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Single-crystal Neutron-diffraction of Ta-substituted and Ga-doped Li7La3Zr2O12 garnet-type solid-state electrolyte material.

Large single crystals of garnet-type Li6La3ZrTaO12 (LLZTO) and Ga-doped Li7La3Ze2O12 (Ga-LLZO) were grown by the Czochralski method and analysed using neutron diffraction between 2.5 and 873 K in order to fully characterize the Li-atom distribution, and possible Li ion mobility in this class of potential candidates for solid state electrolyte battery material. The LLZTO retains its cubic symmetry, with space group Ia-3d,over the complete temperature range. When compared to the other sites, the octahedral sites behave as the most rigid unit and show the smallest increase in thermal parameters and bond length. The La- and Li-sites show mutually similar thermal expansion in their bond lengths up temperature, and the anisotropic and equivalent atomic displacement parameters exhibit a distinctly larger increase at temperatures above 400 K. Detailed inspection of nuclear densities at the Li1 site reveal a small but significant displacement from the 24d to the typical 96h position, which, however, cannot be resolved in the single crystal X-ray diffraction data. The site occupation of LiI ions on Li1 and Li2 remains constant, so there is no change in site occupation with temperature. For Ga-LLZO a phase transition from I-43d to Ia-3d could be identified.

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