Combined in-situ XRD and Raman investigations on the desorption reaction of Li-based Reactive Hydride Composites

U. Bösenberg[a], D.Ravensbæk[b], I. Llamas Jansa[c], C. Bonatto Minella[a], C. Pistidda[a], O. Safonova[d], W. van Beek[d], O. Gutfeisch[c], T.R. Jensen[b], M. Dornheim[a], R. Bormann[a]

[a]Institute of Materials Research, GKSS Research Centre Geesthacht, Max-Planck-Str. 1, D-21502 Geesthacht, Germany
[b]Interdisciplinary Nanoscience Center (iNano) and Department of Chemistry, University of Århus, DK-8000, Denmark
[c]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany
[d]Swiss-Norwegian Beam Lines at ESRF, Boite Postale 220, F-38043 Grenoble, France

Hydrogen is one of the favoured future energy carriers due to its high energy content. However, reliable and safe storage is a critical issue for mobile applications. The chemical storage in metal hydrides has to fulfil high requirements on weight capacity, thermodynamic and kinetic properties to be applicable e.g. with a fuel cell in a car. At present, none of the single light metal hydrides fulfil all the requirements at once. By the development of the reactive hydride composites this drawback was overcome. They show a reduced reaction enthalpy at high gravimetric capacities due to an exothermic reaction during the endothermic desorption. In the present work, the focus is laid on the system 2 $LiBH_4$ + MgH_2 $\leftrightarrow$2 LiH + MgB_2 + $4H_2$. So far, the desorption kinetics of the reaction are poor and take place in reasonable times only at elevated temperatures of approximately 400°C in a two step mechanism. To facilitate the formation of MgB_2 a hydrogen back pressure of 5 bar is applied. This is in contrast to the calculated equilibrium temperature at 1 bar H_2 of 170°C for these composites. To specifically improve the desorption reactions it is wise to identify intermediate and rate limiting steps. To reveal these, in-situ studies offer the best opportunities. By in-situ XRD a large range of the reaction can be covered and the initial and final products be identified. $LiBH_4$ has a low melting point of 270°C and therefore the tracking of the desorption reaction at the high temperatures e.g. 400°C by XRD is not possible. Also possible amorphous intermediates as they have been observed for pure $LiBH_4$ by Orimo et al. or Bowman et al. cannot be detected. However, the BH^-_4 -tetrahedron and other Boron-compounds have defined stretching and bending modes and therefore they should show Raman scattering also at these elevated temperatures. For that reason, we combined in-situ XRD and Raman scattering at BM01B at the ESRF to follow the decomposition reaction of $LiBH_4$/MgH_2-composites in detail.