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

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We investigated why commercial Li7La3Zr2O12 (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 ℃. 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.

Primary 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

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