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6Mg(NH2)2:9LiH:12LiBD4 as hydrogen storage material: in-operando phase transformation

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Hydrogen storage technologies in low weight hydrides promise to help with the global aim of CO2-emissions reduction. High mass energy densities are needed e.g. for heavy-load long distance mobility like trains, trucks, and airplanes. One of the potential reaction based systems is Mg(NH2)2+LiH with a reversible hydrogen capacity of 5.6 wt.% below 200oC. The kinetics of hydrogen desorption/reabsorption is one of the cornerstones of hydrogen storage materials characteristics. The addition of LiBH4 improves it by forming an intermediate phase. It is speculated that subsequent melting improves the hydrogen diffusion, e.g. in the α-phase Li4(BH4)(NH2)3 or β-phase Li4(BH4)2(NH2)2.

The mixtures described in literature are denoted 6:9:x, 6Mg(NH2)2:9LiH:xLiBD4, where x varies from 0.5 to 12. It has been shown that the increase of x leads to faster reaction kinetics at the cost of loss of mass hydrogen capacity (for 6:9:12 down to 2.3 wt.%).

Neutron diffraction measurements at the diffractometer HRPT at PSI were conducted on the ball milled mixture 6Mg(NH2)2:9LiH:12LiBD4. Measurements were performed at several temperatures (RT, 50, 80, 90oC) in a vanadium container and during heating up to 180oC in a steel container while pumping out the released hydrogen. The phase composition was determined in the as-prepared state and in-situ during heating up to the melting transition. The appearance of new phases was registered after cooling back down to the room temperature.

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