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Magnetic and crystallographic properties of the new $La_2SrCo_2FeO_9$ triple perovskite

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In this work, we report synthesis and characterization of the new $La_2SrCo_2FeO_9$ triple perovskite material. The samples were produced by the solid state reaction method from high purity precursor powders of La_2O_3, $SrCO_3$, Co_2O_3 and Fe_3O_4. The analysis of XRD patterns were made by Rietveld refinement through the GSAS code. The results reveal the presence of peaks, which are characteristics of the complex perovskite systems, and showed that $La_2SrCo_2FeO_9$ crystallizes in an orthorhombic structure, space group *Immm* (#71). The lattice parameters were a=5.4314(3) Å, b=5.4583(3) Å and c=7.7018(2) Å. The surface morphology was studied by scanning electron microscopy (SEM) and composition was analyzed using energy dispersive spectrometry (EDX). The SEM micrographs evidence a strongly diffused granular morphology with mean grain size of 2 μm and the EDX spectra show that the chemical composition of samples are in good agreement with the nominal values of the stoichiometric formula. Measurements of magnetization as a function of temperature permitted to determine the ferromagnetic characteristic of material with an effective magnetic moment of 9.7 μ_B, which are in agreement with the value calculated from the Hund's rule.

Keywords: Complex perovskite; magnetic properties; new material.

En el presente trabajo reportamos la síntesis y caracterización de la nueva perovskite triple $La_2SrCo_2FeO_9$. Las muestras fueron producidas mediante el método de reacción sólida a partir de óxidos precursores de alta pureza de La_2O_3, $SrCO_3$, Co_2O_3 y Fe_3O_4. La caracterización cristalográfica fue realizada a través de experimentos de rayos X con posterior análisis Rietveld de los patrones experimentales por medio del código GSAS. Los resultados muestran que el material cristaliza en una perovskite triple con estructura ortorrómbica perteneciente al grupo espacial *Immm* (#71) y parámetros de red a=5.458(8) Å, b=5.427(1) Å y c=7.688(9) Å. La morfología superficial fue estudiada mediante microscopía electrónica de barrido y la composición a través de dispersión de rayos X por electrones. A partir de mediciones de susceptibilidad magnética en función de la temperatura y de magnetización en función del campo magnético aplicado se determinó el carácter ferromagnético del material con un momento magnético efectivo de 9.7 μ_B, el cual está de acuerdo con los valores calculados a partir de la regla de Hund.

Descriptores: Perovskita compleja; propiedades magnéticas; nuevo material.

PACS: 71.15.Mb; 74.25.Ha

1. Introduction

Oxide materials, which belong to the perovskite family, have been extensively investigated in last decades, because small structural distortions, vacancies and compositional modifications can to induce a great variety of physical and chemical properties [1]. When ideal perovskite formula ABO_3 is changed to introduce different type of cations on the octahedral site of the primitive perovskite unit cell, the cationic ordering leads to a complex triple perovskite, which is identified by the $A_2A'B_2B'O_9$ formula. This circumstance permits to infer the possibility to produce new materials by the introduction of an alkaline or rare earth ion in the A, A' sites and transition metal ions in the B, B'. Depending on magnetic or electric characteristic of B and B', it is relatively easy to create new perovskite systems with half-metallic properties [2], magneto-electric response [3] or magnetic ordering [4], which offer promissory perspectives in the recent spintronics technology [5]. In order to analyze the possibility to create new magnetic perovskite materials, in this work we report the synthesis, the structural characterization and magnetic studies of the new ferromagnetic triple perovskite $La_2SrCo_2FeO_9$, which was idealizes as the introduction of a lanthanide ion in the A site, an alkaline earth in the A' and a mixture of two magnetic transition metals in the B and B' sites of $A_2A'B_2B'O_9$ formula, to construct a triple complex perovskite.

2. Experimental

The samples were synthesized by the solid state reaction recipe. The precursor powders La_2O_3, $SrCO_3$, Co_2O_3 and Fe_3O_4 (Aldrich 99.9%) were mixed in stoichiometric proportions according to the chemical formula $La_2SrCo_2FeO_9$. Mixture was ground to form a pellet and annealed at 1250°C for 12 hours. The samples were then regrinded, repelletized and sintered at 1250°C for 24 hours and 1350°C for 24 hours. X-Ray diffraction (XRD) experiment was performed by means a *PW1710* diffractometer with $\lambda_{CuK\alpha}$=1.54064 Å.

Rietveld refinement of diffraction pattern was made by the GSAS code [6]. Scanning Electron Microscopy (SEM) images were obtained by using a FEI QUANTA 200 microscopy, which has a system for Energy Dispersive X-ray (EDX) analysis. Field cooling measurements of susceptibility as a function of temperature and magnetization as a function of applied field were carried out by using a MPMS Quantum Design SQUID.

