Contribution ID : **29** Type : **Poster**

Exploring diffusion mechanisms in oxide-ionic conductive single crystals

Monday, 2 December 2019 18:45 (1)

The development of efficient and cost-effective solid oxide fuel cells (SOFCs) will allow hydrogen or other low-carbon fuels to replace hydrocarbon fuels in commercial energy-generation applications. A wide variety of oxide structure classes are being explored in an effort to discover SOFC electrolyte and electrode materials with competitive ionic conductivity in the "intermediate" temperature range (450-600 ℃). In order to rationally design and tune these materials for better performance, a clear understanding of the causes and mechanisms of ionic conductivity in the most promising materials is essential.

Our work utilises a combination of experimental and theoretical methods to investigate the structural and dynamic origins of oxide ion mobility in diverse solid oxide materials. We have used the optical floating-zone furnace facility recently installed at Durham University to grow single crystals of conductive scheelites ($CeNb_{1-x}M_xO_{4+\delta}$ and $LaNb_{1-x}M_xO_{4+\delta}$, M = V, Mo, W), apatites ($(La, Bi)_{9.33+x}Si_6O_{26\pm\delta}$) and "hybrid" hexagonal perovskites ($Ba_3NbMO_{8.5}$, M = Mo, W), in many cases for the first time. These crystals have enabled a variety of experiments to be performed, including single-crystal x-ray and neutron diffraction, directional quasielastic neutron scattering, and oriented ^{18}O tracer diffusion measurements. Our poster will present new insights obtained from these studies concerning the roles of ionic order and disorder, interstitial site behaviour, low-energy diffusion pathways, and cation coordination environments on efficient ionic conductivity in some of the mentioned materials.

Speakers Gender

Female

Travel Funding

No

Level of Expertise

Early Career <5 Years since PdD

Do yo wish to take part in the poster slam

No

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Session Classification : Welcome Function