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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**

*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  $^6\text{Li}$  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  $\text{Li}^+$  diffusion barrier in the lower symmetric hydrogarnet structure. The symmetry reduction can be reversed back to the higher symmetric garnet structure by annealing at  $1100\text{ }^\circ\text{C}$ . 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.

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