Reaction Mechanism and Kinetics of Reactive Hydride Composites

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Compared to conventional room temperature hydrides, light weight metal hydrides have much higher gravimetric hydrogen storage densities. However, kinetic and thermodynamic restrictions limit the potential use of such high capacity hydrides. Due to the use of high energy ball milling techniques for sample preparation as well as the addition of suitable catalysts or dopants, the sorption kinetics of high capacity hydrides could be improved significantly. Hydrogen absorption and desorption now is possible in metal oxide catalyzed MgH_2 within 2 min [1]. For catalyzed $NaAlH_4$, hydrogenation takes place within 10 min [2]. However there are still a lot of hydrides with high storage capacities which have to be considered as irreversible or at least require high pressures and 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 for the use of light weight metal hydrides as hydrogen absorbing alloys for hydrogen storage applications is their 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. This demonstrates the demand for novel approaches to enhance the kinetics and alter the reaction enthalpies of lightweight hydrides. One very exciting, successful and promising novel approach is the concept of the Reactive Hydride Composites (RHC) [3]. Such systems show reduced total reaction enthalpies as well as significantly improved ab- and desorption kinetics compared to the pure hydrides while a high hydrogen storage capacity is maintained. Furthermore, in RHC reversibility is demonstrated for hydrides, which have to be considered as irreversible using moderate hydrogen pressures and temperatures.

In this talk, we present recent detailed results on the sorption behaviour of doped nanocrystalline Reactive Hydride Composites $2LiBH_4+MgH_2$, $2NaBH_4+MgH_2$ and $Ca(BH_4)_2+MgH_2$.

[1] M. Dornheim et al., Advanced Engineering Materials 8 (2006) 377.
[2] N. Eigen et al., Scripta Materialia 56(2007) 847.
[3] G. Barkhordarian et al., Journal of Alloys and Compounds 440 (2007) L18.