Hydrogen Storage in light complex Hydrides – structural studies

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The most important unsolved problem for the introduction of the Hydrogen Economy is efficient and safe storage of hydrogen. Alanates, compounds based on the AlH_4^- unit, are among the most promising metal hydrides for reversible hydrogen storage. The storage capacity is large, e.g. $NaAlH_4$ can release 5.6 wt% hydrogen below 200 °C. Work during the last years has revealed that Ti additives improve the kinetics of $NaAlH_4$ and also make re-hydrogenation possible. In order to improve the understanding of the effect of additives and absorption/desorption processes in general, detailed structural studies are very important.

Crystal structures of $MAlD_4$, (M=Li, Na, K) Li_3AlD_6, $Mg(AlH_4)_2$ and mixed alanates, like Na_2LiAlD_6, have been determined from high resolution powder neutron and X-ray diffraction. To understand the nature of additives high-resolution synchrotron X-ray and neutron diffraction experiments have been carried out. $NaAlH_4$ added with Ti-compounds shows no sign of solid solution of Ti into neither Na nor Al positions. However, samples being cycled indication the presence of an $Al_{1-x}Ti_x$ alloy. In-situ desorption experiments (both synchrotron X-ray and neutron diffraction) have been important for detailed studies of the desorption processes. $LiAlD_4$ has been shown to decompose completely to LiD, Al and D_2 at 127 °C, releasing 7.9 wt% hydrogen. Addition of VCl_3 by ball milling significantly increases the reaction rate. Recent synchrotron X-ray in-situ experiments will be presented.

Keywords: metal hydrides, powder neutron diffraction, powder x-ray diffraction