Conductivity and Disorder in Rare Earth Apatite Materials

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With the increasing demand for cleaner and more efficient forms of energy production, fuel cell technologies have been attracting great interest for both mobile and stationary power systems. For this latter application, Solid Oxide Fuel Cells (SOFC's) are of particular interest as their high operational temperature bypasses the need for the separate reforming of hydrocarbon fuels and co−generates heat which can be usefully extracted.

The apatite systems $(La/M)_{10-x}(Si/Ge)_6O_{26+y}$ (M=alkaline earth, Mn, Co) have been recently attracting considerable interest as they have been shown to exhibit low activation energies and oxygen ion conductivity equivalent to the conventional yttria−stabilized zirconia electrolyte at 700°C. In particular, it has been found that oxygen disorder and non−stoichiometry decreases the activation energy for conduction. At present, no definite mechanism is known for the transport of oxygen through the structure, though it is widely assumed that conduction occurs along large, 1D channels running through the structure.

In our work we have investigated the mechanism of conduction through these materials using a combination of experimental and modelling techniques. Neutron diffraction and AC impedance have been employed to study the relationship between conductivity and disorder for a wide range of doping methodologies. Our main focus though, has been the use of atomistic modelling to probe the defect chemistry and the underlying mechanisms of conduction in two compositions: $La_8Sr_2Si_6O_{26}$ and $La_{9.33}Si_6O_{26}$.