

Structural Characterisation of a high Na-ion conductor

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Rechargeable lithium ion batteries have been in commercial use for almost three decades now. They are ubiquitous in our society and we can hardly imagine a life without them. Given the challenges ahead, such batteries might help to slow down the rate at which our planet warms. Two large scale approaches that can help here are the storage of sustainably produced renewable energy and the use of batteries in electric cars (re-charged with sustainably produced electricity). Several widely publicised cases of exploding mobile phones (due to highly flammable organic electrolytes) have highlighted critical safety concerns for widespread use of such batteries in cars. To address these safety issues, the highly flammable organic liquid electrolytes can be replaced by solid electrolytes to form all-solid-state batteries (ASSBs). In this context, the development of solid electrolytes for sodium ion batteries is crucial.

One of the systems that we are investigating, and the subject of this presentation, is the perovskite-type $\text{Na}_{1/2-x}\text{La}_{1/2-x}\text{Sr}_{2x}\text{ZrO}_3$ system. The $x=1/6$ member of the system, i.e. $\text{Na}_{1/3}\text{La}_{1/3}\text{Sr}_{1/3}\text{ZrO}_3$ (NLSZO) was recently published by Zhao et al. [1] They reported the structure to have a cubic crystal system with the space group P213, in agreement with the data for SrZrO_3 (PDF No. 74-2231) as proposed in 1992 by Roosmalen et al. [2] However, it has been demonstrated by Kennedy et al. that the transition to the cubic phase for SrZrO_3 is only possible at or above 1373 K with the space group Pm-3m [3]. Under ambient conditions SrZrO_3 is reported to have an orthorhombic superstructure.

Given the high ionic conductivity reported for the system, it is important to determine its structure reliably and with the best available data. The powder data we have collected for our sample indicate that the symmetry is indeed lowered to orthorhombic. The detailed structural characterisation based on those data will be reported.

References:

- [1] Y. Zhao, Z. Liu, J. Xu, T. Zhang, F. Zhang, X. Zhang (2019). Synthesis and characterization of a new perovskite-type solid-state electrolyte of $\text{Na}_{1/3}\text{La}_{1/3}\text{Sr}_{1/3}\text{ZrO}_3$ for all-solid-state sodium-ion batteries. *Journal of Alloys and Compounds* 783, 219 - 225.
- [2] J. A. M. van Roosmalen, P. van Vlaanderen, E. H. P. Cordfunke (1992). On the structure of SrZrO_3 . *Journal of Solid State Chemistry* 101, 59 - 65.
- [3] B. J. Kennedy, C. J. Howard, B. C. Chakoumakos (1999). High-temperature phase transitions in SrZrO_3 . *Physical Reviews B* 59, 4023 - 4028.

Level of Expertise

Student

Do you wish to take part in the poster slam

Yes

Travel Funding

Speakers Gender

Rather not state

Primary author: Mr YANG, Frederick Tiger (The University of Sydney)

Co-author: Prof. SCHMID, Siegbert (The University of Sydney)

Presenter: Mr YANG, Frederick Tiger (The University of Sydney)

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