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Non-specialist Talk - Structure Property correlation in SOFC & SOEC materials

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Solid Oxide Fuel Cells (SOFCs) and Solid Oxide electrolyser cells (SOECs) are exciting electrochemical devices that could provide unique and revolutionary solutions to some of the renewable energy challenges facing society. Central to the design of these devices is the need for a solid electrolyte that is an excellent oxygen ionic conductor whilst simultaneously being and electronic insulator. Additionally the materials needs to be mechanically tough and remain chemically inert in harsh operating environments. The architype materials used as solid electrolyte in most SOFCs include YSZ (Yttrium stabilised Zirconia) and CaSZ (Calcium stabilised Zirconia) with the Y or Ca dopants present at around 8 to 10% level.

In pursuit of improved materials for use in SOFCs and SOECs, our research has focused on gaining a fundamental understanding of the mechanisms governing the transport properties of these and closely related materials with an approximate A2B2O7 stoichiometry for various cationic ions, as well adding dopant species on particularly the A-site. Typically such materials adopt either average defect Fluorite or Pyrochlore structure types, and due to the presence of vacant anionic sites, both these structure types have inherent potential for ionic conduction. Our research has included the development of suitable synthesis, preparation and processing methodologies, particularly for the more novel materials, followed by structural, crystallographic, electrochemical and spectroscopic characterisation. Noteworthy, as SOFCs and SOECs have operational temperatures ranging from around 300°C to 1000°C, we perform XRD, PDF(1), Raman and EIS measurements between ambient to 900°C or 1000°C. Consideration of the results obtained for the array of distinct materials we have prepared, has highlighted the central role of short range order, as well as the importance of microstructure on the overall transport properties of the materials.

I will present a selection of our results to date, including the results obtained from total scattering experiments performed on ID22 at the ESRF in Grenoble. Analysis of the data shows structural differences when comparing the structure as perceived on the nano-scale with the bulk average structure. The implications of this for the transport properties of all energy materials is profound, and will be described.

(1) S. J. L. Billinge, "Nanostructure studied using the atomic pair distribution function", Z. Kristallogr. Suppl. 26 (2007) 17-26

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