Characterization of a novel Mg-conductor using Neutron Methods

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Neutrons are a unique probe for non-destructive structural studies of energy materials, especially for future investigation and development of highly conductive solid state Mg electrolyte, neutrons are one of the main requirements for successful post-Li battery research. Recently, a new compound synthesized from γ-$Mg(BH_4)_2$ and ethylenediamine ($C_2H_8N_2$, abbreviation "en") was reported to have an exceptionally high magnesium ion conductivity of up to 6 x 10^{-5} S cm^{-1} at 70 °C in the solid state. In our work, the structure of this new compound has been solved and shows a different ratio of the precursors, γ-$Mg(BH_4)_2$: $[Mg(en)_3(BH_4)_2]$, while initially reported was 2:1. A new ratio of precursors will increase the ionic conductivity, simply because there is less unreacted γ-$Mg(BH_4)_2$. High resolution neutron powder diffraction data was previously collected at the NOVA beamline at J-Parc Spallation Source, Japan, and shows a very good correlation with the proposed model. Conductivity measurements will be presented as well as quasi elastic neutron scattering (QENS) experiments.

Reference

1. Igor E Golub, Michael Heere, Volodia Gounaris, Xiao Li, Timothy Steenhaut, Jian Wang, Koen Robeyns, Hai-Wen Li, Iurii Dovgaliuk, Kazutaka Ikeda, Geoffroy Hautier, Yaroslav Filinchuk, Structural insight into the magnesium borohydride–ethylenediamine solid-state Mg-ion electrolyte system, Dalton Transactions, 2023, DOI: 10.1039/D2DT03567G
2. Alexander Skripov; Olga Babanova; Roman Skoryunov; Alexei Soloninin; Igor Golub; Michael Heere; Yaroslav Filinchuk, Dynamical properties of the magnesium borohydride – ethylenediamine composite Mg(en)1.2(BH4)2: a nuclear magnetic resonance study (submitted); Solid State Ionics, 2022
3. Heere, M., A.-L. Hansen, S. Payandeh, N. Aslan, G. Gizer, M.H. Sørby, B.C. Hauback, C. Pistidda, M. Dornheim, and W. Lohstroh, Dynamics of porous and amorphous magnesium borohydride to understand solid state Mg-ion-conductors. Scientific Reports 10, 9080, DOI:10.1038/s41598-020-65857-6 (2020)