PHYSICAL CHEMISTRY 2016

2nd International Meeting
on

Materials Science for Energy Related Applications

BOOK OF ABSTRACTS

September 29-30, 2016
University of Belgrade - Faculty of Physical Chemistry, Belgrade

KTH
ROYAL INSTITUTE OF TECHNOLOGY
Stockholm, Sweden

UNIVERSITY OF BELGRADE
FACULTY OF PHYSICAL CHEMISTRY
Belgrade, Serbia

THE SOCIETY OF
PHYSICAL CHEMISTS OF SERBIA
Belgrade, Serbia

2nd International Meeting

on

Materials Science for Energy Related Applications

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CHEMICAL STABILITY OF DOPED $BaCe_{0.9}Y_{0.1}O_{3-\delta}$ AS A PROTON CONDUCTING ELECTROLYTE FOR IT-SOFC

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$BaCe_{0.9}Y_{0.1}O_{3-\delta}$ (BCY) has been one of the most studied materials known for its highest proton conductivity at temperatures between 500 and 700 ºC, which allows its application as a proton conducting electrolyte for intermediate-temperature solid oxide fuel cells (IT-SOFC). The proton conductivity is an exclusive property of mixed oxides with perovskite structure and large unit cell volume, such as $BaCeO_3$ or $SrCeO_3$. Doping with aliovalent cations (Y^{3+}) that replace Ce^{4+} induces formation of point defects (oxygen vacancies), which in wet or hydrogen containing atmosphere allow proton mobility. The main disadvantage of this material is its instability in CO_2-rich atmosphere due to the basic character of the crystal lattice, thus limiting its application in SOFCs in respect to fuel selection. However, the stability of BCY can be enhanced by doping with cations that may raise the acidic character of the material, such as Nb^{5+}, Ta^{5+} or In^{3+}. Introduction of pentivalent cations will lead to reduced amount of point defects and consequently lower proton conductivity and it is therefore recommended that their molar concentration should not exceed 5 %. On the other hand, trivalent In^{3+} is more suitable as it can completely replace Y^{3+} since it can both serve as a point defect source and increase acidity of the crystal lattice. Because of these properties it can be introduced in much larger amounts than Nb^{5+} or Ta^{5+}.

In this study $BaCe_{0.9-x}Nb_xY_{0.1}O_{3-\delta}$ (where x = 0.01, 0.03 and 0.05) and $BaCe_{1-x}In_xO_{3-\delta}$ (where x = 0.15, 0.20 and 0.25) powders were synthesized by the method of autocombustion, while $BaCe_{0.9-x}Ta_xY_{0.1}O_{3-\delta}$ (where x = 0.01, 0.03 and 0.05) powders were prepared by the classical solid state route. Much higher specific surface areas were observed for the samples synthesized by the autocombustion method. In the case of Nb and Ta doped samples, the dense electrolytes were formed after sintering at 1550 ºC for 5 h in air. Temperature of 1300 ºC was enough to complete sintering of the samples doped with In after 5 h in air, which was another advantage of In as a dopant. The conductivities determined by impedance measurements in temperature range of 550-700 ºC in wet hydrogen showed a decreasing trend with increase of Nb and Ta content, while it was the opposite in the case of In. Interestingly, the total conductivity of the samples $BaCe_{0.85}Nb_{0.05}Y_{0.1}O_{3-\delta}$, $BaCe_{0.85}Ta_{0.05}Y_{0.1}O_{3-\delta}$ and $BaCe_{0.75}In_{0.25}O_{3-\delta}$ reached around 5×10^{-3} S/cm in wet hydrogen atmosphere at 700 °C. After exposure in 100 % CO_2 atmosphere at 700 °C for 5 h, the samples were

investigated by X-ray analysis. It was found that even 15 % In could completely supress degradation of electrolyte, while the highest concentrations of Nb and Ta (5%) were necessary to secure sufficient stability in CO_2.