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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. As the performance characteristics of these materials are not completely satisfactory, there is a definite need for improved alternatives. It is worth noting that although it is well established that these materials are cubic with average structure features consistent with the Flourite structure, there have been very few reports of studies into the nano-structure of these materials, as would be revealed by for example PDF studies(1).

Within this context 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 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 900°C, we also do XRD, PDF, Stress – Texture, Raman and EIS measurements between ambient to 900°C or 1000°C. Careful consideration of the results obtained for the vast array of distinct novel materials we have prepared, has highlighted the central role of short range order or so-called nano-structure, 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 ID31 at the ESRF in Grenoble. Analysis of the data for (as an example) the Y2Zr2O7 as prepared via sol-gel methods case, clearly 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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