Crystal structure of $SrCo_{1-x}Mo_xO_{3-\delta}$ ($0 \le x \le 1$) perovskites obtained under oxidizing and reducing conditions with potential use as electrodes for intermediate-temperature symmetrical solid-oxide fuel cells

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In this work, $SrCo_{1-x}Mo_xO_{3-\delta}$ ($0 \le x \le 1$) powders were synthesized by the gel-combustion method in order to explore two major aspects: the synthesis method and the crystal structure of these systems upon the variation of the Co/Mo relation. Sample $SrCo_{0.95}Mo_{0.05}O_{3-\delta}$, exhibiting a tetragonal phase (space group *P4/mmm*) at room temperature (RT) was used as the parent compound as it was reported to be a good cathode for intermediate-temperature solid-oxide fuel cells (IT-SOFCs) [1]. The amount of glycine used as fuel in the synthesis route was studied in order to obtain a single-phased material with high homogeneity and reproducibility. Afterward, the relationship between the Co/Mo ratio in the B site of the perovskite was also investigated with the aim of implementing these materials as potential electrodes for intermediate-temperature symmetrical solid-oxide fuel cells (IT-SSOFCs). Thus, both the crystal structure and the reducibility properties of the powders were investigated by X-ray powder diffraction (XPD) and temperature-programmed reduction under diluted H_2 (H_2-TPR) techniques respectively. Additionally, scanning electron microscopy (SEM) was performed for the $SrCo_{0.95}Mo_{0.05}O_{3-\delta}$ sample in order to study its morphology.

The $SrCo_{0.95}Mo_{0.05}O_{3-\delta}$ sample synthesized by the addition of a non-stoichiometric amount of glycine, was able to stabilize the desired tetragonal phase as shown in Fig. 1. On the other hand, the undoped $SrCoO_{3-\delta}$ sample showed the typical hexagonal structure corresponding to the *R32* space group. Samples containing $0.1 \le x \le 1$ Mo, prepared in air flow at RT, presented two additional tetragonal phases (space groups: *I4/m* and $I4_1/a$), which correspond to the $Sr_2CoMoO_{6-\delta}$ double perovskite and the $SrMoO_4$ scheelite phase respectively, as depicted in Fig. 2. Recent research has shown that this double perovskite material can become a promising ceramic oxide for anode applications in IT-SOFC [2]. Samples calcinated in a 5 mol% H_2 in Ar flow (50 cm^3 (STP) min^{-1}) during the H_2-TPR experiments showed that, those with the lowest Mo content presented some reduction peaks at 275, 390 and 825 ºC; and the ones with the highest Mo content were partially reduced at 900 ºC. In the latter, a cubic phase was stabilized at RT (*Pm-3m* space group), which has been considered an ideal phase for its use as IT-SOFCs anode materials [3], meaning a big possibility to obtain other materials at intermediate Co/Mo compositions with optimal properties for IT-SSOFCs electrodes.

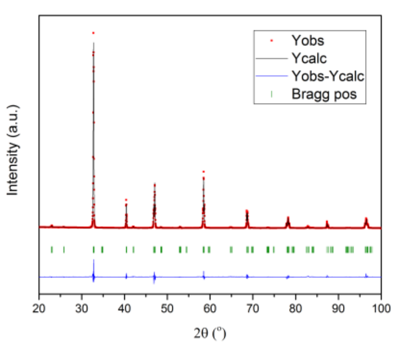

Figure. 1. Rietveld refinement for $SrCo_{0.95}Mo_{0.05}O_{3-\delta}$ in the *P4/mmm* space group.

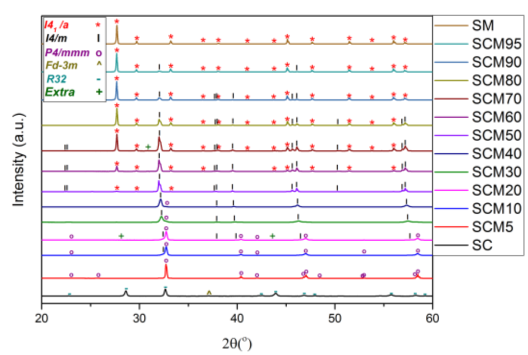

Figure. 2. XRD patterns for $SrCo_{1-x}Mo_xO_{3-\delta}$ ($0 \le x \le 1$) RT, air.

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