3. Results and discussion

The analysis of XRD pattern showed in Fig. 1 reveals the presence of characteristic peaks of complex perovskite systems. In Fig. 1, crosses represent the experimental data and line corresponds to simulated pattern by means of GSAS code. Base line is the difference between theoretical and experimental results. Rietveld refinement permitted to establish that this material crystallizes in a orthorhombic triple perovskite with space group *Immm* (#71) and lattice constants are$a$=5.4314(3) Å, b=5.4583(3) Å and c=7.7018(2) Å. These results are 99.78% in agreement with the theoretical values obtained from the Structure Prediction Diagnostic Software *SPuDS* [7], which predicts that lattice constants a=5.458(8) Å, b=5.427(1) Å and c=7.688(9) Å for the $La_2SrCo_2FeO_9$ material.

In Fig. 1, symbol represents experimental data, continuous line is the simulated refined diffractogram and line of bottom corresponds to difference between experimental and simulated patterns. Parameters of refinement are: R_F^2=2.67%; x^2=1.313; R_{WP}=3.82% and R_P=3.20%. The numeric results of the Rietveld analysis are shown in the Table I.

Surface morphology of $La_2SrCo_2FeO_9$ samples was studied by SEM images as shown in Fig. 2. Performed analysis reveals the occurrence of granular topology with different grain sizes. As observed in the microphotography, grains are strongly diffused between them, but great empty spaces appear too. It is important to notice that sample evidences a single type of grain.

TABLE I. Atomic positions and occupancy for the $La_2SrCo_2FeO_9$.

Ion	*x*	*y*	*z*	*Occupancy*
Sr	0.5000	0.0000	0.2476	0.3379
La	0.5000	0.0000	0.2476	0.6804
Co(1)	0.0000	0.0000	0.0000	0.6025
Fe(1)	0.0000	0.0000	0.0000	0.4371
Co(1)	0.5000	0.5000	0.0000	0.7491
Fe(2)	0.5000	0.5000	0.0000	0.2015
O(1)	0.2295	0.2809	0.0000	1.7620
O(2)	0.0000	0.0000	0.2509	1.3551

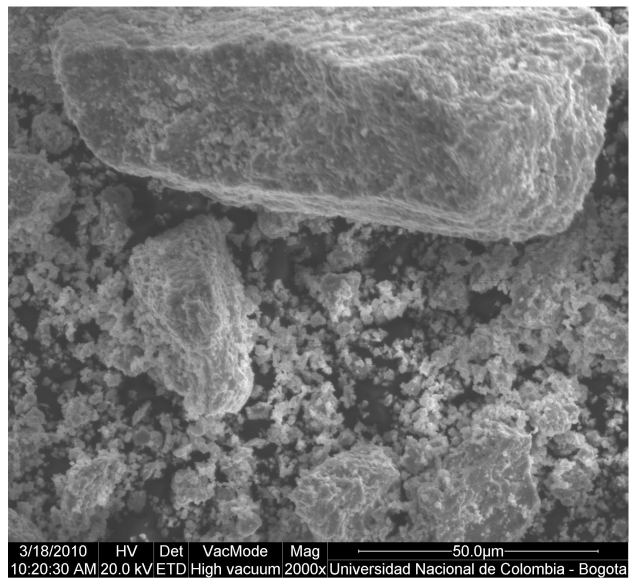

FIGURE 2. SEM micrography of $La_2SrCo_2FeO_9$ obtained from ETD detector (secondary electrons).

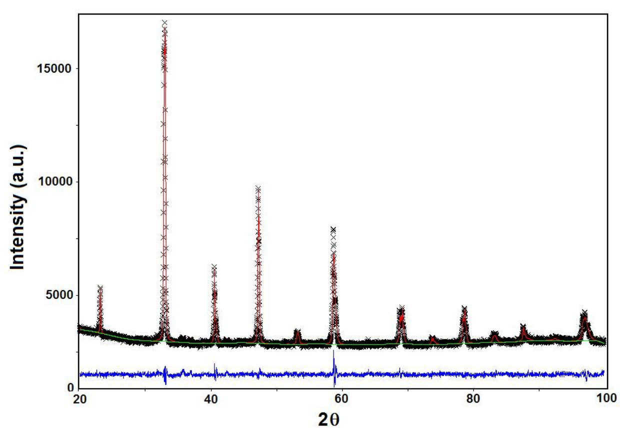

FIGURE 1. Characteristic XRD pattern for the triple perovskite $La_2SrCo_2FeO_9$. Symbols represent experimental diffraction data and base line is the difference between experimental and simulated patterns (continuous line).

From the EDX semi-quantitative analysis, which considers the spectrum areas for each element, we obtain the experimental composition of material. These values were compared with the theoretical composition, calculated from the $La_2SrCo_2FeO_9$ stoichiometric formula. Results are presented in Table II.

The results of Table II corroborate with 97% that there exists a single phase, which corresponds to the stoichiometry of $La_2SrCo_2FeO_9$. From structural, morphologic and compositional characterizations we deduced that no other crystallographic phases or impurities are present in the samples.

