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

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The sodium superionic conductor materials, also known as NASICON, 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 Na_{1+x}Zr₂Si_xP_{3-x}O₁₂ ($0 \leq x \leq 3$), and 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. We also investigate the role of Al/Y and Sc substitution and the overall temperature dependence of the ionic conductivity in the temperature range of 297-640K.

The quasi-elastic neutron scattering (QENS) is used to measure the spatial and temporal dynamic properties of diffusion of Na⁺ ions in the crystal structure. The measurements were performed at the BASIS spectrometer at the SNS, Oak Ridge National Laboratory in Tennessee, USA.

The Na⁺ ion diffusion mechanism can be described by the right choice of the diffusion model, 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. Additionally, temperature dependent X-ray diffraction data have been obtained and analysed. Information about interatomic distances have been extracted in order to confirm the results obtained from the QENS data.

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