Evaluation of the Mass Transport Properties of $La_{0.8}Sr_{0.2}MnO_{3+\delta}$ nanostructures by Finite Element Method Simulations

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Decreasing particle sizes to the nanometer scale modifies the ceramic materials properties leading, in some cases, to completely new ones [1]. Recently, enhanced oxygen mass transport has been reported in La0.8Sr0.2MnO3 δ (LSM), an essentially pure electronic conductor material [2-4]. The high ion diffusion measured is attributed to the existence of an interface-dominated nanostructure, i.e. dense thin films with a high density of grain boundaries. While grain boundaries are assumed to provide the fast diffusion paths, there is still a lack of understanding of how the nanostructure characteristics affect the mass transport and functional properties.

Since analytical solutions for diffusion in such an inhomogeneous material with finite geometry are not available, modelling by Finite Elements Method (FEM) has been performed. The model basis consists of a bilayer formed by (i) a nanometric-thick LSM film exposed to the atmosphere with vertically aligned squared grains interfaced with grain boundaries (gb) and (ii) a nanometric-thick film of a fast oxygen ion conductor. The FEM model was initially used to obtain the oxygen diffusion and surface exchange coefficients (D*bulk, k*bulk, D*gb and k*gb) of a dense LSM/YSZ heterostructure from the normalized isotopic profiles obtained by isotope exchange experiments combined with Secondary Ion Mass Spectroscopy measurements. These coefficients were further confirmed by Electrochemical Impedance Spectroscopy measurements and are considered as initial reference values [4]. In addition, the developed FEM model has allowed us to obtain an in-depth analysis of the influence of the nanostructure on the functional

behavior of LSM thin films taking into account parameters such as the grain and grain boundary sizes, the thin film porosity and the thickness.

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