CRYSTALLINE STRUCTURE AND OXYGEN STOICHIOMETRY OF THE $Ba_{0.50}Sr_{0.50}Co_{0.80}Fe_{0.20}O_{3-\delta}$ POWDERS OBTAINED BY EDTA-CITRATE METHOD MEASURED BY X-RAY AND NEUTRON DIFFRACTION

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The $Ba_{0.50}Sr_{0.50}Co_{0.80}Fe_{0.20}O_3$ (BSCF) is good candidate as air electrode for Intermediate Temperature Solid Oxide Fuel Cells (ITSOFC). Studies have shown that the different methods may modify the powder characteristics such as: morphology, crystalline size and surface microstructure.[1] The transport properties and catalytic activity of BSCF are directly associated to perovskite structure (ABO_3) and substitution of A and/or B site, besides the oxygen vacancies. Zhou et al. (2009) mentioned that the substitution of Sr^{2+} by Ba^{2+} may increase the oxygen vacancy concentration, thus optimize the composition of BSCF.[2] The investigation of these parameters is usually made by X-ray diffraction, obtaining important information such as the crystal structure, lattice parameter and atomic substitution among other characteristics of the studied material. The ionic conduction of perovskite oxides occur due oxygen vacancy in atom structure of material.[3]
The presented results deal the crystal structure and oxygen vacancy of BSCF characterized by X-ray and Neutron diffraction with the Rietveld refinement method. The $Ba_{0.50}Sr_{0.50}Co_{0.80}Fe_{0.20}O_{3-\delta}$ has been synthesized by combined EDTA – citrate method. The main phase is identified as cubic perovskite structure with a = 3.9857 Å, without the presence of secondary phases. Theoretical density of 5.476 $g.cm^{-3}$ have been achieved for BSCF calcined at 900°C for 5h. The results obtained by Neutron Diffraction confirm the occupancy oxygen refined at 0.818 and the calculations for oxygen stoichiometry at 2.454. In these results we can see existence of oxygen vacancies, the most important feature for the performance of this compound applied in cathodes ITSOFCs.

Keywords: ITSOFC, crystalline structure, neutron, diffraction, BSCF

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