

MS13-02 Characterization of hydrogen storage materials both at the laboratory level and at the scale for prototype tanks M. Dornheim, J. Bellosta von Colbe, J. Jepsen, G. Lozano, C. Pistidda, F. Karimi, C. Bonatto Minella, R. Gosalawit, I. Saldan, K. Taube, T. Klassen *Institute of Materials Research, Materials Technology, Helmholtz-Zentrum Geesthacht GmbH, Geesthacht, Germany*
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Light weight metal or complex hydrides offer the potential for a safe and energy efficient hydrogen storage alternative for stationary as well as mobile applications. Highest energy efficiencies, however, are achievable only if both working temperature and the reaction enthalpy of the respective hydrogen sorption process can be attuned to the accompanying hydrogen consuming process in such a way that the required heat for hydrogen release of the hydride can be provided by the corresponding waste heat [1]. Since the kinetic optimisation of novel high capacity hydrides as well as the tailoring of reaction enthalpies is an important research task. One way to do this is to combine different hydrides which react during decomposition in an exothermal way with each other and thereby reduce the value of reaction enthalpy while maintaining the average of the hydrogen capacities of the single hydrides.

In parallel to such materials development and optimization activities upscaling of novel high capacity materials has to be demonstrated and tank concepts based upon these have to be investigated and optimized.

Reactive Hydride Composites like combinations of MgH_2 with $M(BH_4)_x$ (M being Li, Na or Ca) show significantly reduced values of reaction enthalpies as well as improved ab- and desorption kinetics compared to the pure borohydrides. Furthermore, due to their high reversible gravimetric storage capacities of up to 11 wt.% they are interesting candidates for future hydrogen storage applications.

In this presentation, recent results concerning reaction mechanisms, thermodynamic properties and sorption behaviour, cycling stability of borohydrides and Reactive Hydride Composites are presented. The progress in the optimisation of reaction kinetics reached so far will be described. Function and suitability of additives as potential catalysts on hydrogen ab- and desorption will be discussed.

MS13-03 Investigating Repeated Gas adsorption in zeolites for solar cooling applications. Marco Milanesio,^a Luca Palin,^a Davide Viterbo,^a Wouter van Beek^{ab}, Dmitry Chernyshov,^b Atsushi Urakawa^c, Rocco Caliandro^d
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Solar cooling exploits repeated adsorption/desorption cycles in porous materials to produce “cooling” by using hot water produced from *solar* energy. The first issue for application is identifying the best couples adsorber/fluid to match the working conditions, i.e. the hot water temperature and the cold sink where heat is discharged during the cycle. The second issue is the stability and reversibility of the cycle itself, since adsorber must work for a large ($>10^7$) number of cycles. To test adsorption/desorption properties of different materials, repeated gas adsorption in MFI zeolite materials was carried out, by collecting X-ray powder diffraction data set at in situ conditions. Different gases were used to test the temperature desorption range and the reversibility of the process. Thanks to the efficiency of modern detectors, it is possible to collect a huge amount of data and new data analysis tools are needed. Recently a new theory, named MED [1] exploiting modulation enhancement and able to manage such large experimental data sets, was developed for diffraction. The first experiments were carried out on porous materials [2] on MFI zeolite with Xe and Kr gases by modulating T and with mixture of gases (CO_2/N_2 bis shown in figure 1) modulating their concentration. Different reversibility behaviors were observed because of chemical interactions between the gas and the zeolite framework. Applications of MED to temperature modulation experiment are shown and possibilities of concentration modulation are explored.

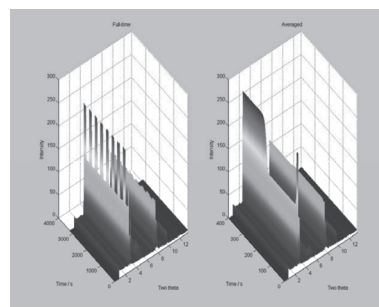


Figure 1: In situ XRPD data for CO_2/N_2 adsorption in MFI zeolite (left) and single period cycle after data merging (right).

- [1] Chernyshov, D., van Beek, W., Emerich, H., Milanesio, M., Urakawa, A., Viterbo, D., Palin, L. & Caliandro, R. (2011). *Acta Cryst.* A67, 327-335. [2] Caliandro, R., Chernyshov, D., Emerich, H., Milanesio, M., Palin, L., Urakawa, A., van Beek, W., & Viterbo, D. (2012). *J. Appl. Cryst.* 45, 458-470.

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