Structural Characterization of Metal Hydrides using Diffraction 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 by E. Roedern et al. 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. Heere, M., M.J. Mühlbauer, A. Schökel, M. Knapp, H. Ehrenberg, and A. Senyshyn, *Energy research with neutrons (ErwiN) and installation of a fast neutron powder diffraction option at the MLZ, Germany.* Journal of Applied Crystallography, 2018. **51**(3).