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Hydrogen motion in $Li_4(BH_4)(NH_2)_3$ investigated by Quasielastic Neutron Scattering (QENS)

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Fast and efficient hydrogen storage is one of the key components for the use of hydrogen in a sustainable energy economy. Reactive Hydride composites have been considered for some time as potential solid state storage systems, among others also the amide based mixture $Mg(NH_2)_2$ + 2 LiH. The kinetic performance of the hydrogen exchange reaction in this system is significantly enhanced by the addition of $LiBH_4$ [Gizer et al. Inter. J. Hydrogen Energy 44, 11920-11929 (2019)] and the subsequent formation of the amide-borohydride compound $Li_4(BH_4)(NH_2)_3$. Here, we present a study of the structure and of the anion motion of in $Li_4(BH_4)(NH_2)_3$ investigated with synchrotron radiation powder X-ray diffraction (SR-PXD) and quasielastic neutron scattering (QENS) at temperatures close to operating condition. SR-PXD confirms the recrystallization of $Li_4(BH_4)(NH_2)_3$ into the α-phase during cooling from the melt. The QENS measurements prove a long-range diffusive motion of hydrogen containing species at 514 K with the diffusion coefficient $D \sim 10^{-6}\,\frac{\mathrm{cm}^2}{\mathrm{s}}$. At temperatures below 514 K, localized rotational motions were observed which have been attributed to (BH_4^- tetrahedra units undergoing rotations mainly around C_3 axes. The results will be discussed in the context of the improved hydrogen exchange reaction that is observed in $Mg(NH_2)_2$ + 2 LiH with $LiBH_4$ additions.

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