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In-situ characterization of energy materials by neutron diffraction

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The development of energy conversion and storage devices necessary to provide clean and sustainable energy is based on the design, synthesis and characterization of new materials with appropriate properties in terms of ionic and/or electronic conductivity, ion insertion, redox activity, catalytic properties, etc. Structural characterization of these energy-related materials is of paramount importance in understanding and improving the desired behavioral properties of interest. In this sense, neutron diffraction is a unique tool for providing detailed structural information on characteristics closely related to these properties and their evolution to external factors (temperature, composition of the atmosphere, pressure, etc.). Well-known neutron diffraction applications are the location of oxygen atoms and oxygen vacancies into conductive oxide ions, Li ions in Li electrolyte or Li-battery cathodes; proton fast conductors, etc. Low neutron absorption is invaluable for the "in-situ" study of materials in furnaces, cryostats, pressure chambers, etc., simulating the operation conditions of the devices where they find applications. In this talk, we present some recent findings on various types of energy-related materials, including electrodes and electrolytes of solid oxide fuel cells (SOFC), and Li, Na and H conductors.

As SOFC cathodes, we have developed several series of $SrCoO_{3-\delta}$ derivatives with high electrical conductivity and oxygen permeability of oxygen flow. Suitable doping in the Sr or Co sites stabilized the desired cubic (or 3C-type) structure; the oxygen conduction pathways were revealed by neutron powder diffraction (NPD), collected "in-situ" under SOFC working conditions. Similar procedures were followed for SOFC anode materials derived from $SrMoO_3$ perovskite and new families of electrolytes $(Sr,K)SiO_3$, where NPD assisted in determining the oxide-ion diffusion pathways. An example of performant proton conductor is the $(H_3O)SbTeO_6$ pyrochlore, showing a H^+ conductivity greater than that of Nafion at 200 ° C; the hydronium H_3O^+ positions were determined from difference Fourier maps from NPD data. Neutrons are also useful for determining the location of Li in $La_{0.5}Li_{0.5}TiO_3$ perovskite and $Li_7La_3Zr_2O_{12}$ garnet, the latter being technologically important for lithium-air battery equipment. An extraordinary conductivity of Na is also reported in $Na_3[Ti_2P_2O_{10}F]$, with applications in Na-ion batteries; an in-situ NPD study allowed following Na diffusion across the structure. We will review some features of these different materials, focusing on the specific structural characteristics determined by neutrons that explain their interesting properties.

Keywords: SOFC cathodes and anodes; Li Na and proton conductors; neutron diffraction