Location: H 1058

## MM 40: SYM Hydrogen in Materials: New Developments IV

Time: Thursday 16:30-18:00

Invited Talk	MM 40.1	Thu	16:30	$H \ 1058$
Complex Metal Hydrides —	• MICHAEL	Felder	HOFF	— Max-
Plack-Institut für Kohlenforschung	g, Kaiser V	Wilhelm	Platz	1, 45470
Mülheim / Ruhr				

One important feature for a commercial success of PEM fuel cell for mobile applications is the improvement of the hydrogen storage system. Since the physical storage methods are limited, solid state hydrogen storage are in the focus of research activities. The classical metal hydrides have storage capacities not higher than 2 wt.%. Compared to these materials the storage capacities of the complex metal hydrides are much higher. Sodium aluminium hydride (NaAlH4) is one of the most interesting material, because it is fully reversible, the thermodynamic properties and the storage capacities are close to the technical requirements for on-board hydrogen storage. The recent work for optimization of the complex metal hydrides and to understand the molecular processes during the de- and rehydrogenation reactions will be summarized.

## MM 40.2 Thu 17:00 H 1058

XRD, XPS and Raman analysis of metal and complex hydrides — •ISABEL LLAMAS JANSA<sup>1</sup>, CARINE RONGEAT<sup>1</sup>, STEFFEN OSWALD<sup>2</sup>, ANGELIKA TERESIAK<sup>2</sup>, MARTIN KALBÁC<sup>3</sup>, and OLIVER GUTFLEISCH<sup>1</sup> — <sup>1</sup>IFW Dresden, Institute for Metallic Materials, P.O. Box 270016, D-01171 Dresden, Germany — <sup>2</sup>IFW Dresden, Institute for Complex Materials, P.O. Box 270016, D-01171 Dresden, Germany — <sup>3</sup>IFW Dresden, Institute for Solid State Research, P.O. Box 270016, D-01171 Dresden, Germany

X-ray diffraction (XRD), photoelectron spectroscopy (XPS), and Raman spectroscopy, preferentially as in-situ techniques, are valuable tools for the characterisation of the chemical state and structure of doped metal- and complex-hydrides and their intermediate products upon absorption and desorption. Examples for ex- and in-situ characterisation of the evolution with temperature and pressure of doped-NaAlH<sub>4</sub> [1] and reactive hydride composites [2] (e.g. LiBH<sub>4</sub> + MgCl<sub>2</sub>) are discussed. XPS surface analyses indicated the complete decomposition of the catalyst in the case of TiCl<sub>3</sub> doped NaAlH<sub>4</sub> samples, whereas samples doped with ScCl<sub>3</sub> and CeCl<sub>3</sub> still showed traces of the chloride phases. Raman results demonstrated the formation of the Mg(BH<sub>4</sub>)<sub>2</sub> phase after high-pressure ball milling (HP-BM) of a LiBH<sub>4</sub> + MgCl<sub>2</sub> mixture for 12 h. Finally, in-situ XRD was used to monitor the transition from tetrahydride (NaAlH<sub>4</sub>) into the hexahydride (Na<sub>3</sub>AlH<sub>6</sub>) phase during desorption of sodium alanate.

[1] C. Rongeat, I. Llamas-Jansa, and O. Gutfleisch, in preparation

(2007)

[2] U. Boesenberg et al., Acta Materialia 55, 3951 (2007)

MM 40.3 Thu 17:20 H 1058

**Seeing Hydrogen** — •ANDREAS BORGSCHULTE — EMPA Materials Science and Technology, Hydrogen & Energy, Überlandstrasse 129, CH-8600 Switzerland

The fact that hydrogen absorption in metals leads to large optical changes is the basis of a new combinatorial method called hydrogenography. We show that hydrogenography provides a high-throughput method to measure quantitatively the key thermodynamic properties (equilibrium properties like heat of absorption and kinetics) of hydride formation. The optical setup involves a good accessibility of the sample, which enables us the measurement of the impact of electric fields on the hydrogen absorption process. We demonstrate that an electric current and the thereby induced heat and electromigration of H<sup>-</sup> ions can start and control the absorption of hydrogen in Mg thin films. We describe how the optical technique on thin films can be transferred to measure hydrogen dynamics in bulk materials by means of Raman spectroscopy.

## MM 40.4 Thu 17:40 H 1058

Opto-mechanical high-throughput characterization of composition spread thin films for the development of new hydrogen storage materials — •ALFRED LUDWIG<sup>1,2</sup>, JIALIN CAO<sup>2</sup>, ALAN SAVAN<sup>2</sup>, MICHAEL EHMANN<sup>2</sup>, and HANS-WERNER BECKER<sup>3</sup> — <sup>1</sup>Institut für Werkstoffe, Ruhr-Universität Bochum — <sup>2</sup>Combinatorial Materials Science, caesar, Bonn — <sup>3</sup>Institut für Physik mit Ionenstrahlen, DTL Labor, Ruhr-Universität Bochum

An opto-mechanical high-throughput characterization method was used for the investigation of hydrogen storage materials within the system Mg-B-Ti-Pd. The materials were deposited by magnetron sputtering in form of thin film composition spreads on micromachined Si cantilever arrays. The thin films were characterized by EDX and XRD prior and after hydrogen loading. In a special pressure vessel, the mechanical stress-changes of the coated cantilevers as a function of hydrogen pressure (0.1 to 5.1 MPa) and temperature (20 to  $450^{\circ}$ C) was measured in parallel using the optical technique. These stress-changes are related to the hydrogen uptake/release of the different materials. The most promising thin films which showed hydrogen storage were further analyzed by RBS and NRA. The latter was used to determine the hydrogen content of the thin films and its depth distribution.