



Contribution ID: 221

Type: **Poster**

Rotational and long range diffusion in a lithium amide–lithium borohydride mixture

Wednesday, 9 December 2020 17:40 (20 minutes)

On-board hydrogen storage is still a challenge for fuel cell vehicles and other mobile applications. Complex hydrides, which contain ions such as BH_4^- and NH_2^- , have a high hydrogen capacity in combination with a low weight of the storage material. For example, $\text{Li}_4\text{BH}_4(\text{NH}_2)_3$ contains 11.1 wt.% hydrogen and desorbs more than 10 wt% at 573-673 K. In previous studies the high desorption temperature was reduced with additives. To understand the chemical behaviour and atomic motions of $\text{Li}_4\text{BH}_4(\text{NH}_2)_3$, we present an in situ phase analysis and quasielastic neutron scattering (QENS) during heating.

In situ X-ray diffraction was measured up to 573 K at P02 (DESY) and QENS was taken at TOFTOF (MLZ) in the temperature range 300-514 K. $\text{Li}_4\text{BH}_4(\text{NH}_2)_3$ melts at 494 K and during heating crystallization of a second phase was detected and identified as LiNH_2 , which remained a crystalline residue in the melted material. From the quasielastic signal rotational and long range motions were analysed and assigned to BH_4^- and NH_2^- of $\text{Li}_4\text{BH}_4(\text{NH}_2)_3$ and of the crystallized LiNH_2 phase.

Primary author: ASLAN, Neslihan (HZG, GEMS at MLZ)

Co-authors: Dr PISTIDDA, Claudio (Helmholtz-Zentrum); LOHSTROH, Wiebke; BUSCH, Sebastian (GEMS at MLZ, HZG); MÜLLER, Martin (Helmholtz-Zentrum Geesthacht)

Presenter: ASLAN, Neslihan (HZG, GEMS at MLZ)

Session Classification: Joint poster session of MLZ User Meeting and DN2020

Track Classification: UM: Materials Science