REVISITING THE CRYSTAL STRUCTURE OF $BaCe_{0.4}Zr_{0.4}Y_{0.2}O_{3-\delta}$ PROTON CONDUCTING PEROVSKITE AND ITS CORRELATION WITH TRANSPORT PROPERTIES

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Oxides with proton conductivity have a great potential for applications in environmental energy technology. Despite the $BaCe_{0.4}Zr_{0.4}Y_{0.2}O_{3-\delta}$ (BCZY) perovskites are well-known proton conductors, it is a challenge to determine the optimal operating temperature range where the energy applications benefit most from this unique property **[1]**. The protonic transport properties strongly depend on crystal structure and local distortions in the participating cation coordination sphere, according to related temperatures and gas feed. The transport and crystallographic properties of BCZY were simultaneously studied by Impedance Spectroscopy (IS) and Synchrotron X-Ray Diffraction (S-XRD). A strong correlation between conductivity and lattice parameter, corresponding in principle to a cubic symmetry, was observed, mainly between 400 and 700 °C. The protonic conductivity range was analyzed by the H/D isotopic effect on the impedance spectra, which helped to identify protonic conduction as the governing transport mechanism below 600 °C, while the transport via oxygen vacancies dominates above this temperature. Anyway, in order to assess the real crystallographic structure, the simultaneous refinement of laboratory XRD and Neutron Diffraction (ND) patterns was performed **[2]**. It shows that BCZY changes from rhombohedral symmetry below 400 °C to cubic at 600 °C in a second order phase transition. Complementary Quasielastic Neutron Scattering (QENS) let determine a protonic jump length of 3.1 Å, which matches the O-O distances in the octahedral oxygen coordination sphere around the cations **[3]**. These results support the protonic self-diffusion through proton hopping between intra-octahedral O sites as the main transport mechanism up to 600 °C.

Keywords: $BaCe_{0.4}Zr_{0.4}Y_{0.2}O_{3-\delta}$ (BCZY) electrolyte, protonic conductivity, in-situ measurements, ND, XRD, QENS, EIS.

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