Contribution ID : **69** Type : **Poster**

Composition and temperature dependent structural investigation of perovskite-type sodium-ion solid electrolyte series Na1/2-xLa1/2-xSr2xZrO3

Thursday, 12 November 2020 17:34 (1)

The development of new solid electrolytes is becoming increasingly important, e.g. in rechargeable batteries for electric vehicles, where current organic electrolytes cause major safety concerns. The ABO3 perovskite metal oxides have shown excellent lithium and sodium ion conductivity owing to their stability and structural flexibility. This has led to the development of several perovskite-type solid electrolytes such as Li3xLa2/3-xTiO3 and Na1/2-xLa1/2-xSr2xZrO3, which have shown high ionic conductivity.

The Na1/2-xLa1/2-xSr2xZrO3 perovskite-type sodium-ion solid electrolyte system was recently published by Zhao et al. [1] with the x=1/6 member, i.e. Na1/3La1/3Sr1/3ZrO3, found to have the highest ionic conductivity. The structure was reported to adopt a cubic crystal system with the space group P213. However, this is highly unlikely as both theoretical end members of the series, Na1/2La1/2ZrO3 and SrZrO3, have orthorhombic symmetry[2, 3]. Given the high ionic conductivity reported for the system, it is important to determine its structure reliable and with the best available data. Using neutron and X-ray powder diffraction data we have been able to confirm that the symmetry across the series is lowered to orthorhombic indeed. Variable temperature neutron powder diffraction data collected for the x=1/6 member of the system from room temperature to 1100 ◦C helped to identify a structural phase transition from orthorhombic to tetragonal symmetry at 800 ◦C.

[1] Y.Z. Zhao, Z.Y. Liu, J.X. Xu, T.F. Zhang, F. Zhang, X.G. Zhang, Synthesis and characterization of a new perovskite-type solid-state electrolyte of Na1/3La1/3Sr1/3ZrO3 for all-solid-state sodium-ion batteries, J Alloy Compd, 783 (2019) 219-225.
[2] B.J. Kennedy, C.J. Howard, B.C. Chakoumakos, High-temperature phase transitions in SrZrO3, Phys Rev B, 59 (1999) 4023-4027.
[3] M.C. Knapp, P.M. Woodward, Ohio State University. Department of Chemistry, Investigations into the structure and properties of ordered perovskites, layered perovskites, and defect pyrochlores, in, Ohio State University„ Columbus, Ohio, 2006, pp. xvii, 161 p.

Speakers Gender

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Level of Expertise

Student

Do you wish to take part in the poster slam

Yes

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Session Classification : Poster Session

Track Classification : Chemistry & Crystallography