



Contribution ID: 22

Type: Poster

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

Monday, 4 November 2024 19:55 (20 minutes)

NaSICON-type materials (ceramic lattices of joined MO_6 and PO_4 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.

(1) Leclaire, A.; Borel, M. M.; Grandin, A.; Raveau, B. A mixed-valence niobium phosphate with an empty nasicon structure: $\text{Nb}_2(\text{PO}_4)_3$. *Acta Crystallographica Section C Crystal Structure Communications* 1989, 45 (5), 699-701. DOI: 10.1107/s0108270188013708.

(2) Woodcock, D. A.; Lightfoot, P.; Smith, R. I. Negative thermal expansion behaviour in the NZP phase $\text{NbTi}(\text{PO}_4)_3$. In *Symposium on Solid-State Chemistry of Inorganic Materials II*, Boston, Ma, Nov 30-Dec 04, 1998; Materials Research Society: WARRENDALE, 1999; Vol. 547, pp 191-196.

(3) Zhao, D.; Liang, P.; Su, L.; Chang, H.; Yan, S. $\text{Al}_{0.5}\text{Nb}_{1.5}(\text{PO}_4)_3$. *Acta Crystallographica Section E Structure Reports Online* 2011, 67 (3), i23-i23. DOI: 10.1107/s1600536811003886.

Topics

Chemistry and Crystallography

Primary author: CLARK, Kaylee (The University of Sydney)

Co-authors: LING, Chris (University of Sydney); AVDEEV, Max (Australian Nuclear Science and Technology Organisation, Australian Centre for Neutron Scattering)

Presenter: CLARK, Kaylee (The University of Sydney)

Session Classification: Posters