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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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