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Mechanisms of molecular dynamics in anomalous thermal expansion of NaSICON-type ceramics

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NaSICON-type materials (ceramic lattices of joined MO6 and PO4 polyhedra with interstitial alkali metals) are of interest due to their ability to have anisotropic metallic semi-conductivity due to delocalization of electrons along the octahedral chains.(1) “Filled” alkali metal containing NaSICONs have been shown to have positive thermal expansion, whereas some “empty” NaSICONs have been shown to have some anomalous thermal expansion.(2) Applications of these materials are due to their thermomechanical stability, with increased resistance to thermal shock. The temperature dependant properties have been studied for some empty NaSICON type materials(2, 3), but often there is no variable temperature neutron powder diffraction and Xray powder diffraction data. We aim to gather variable temperature neutron powder diffraction data along with X-ray powder diffraction data in combination with molecular dynamics simulations to characterise lattice distortion modes and the mechanism of anomalous thermal expansion of NaSICON-type ceramics.

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Topics

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