



Contribution ID: 129

Type: **Talk**

Garnet to hydrogarnet: effect of post synthesis treatment on cation substituted LLZO solid electrolyte and its effect on Li ion conductivity

Tuesday, December 7, 2021 1:40 PM (25 minutes)

We investigated why commercial $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (LLZO) with Nb- and Ta substitution shows very low mobility on a local scale, as observed with temperature-dependent NMR techniques, compared to Al and W substituted samples, although impedance spectroscopy on sintered pellets suggests something else: conductivity values do not show a strong dependence on the type of substituting cation. We observed that mechanical treatment of these materials causes a symmetry reduction from garnet to hydrogarnet structure. To understand the impact of this lower symmetric structure in detail and its effect on the Li ion conductivity, neutron powder diffraction and ^6Li NMR were utilized. Despite the finding that, in some materials, disorder can be beneficial with respect to ionic conductivity, pulsed-field gradient NMR measurements of the long-range transport indicate a higher Li^+ diffusion barrier in the lower symmetric hydrogarnet structure. The symmetry reduction can be reversed back to the higher symmetric garnet structure by annealing at 1100 °C. This unintended phase transition and thus a reduction in conductivity is crucial for the processing of LLZO materials in the fabrication of all-solid state batteries.

Authors: FRITSCH, Charlotte; Dr ZINKEVICH, Tatiana; Dr INDRIS, Sylvio; Dr ETTER, Martin; BARAN, Volodymyr (DESY, FS-PETRA-D, P02.1); Dr BERGFELDT, Thomas; EHRENBERG, Helmut (KIT); KNAPP, Michael (KIT, IAM-ESS); Dr HANSEN, Anna-Lena

Presenter: FRITSCH, Charlotte

Session Classification: Structure Research

Track Classification: Structure Research