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Synthesis and Characterization of potential anodic materials for SOFC´s based on $La_{0.80}Sr_{0.20}Cr_{0.80}Fe_{0.20}O_3$ system

J. A. Gómez C. [(1)]*, J. S. Valencia R. [(1)] and J. B. Carda. C. [(2)]

(1) Universidad Nacional de Colombia, Departamento de Química, Laboratorio de Catálisis Heterogénea, Grupo de Aplicaciones Fisicoquímicas del Estado Sólido (AFES); Ciudad Universitaria; Transversal 38 No. 40-04, Bogotá, Colombia. jagomezcua@unal.edu.co
* Corresponding author.
(2) Grupo de Química del Estado Sólido, Departamento de Química Inorgánica y Orgánica, Universitat Jaume I de Castelló, Castelló de la Plana, España. carda@qio.uji.es

Abstract – The research in anodic materials for solid oxide fuel cells (SOFC´s) is one of the most exciting technologies that offer the possibility to utilize CH_4 or CO as well as an effective and early response to reduction in carbon dioxide emissions. Among the most promising materials there are those with *A* and *B*-site substitutents, where Sr and Fe were found to be the most suitable for these purpose. Hence, nanoparticles of $La_{0.8}Sr_{0.2}Fe_{1-x}Cr_xO_3$ (<40.0 nm) were obtained using a wet chemical route (citrate method). The characterization using X-ray diffraction (XRD); scanning electron microscopy (SEM) and thermogravimetric analysis (TGA) showed the best synthesis conditions.

For the synthesis of $La_{0.8}Sr_{0.2}Fe_{0.80}Cr_{0.20}O_3$ oxide, nitrate type solutions 1.00 M and monohydrate citric acid 2.00 M were used. The precursor solutions are dosed into a reactor equipped with magnetic stirring (150 rpm), temperature control and reflux at 80º C for two hours. The order of addition of precursors was established by the corresponding hydrolysis constants, so that the total amount of nitrate in the reaction media was 0.01 mol and the addition of citric acid was done in a 4:1 molar ratio, while the pH was adjusted with an ammonia solution at 2.00 based on the analysis and modeling proposed to resolve the potential reactions in aqueous medium using the Hydra-Medusa software [1], this will prevent hydrolysis and precipitation of insoluble secondary species. The resulting sol was heat at 120 ºC for 24 hours and then at 250°C, until the obtention of a solid foam precursor that was calcined at 900ºC for 2 hours using a ramp of $50ºC{\cdot}hour^{-1}$. The precursor analysis by infrared spectroscopy (Fig. 1b) and thermogravimetric analysis showed the formation of citrate type species as well allowing evaluate the optimum temperature for the consolidation of the crystalline phase (Fig. 1a). The phase formation, purity and morphology were determined by X-ray diffraction, in a PANAlytical X'pert PRO MPD equipment with ultra-fast X'Celerator detector, using Cu K_α radiation (λ = 1.54186 Å) between 10 and 90° 2θ in Bragg-Brentano configuration with steps of 0.02° 2θ, with irradiations of 40.80 seconds per step. The scanning electron microscopy (SEM), showing that the method allows to generate and maintain in the solid important surface and textural features for potential applications (Fig. 1d). The diffraction results were analyzed and refined using the software X'Pert High Score® and Cellref3.0®, indicating that the $La_{0.8}Sr_{0.2}Fe_{0.8}Cr_{0.2}O_3$ has a characteristic grain size distribution proper of synthesis method with preferential orientation in the plane (011) (Fig. 1c); with this reflection, the determination of the crystalline particle size, by Debye-Scherrer equation, yield a crystal size of 39.8nm. The survey in the databases of the ICCD, suggests a classification consistent with the cubic phase reference compound $La_{0.9}Sr_{0.1}CrO_3$, space group *Pm-3m* (221), with cell parameters $a = b = c = 3.874$ Å, cell volume: 58.14 $Å^3$, ICSD: 041062 and JCPDS: 01-074-1975 . The tolerance factor using the SPuDS software [2] confirmed a structural tolerance factor (τ) of 0.9621 to 298 K and a global instability index of 0.4238 confirm the feasibility of the perovskite type structure.

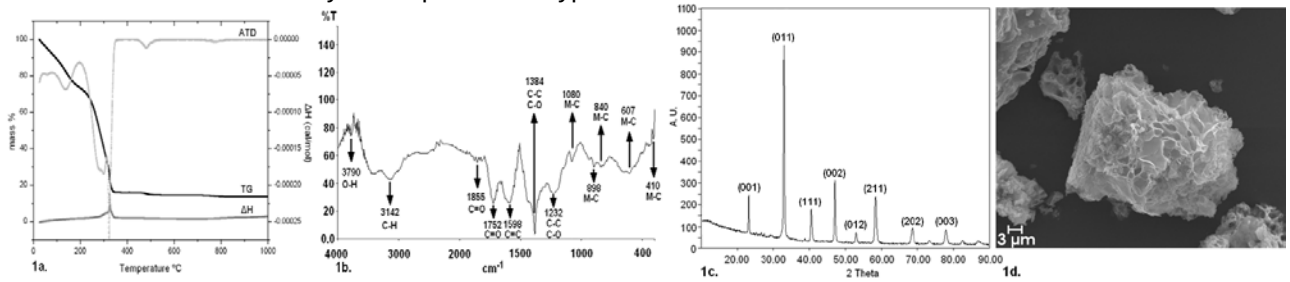

Figure 1: a) Thermogravimetric analysis of $La_{0.8}Sr_{0.2}Fe_{0.8}Cr_{0.2}O_3$ precursor. **b)** FT-IR spectrum of citrate precursor. **c)** Indexed $La_{0.8}Sr_{0.2}Fe_{0.8}Cr_{0.2}O_3$ XRD pattern **d)** $La_{0.8}Sr_{0.2}Fe_{0.8}Cr_{0.2}O_3$ scanning electron microscopy at 3 µm.

References

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