

**Structural analysis of polycrystalline hexagonal manganites of the type $R_{1-x}Sm_xMnO_3$
(R: Y, Yb, Ho)**

M. E. Bolívar^a e J. Roa-Rojas^b.

^a*Departamento de física, Universidade Federal de Minas Gerais, Belo Horizonte, Brasil.*

^b*Departamento de física, Universidad Nacional de Colombia, Bogotá, Colombia.*

Yttrium and rare earth manganites crystallize in two main symmetries: hexagonal and orthorhombic[1]. For ions with small atomic radii like Y, Yb and Ho the typical crystallization gives rise to crystal with hexagonal symmetry[2,3,4,5] and for Sm, which has a greater ionic radius, the crystallization gives rise to orthorhombic phase[6]. In this work we described the synthesis and structural characterization of the polycrystalline manganites $R_xSm_{1-x}MnO_3$ ($x=0, 0.25, 0.50, 0.75, 1$). The samples, prepared by a solid state reaction method, were characterized by X-ray diffraction (XRD). The Rietveld method was employed in the refinement of XRD results and revealed the effects of the presence of Sm into the pure structures; it was observed that the structure changes by the increase in degree of substitution, from the hexagonal ($P6_3cm$) to the orthorhombic perovskite ($Pnma$) evidencing crystallographic changes with orthorhombic trends for strong concentrations of Sm. These two types of ordering are found to coexist and affect one another, one important aspect is the increasing of the hexagonal to orthorhombic structure transition in the case of Holmium manganate, which may be caused by competing between the size of cations and its bonds.

- [1] Z. J. Huang, et al., *Phys. Rev. B*, **56**, 2623(1997).
- [2] H. L. Yakel, W. