STORHY FINAL EVENT
HYDROGEN STORAGE SYSTEMS FOR AUTOMOTIVE APPLICATION
PSA POISSY, JUNE 3-4, 2008

Development of Solid State Materials for Hydrogen Storage

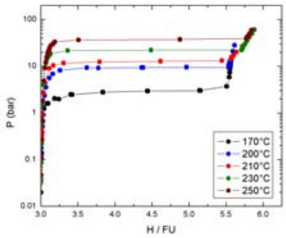
Objectives

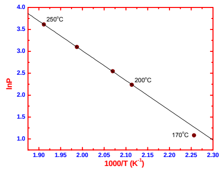
- Investigations on some of the light weight complex alanates and alanes as candidate materials for solid hydrogen storage with the aim to contribute to their state-of-the-art, improving their hydrogen storage density as well as hydrogenation / dehydrogenation kinetic performances.

Achievements

$2NaAlH_4+LiH+2mol\%TiF_3$:

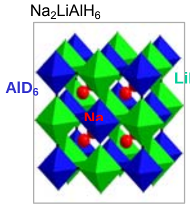
- revealed a maximum storage capacity 2.8 wt.% H_2
- leads to formation of reversible Na_2LiAlH_6
- exhibits a dissociation enthalpy of 56.4 kJ/molH_2 (calculated from pressure composition isotherms -PCI- at 3-40 bar and 170-250 ºC)
- can be rehydrogenated in 1-2 h at 200 ºC





TiF$_3$ in Na$_2$LiAlH$_6$ PCI (left) and van't Hoff plot (above)

Na$_2$LiAlH$_6$

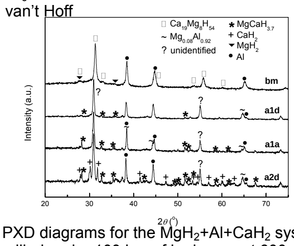


Screening experiments for synthesis and characterization for new mixed alanates:

Systems studied are mixtures of:
Mg-Al-Li-H, Mg-Al-Ca-H, Mg-Al-Na-H, Mg-Al-K-H, Ca-Al-Li-H, Ca-Al-Na-H, Ca-Al-K-H.

- Milling parameters, in particular milling speed and milling time, were found to have great importance for the formation of any new phase obtained by reactive milling (milling under hydrogen atmosphere up to 160 bar)
- Peaks of new compounds were found in several mixtures, although not reversible.

One of the in-house built high-pressure milling vials

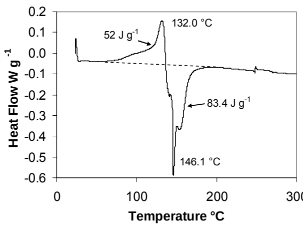


PXD diagrams for the MgH$_2$+Al+CaH$_2$ system ball milled under 100 bar of hydrogen at 600 rpm at different stages of the reaction: ball milled (bm); after the first desorption (a1d); after the first absorption (a1a) and after the second desorption (a2d).

Alane (AlH_3):

Contains 10.1 wt.% H_2, theoretical H density of 148 g/L

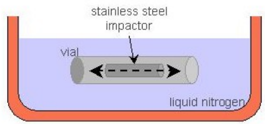
- Simplified method to synthesize AlH$_3$ by milling at liquid nitrogen temperature, compared to wet chemistry.
- Improved comprehension of the desorption behaviour and stability of alanes.
- The experimental results show that □´-AlD$_3$ decomposes (80 ºC) before □-AlD$_3$ (95-100 ºC) and that both directly decompose to Al. At temperatures above 100 ºC, a transformation of □´-AlD$_3$ to □-AlD$_3$ is observed.
- A first-order type, reconstructive transformation at an interface between the two phases was demonstrated to be feasible by molecular dynamics.
- Possibility to modify the composition of alane through the variation of the starting materials and the addition of several compounds (e.g. FeF$_3$, MgD$_2$).



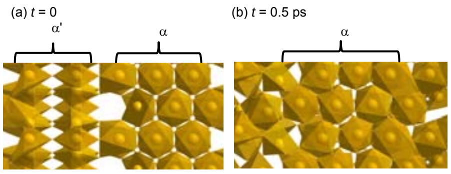
Differential scanning calorimetry plot for the cryomilled sample in the temperature range of 25-300 ºC ramped at a rate of 5 ºC min^{-1}.

Cryomilling 3LiAlH$_3$+AlCl$_3$

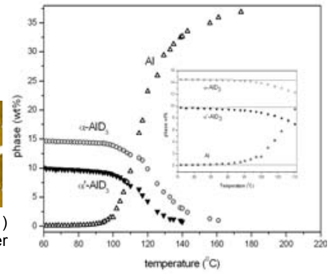
- milling atmosphere: Ar
- ball-to-powder ratio: 30:1
- milling time: 1 hour
- impact frequency: 20 Hz



Phase fractions from the Rietveld refinements of the *in situ* SR-PXD patterns of the sample during the thermal decomposition.



Model interface between α-AlH$_3$ (1-10) and α´-AlH$_3$ (001) sections. The input model (a) is compared to the model after 500 fs molecular dynamics simulation (b).



Future Perspectives

- The results of this work have increased our understanding of reaction mechanisms of complex alanates, which pave the way for further development of solid materials for hydrogen storage. The experience gained can be applied to other promising complex hydride materials.

Partners

- Institute for Energy Technology IFE (NO)
- Forschungszentrum Geesthacht GKSS (DE)
- Forschungszentrum Karlsruhe FZK (DE)
- Daimler AG (DE)

Website

www.storhy.net

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