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Investigation of Na⁺ diffusion in NASICON solid electrolyte materials by Quasi-Elastic Neutron Scattering

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Over the last decades, sodium superionic conductor (NASICON) materials have been a widely studied class of solid electrolytes for Na-ion based all-solid-state batteries due to their high conductivity and facile synthesis conditions. The aim of this work is to clarify the reason for extremely high conductivity exhibited by some compositions, specifically by $\text{Na}_{1+x}\text{Zr}_2\text{Si}_x\text{P}_{3-x}\text{O}_{12}$ ($0 \leq x \leq 3$). The focus of this study is to explain the role of the monoclinic to rhombohedral phase transition for the material with $x=2.4$, which occurs at around 170 °C, on the Na⁺-ion occupancy in the crystal structure. Additionally, we investigate the role of Al/Y and Sc substitution on the sodium occupancy and the overall temperature dependence of the ionic conductivity in the temperature range of 297-640 K.

In general, neutron scattering techniques are highly suitable for measuring the properties of crystalline materials. Here, QENS (quasi-elastic neutron scattering) is applied to measure the spatial and temporal dynamic properties of diffusion of sodium ions in the crystal lattice. This technique is feasible, because sodium is the only diffusive element in the material and the only one scattering incoherently. The measurements were performed at the BASIS spectrometer at the Spallation Neutron Source, Oak Ridge National Laboratory in Tennessee, USA. For the evaluation of the QENS data, the DAVE software (NIST Center for Neutron Research) is used.

The Na⁺-ion diffusion mechanism can be described by the right choice of the diffusion model, in this case the Chudley-Elliott jump diffusion model has been used. Important parameters, such as diffusion coefficients, activation energies, jump distances between the occupation sites and residence times are extracted from the measured and modelled QENS data.

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