STRUCTURAL, MAGNETIC, ELECTRIC AND ELECTRONIC BEHAVIOR OF Sr_2ZrMnO_6 DOUBLE PEROVSKITE

J. Roa-Rojas,[1]* J. Arbey Rodríguez M,[2] F. Fajardo,[2] D. Llamosa,[1] D. A. Landínez Téllez[1]

1. Grupo de Física de Nuevos Materiales, Departamento de Física, Universidad Nacional de Colombia, Bogotá DC, Colombia

2. Grupo de Estudios de Materiales - GEMA, Departamento de Física, Universidad Nacional de Colombia, Bogotá DC, Colombia

**jroar@unal.edu.co*

Abstract

We report synthesis, structural, electric and magnetic characterization, and *ab initio* calculations of electronic structure for the Sr_2ZrMnO_6 manganite-like material. Samples were produced by the solid state reaction method with sinterization temperatures up at 1400°C. X-ray diffraction experiments reveal that material crystallizes in a cubic double perovskite system, space group $Fm\bar{3}m$ (#225). Lattice parameter *a=7.840(1) Å* was obtain by means a Rietveld-type refinement, through the GSAS code. This value is 99% in agreement with the calculated result from Density Functional Theory (DFT), by using the an exchange correlation potential, which was treated from several approximations in the framework of local density approximation with B3PW91 potential correction (LDA+U) and the generalized gradient approximation (GGA) with spin polarization. Magnetic properties were studied by using a MPMS Quantum Design SQUID. From measurements of magnetization as a function of temperature, we determine the occurrence of a paramagnetic-antiferromagnetic transition with Néel temperature 50 K. Curie-Weiss fitting permitted to obtain the magnetic characteristic parameters. At temperature regimes below the Néel temperature, strong evidences of frustration and an irreversibility temperature between zero field cooling (ZFC) and field cooling (FC) measurements are observed. Frustration may be occurs as a consequence of cationic disorder of Zr and Mn in the structural sites of double perovskite cell. Curves of magnetization as a function of applied field were performed at T=4 K. Results show a hysteretic feature for Sr_2ZrMnO_6 magnetic material. This response is attributed to a possible antiferromagnetic canted ordering of magnetic spins, which give rise to an effective magnetization with the consequent hysteresis curve. From saturation magnetization and Curie-Weiss fitting we determine a magnetic moment of 0.8 μ_B, which is in accordance with the DFT calculated value. Electrical characterization was performed by the technique of Impedance Spectroscopy. Experimental data reveal the semiconducting behavior of Sr_2ZrMnO_6 material. Theoretical Density of States was analyzed for two (A and B) types of antiferromagnetic ordering. Results show that this magnetic material behaves as a semiconductor with a characteristic energy gap of 1.2 eV for both up and down spin polarizations.

This work was partially supported by the Division of Investigations, National University of Colombia (Bogotá DC) and Excellence Center of Novel Materials (CENM).