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Hydrogen storage chemistry: the path of phase transformation in 6Mg(NH2)2:9LiH:12LiBD4 during hydrogen-emission reaction

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Hydrogen storage technologies in low weight hydrides promise an aid 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 formation of an intermediate phase with LiBH4 improves it. It is speculated that subsequent melting of e.g. α-phase Li4(BH4)(NH2)3 or β-phase Li4(BH4)2(NH2)2 improves the hydrogen diffusion.

The mixtures described in literature are denoted 6:9:x, 6Mg(NH2)2:9LiH:xLiBD4, where x grows 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 disappearance of precursors and appearance of new ones was registered after cooling back down to the room temperature.

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