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Neutron and X-ray Diffraction Studies of BaCe0.85Y0.15O2.925 for Application in Innovative Design of Fuel Cell

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The aim of this study is a deeper insight into the conductivity mechanisms and water behavior in BaCe0.85Y0.15O3−δ (BCY15) which is applied in an innovative design of solid oxide fuel cell, named dual membrane fuel cell (dmFC). The new design overcomes the disadvantages connected with the production of water at the electrodes. The innovative idea is the introduction of a separate compartment (central membrane CM) for the water formation and evacuation. It has mixed ionic (proton and oxide ion) conductivity and porous structure. Specialized impedance measurements discovered good mixed ion (proton and oxide ion) conductivity in BCY15 at operating temperatures. Thus a "monolithic design", which strongly simplifies the technology, has been proposed, since in O2 flow BCY15 is oxide ion conductor, in H2 flow it is proton conducting and in the central membrane it is mixed ion conducting. Applying several experimental approaches (complex permittivity, water vapour permeability and impedance measurements), new phenomena connected with the presence of water in the porous BCY structure were discovered - formation of an electrochemically active volumetric layer in the CM which facilitates the water formation and thus improves the operation of the dmFC design by decreasing its resistance. This phenomenon can facilitate also the splitting of water, which is of importance for operation in electrolyzer mode.
For deeper insight of the conductivity properties/mechanisms and water behaviour, fundamental studies on atomic level are in progress. The structural details of powder, dense and porous samples were investigated from full profile analysis of neutron and x-ray diffraction patterns. The basic constituent is BCY15 powder prepared by auto-combustion and calcination at high temperature, which crystallizes in the orthorhombic Pnma space group similarly to the parent BaCeO3 stoichiometric perovskite and BaCe0.9Y0.1O2.95. New studies are under development.

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Author: Dr KREZHOV, Kiril (INRNE-BAS)

Co-authors: Prof. THOREL, Alain (ARMINES); Dr CHASNAUD, Anthony (ARMINES); Dr RAIKOVA, Gergana (IEES); GENOV, Ivaylo (IEES)

Presenter: Dr KREZHOV, Kiril (INRNE-BAS)

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