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Understanding disorder in the Y2Sn2-xZrxO7 pyrochlore oxides

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Solid oxide fuel cells (SOFCs) offer clean alternatives to current carbon emitting energy sources; however, reducing their operation temperature is a major challenge for widespread application. Hence, the development of novel electrolyte materials with high room temperature ionic conductivity is crucial. Pyrochlore oxides, of the general chemical formula A2B2O7, exhibit chemical and structural flexibility, resulting in a diverse range of physical properties and technological applications, such as host matrices in the immobilization of actinide-rich nuclear wastes. In particular, they have gained interest as fast-ion conductors for electrolytes in SOFCs.

The pyrochlore structure is highly ordered, which limits long-range oxygen diffusion. This can be altered via disordering, which results in the formation of oxygen Frenkel pairs that improve conductivity. The pyrochlore structure can adopt the disordered-fluorite structure via changes in composition, temperature, pressure and radiation. The disordered-fluorite exhibits lower formation energy of the Frenkel defect; however, this increase in structural disorder can increase the activation energies needed for long-range migration, which results in optimal conductivity occurring in partially disordered materials. Hence, the interplay between disorder and order in the atomic structure is key to the physical properties of these materials.

There have been many studies dedicated to understanding the structural order and disorder in pyrochlore and disordered-fluorite oxides, with a recent study claiming the local structure of the disordered-flourite to be weberite. It was proposed that the overall structure of a disordered-fluorite consists of randomly arranged orthorhombic weberite domains that result in the long-range cubic disordered-fluorite.

In this study we use low temperature (15 K) neutron pair distribution function (PDF) and big box modelling to understand the local-scale structure of the Y2Sn2-xZrxO7 system. We show that the local structure of the Y2Zr2O7 disordered fluorite does not contain ordered weberite domains, which emphasizes the importance of low temperature measurements in the local structure analysis of disordered oxide materials. Our analysis of the Y2Sn2-xZrxO7 series serves as a direct method for quantifying disorder and Frenkel defects. Understanding and quantifying these atomic-scale distortions is essential in simulations and design as it directly influences the energy landscape for anion mobility. These techniques can be used in the development and engineering of novel and advanced electrolyte materials for SOFCs.

Speakers Gender

Male

Level of Expertise

Early Career <5 Years

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