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Structure Property correlation in SOFC & SOEC materials, and the importance of Synchrotron Techniques.

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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.

Our research has focused on gaining a fundamental understanding of the mechanisms governing the transport properties of these and closely related materials. Typically the cubic forms (Space group Fm-3m) of these materials exhibit higher oxide ion conductivity due to the presence of vacant anionic sites. 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℃ to 1000℃, we perform XRD, PDF(1), Raman and EIS measurements between ambient to 900℃ or 1000℃. 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 as well as 28-ID-1 at NSLS-II at BNL. 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.

Synchrotron techniques are central to insight into the real structure – property relationships, to this end we have additional experiments planned (beamtime approved) for NSLS-II, Diamond and SSRL. I will also present some of the unique aspects of some of the planned experiments.

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

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