11th International Conference
on Advanced Materials
Rio de Janeiro Brazil
September 20 - 25
ICAM2009

Structural and morphological study of the double perovskite Sr_2DyRuO_6

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Abstract – In this work we report crystal structure and morphological characterization of Sr_2DyRuO_6 perovskite. These compounds sometimes show long range magnetic ordering at low temperature with transitions considered to be antiferromagnetic from large negative Weiss constant. However, previous works are limited to compounds in which the paramagnetic ions are only Ru^{5+} [1], but inclusion of another one like Dy^{3+} in their structure helps to improve the understanding of the magnetic properties on these perovskites. The Sr_2DyRuO_6 compound was prepared by the standard solid state reaction method, by firing the appropriate amounts of strontium carbonate $SrCO_3$, dysprosium oxide Dy_2O_3 and ruthenium dioxide RuO_2, at temperatures between 1173 K and 1273 K. We present experimental and theoretical results of the crystal structure. Rietveld refinement of experimental X-ray diffraction patterns shows that material crystallizes in a monoclinic structure [2], which belongs to the P2/c (#14) space group, with lattice parameters: a = 5.5768 Å, b = 5.7778 Å, c = 8.1768 Å and β = 90.180. Morphological characterization was performed by scanning electron microscopy (SEM) revealing a~5μm grain size. Calculations of electronic structure were performed by the Density Functional Theory. The exchange and correlation potentials were included through the LDA+U approximation. Density of states (DOS) study was carried out considering the two spin polarizations and several types of antiferromagnetism. The spin-polarized DOS were obtained by using the experimental lattice constants obtained by Rietveld analysis. DOS results show that Ru and Dy are responsible for the magnetic character on the Sr2DyRuO6 perovskite.

[1] Yoshihiro Doi and Yukio Hinatsu, J. Phys. Condens. Matter **11** (1999) 4813–4820.
[2] Izumi F 1993 *The Rietveld Method* ed R A Young (Oxford: Oxford University Press) ch 13.