Magnetic properties of STMO have been investigated by measuring the DC susceptibility in the temperature range from 2 to 300 K and at an applied magnetic field of 50 Oe. Figure 3 shows the dependence of susceptibility as a function

TABLE II. Results of semi quantitative EDX analysis for $La_2SrCo_2FeO_9$ samples.

Atom	Theor. %Wt	Exper. %Wt
La	40.67	41.89
Sr	12.83	13.21
Co	17.25	17.77
Fe	8.17	8.41
O	21.08	18.72

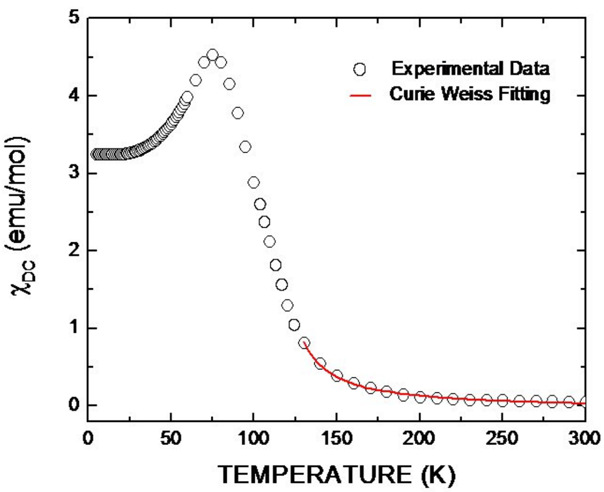

FIGURE 3. Magnetic behavior of $La_2SrCo_2FeO_9$ obtained from measurements of susceptibility as a function of temperature.

of temperature for $La_2SrCo_2FeO_9$ when it is measured using the Field Cooling recipe.

The fitting susceptibility as a function of temperature was made by the Curie Weiss equation,

$$\chi = \chi_0 + \frac{C}{T - T_C}, \tag{1}$$

which permitted to establish the ferromagnetic character of material with a Curie temperature $T_C = 123.3$ K, a Curie constant *C*=11.7438 emu.K/mol and a susceptibility independent of temperature of $\chi_0 = 2.56x10^{-2}$ emu/mol. From the Curie constant we obtain the effective magnetic moment of material μ_{eff}=9.7μ_B. Theoretical calculations by the Hund's rule, with $P_{eff} = g\sqrt{J(J+1)}$, predict that magnetic moments of the isolated ions Co^{4+} and Fe^{2+} must be μ_{Co}^{4+}=3.87μ_B and μ_{Fe}^{2+}=5.5μ_B, respectively [8]. The effective magnetic moment of $La_2SrCo_2FeO_9$ is obtained to be μ_{eff}=9.33μ_B, where we have used

$$\mu_{eff} = \sqrt{\mu^2_{Co^{4+}} + \mu^2_{Fe^{2+}}},$$

by considering two Co^{4+} cations in the crystallographic unit cell.

This result corresponds to 96% of agreement between experimental and theoretical values.

In order to verify the ferromagnetic behavior of the $La_2SrCo_2FeO_9$ triple perovskite, in figure 4 we show the curve of $1/\chi$ as a function of temperature. In the picture, the value of T_C is corroborated by the extrapolation of the high temperature linear-like behavior on the temperature axis.

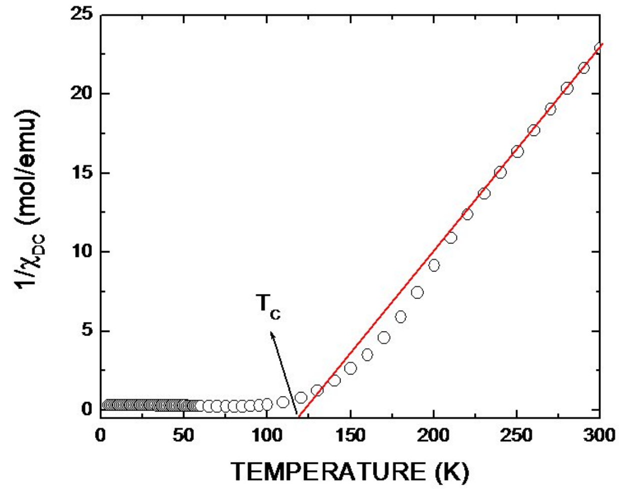

FIGURE 4. High temperature linear fit of $1/\chi$ as a function of temperature for $La_2SrCo_2FeO_9$.

4. Conclusions

The synthesis and structural characterization of the new $La_2SrCo_2FeO_9$ perovskite-like material was performed. The Rietveld analyses reveal that this material crystallizes in an orthorhombic complex perovskite which corresponds to *Immm* (#71) space group. Measurements of magnetic susceptibility showed a ferromagnetic ordering transition for a T_C= 123.3 K, which was fitted by the Curie Weiss model. From the fitting we obtain the magnetic moment of the unit cell to be μ=9.7μ_B.

Acknowledgments

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