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Mechanism of mixed (oxide ion and proton) conductivity of BCY15

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The aim of the proposed object is a deeper insight into the conductivity mechanisms and water behavior in BaCe0.85Y0.15O3-α (BCY15), material which is well known with its good proton conductivity.

This study is directly related to the application of BCY15 in an innovative design of solid oxide fuel cell, named dual membrane fuel cell (dmFC) which is based on a patented idea, proved in the frames of a FP7 FET project [1-6]. The new design overcomes a principle construction disadvantage connected with the production of water at the electrodes, which brings to dilution of the fuel or oxidizer and reduction of the electrodes catalytic activity. The innovative idea is the introduction of a separate compartment (central membrane CM) for the water formation and evacuation [2]. It has mixed ionic (proton and oxide ion) conductivity and porous structure.

Specialized impedance measurements discovered good mixed ion conductivity in BCY15 at operating temperatures. Thus the proton conducting electrolyte replaced the composite material of the CM which also brought to simplification of the technology [4]. Applying several experimental approaches (complex permittivity, water vapor 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 be of importance also for proton conducting solid oxide fuel cells, as well as for operation in electrolyzer mode.

For the moment basic understanding of proton conductivity in ceramics is lacking. Thus fundamental studies on molecular level applying methods as neutron powder diffraction (NPD), anomalous resonant X-ray diffraction (XRD), quasi-elastic neutron scattering (QENS), x-ray spectroscopy (XS) can contribute to deeper insight into the new phenomena (mixed ion conductivity and water behavior). Recent studies on BaZr0.9Y0.1O2.95 (BZY10) performed in EMPA discovered some superstructures for protons, deuterons and yttrium, as well as correlation of toughening of the lattice and proton conductivity. Interesting results are obtained combining QENS and impedance spectroscopy [www.empa.ch/plugin/template/empa/*/134090].

Two NPD measurements at the H2FC infrastructure IFE is proposed. BZY15 measured in humid atmosphere will be used to reveal the distribution of protons (or deuterons; see below) in the crystal structure. Heavy water (D2O) will be used rather than normal water because hydrogen gives a very high background due to incoherent scattering. BZY15 will also be measured in the unprotoated state (i.e. in dry atmosphere) as a reference.

It is expected that the combination of the macroscopic with the microscopic approach and the analysis of the results obtained by the impedance-based and neutrons-based techniques on BCY15 in dry and humidified hydrogen, oxygen and in water at operating temperatures (500-700oC) will ensure information about the topology of the pores space (internal surface areas, porosity, particle size, void size, fractality) as well as about the transport (diffusion) and hopping in microscopic scale.

References

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