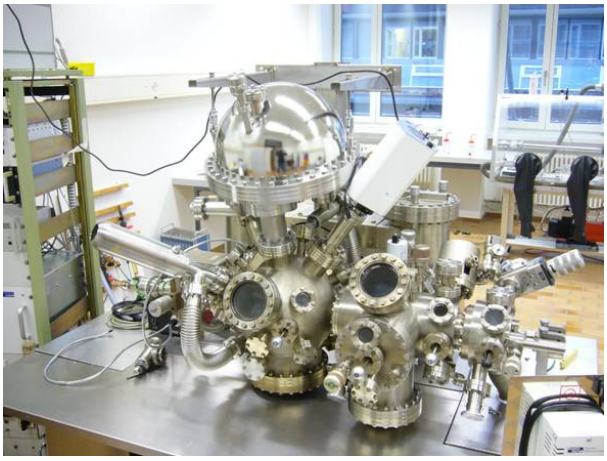

Fig. 1 : ESCA setup at EMPA for the analysis of surface reactivity and dersorption byproducts of the SafeSYST project

The finalization of the system was delayed due to delivery problems with the baking-out system which had to be acquired. Unfortunately, only few companies worldwide provide such systems and it was not possible to change to an alternative source. The system is now in delivered and in place.

The thermal desorption spectroscopy (TDS) setup which is used complementary to the ESCA Surface Analytical System has been also completed and has undergone testing and commissioning. Measurements can start in Q1/2008 and results thereof are expected in the same timeframe. These two setups are the cornerstones of WP1 and WP2 and starting of experiments are therefore imminent.

Pure Samples :

During the year 2007 a break through in the synthesis of complex hydrides was achieved in our group Hydrogen and Energy. $LiBH_4$ was directly synthesized from the elements. This not only proves that borohydrides can be produced by no-wet chemical processes; it is also a very important break through for analytical studies. Solvent where always a major nuisance in the analysis process. Their nature and amount was unknown and the production process is not disclosed from the producers, rendering analysis incredibly difficult, adding unknown parameters to the system. The proof of principle is now made that production is possible in the absence of solvents. This opens up the possibility of using pure samples for analysis, greatly simplifying the evaluation of the data. Also, it opens up the possibility to produce deuterated samples ourselves, which are almost impossible to acquire on the market. These two factors will greatly aid the task of solving the nature of desorbed species from borohydrides by massspectrometry, which so far is unresolved and is a central question of WP1 and WP2.

Papers:

"Hydrogen dissociation on oxide covered MgH_2 by catalytically active vacancies", A. Borgschulte, M. Bielmann, A. Züttel, G. Barkhordarian, M.Dornheim, R. Bormann, Applied Surface Science, in press

"Direct Synthesis of $Li[BH_4]$ and $Li[BD_4]$ from the elements", O. Friedrichs, F. Buchter, A. Borgschulte, A. Remhof, Ch. Zwicky, Ph. Mauron, M. Bielmann, A. Züttel, Acta Materialia, accepted for publication

Präsentationen:

"Desorption Byproducts from $LiBH_4$ under UHV Conditions", 3.08.2007, 2nd ESSHS, Univeristy of Ulster, Belfast, Northern Ireland

Nationale Zusammenarbeit

- Flurin Trepp, SwissRe (Safety)
- Michael Höckl, BFH-TI (Systems)

Internationale Zusammenarbeit

IEA Task 19 (Safety) Expert Meeting, International Conference on Hydrogen Safety (ICHS), 8.9.-14.9.2007, San Sebastian, Spain

Bewertung 2007 und Ausblick 2008

The year 2007 can, in short, be described as „get ready for action". Central experimental setups and aspects have been finalized and are ready for commissioning and experiments thereafter. The experimental facilities build the corner stones for the scientific work to follow and in 2008 the scientific experimental part can proceed as planed.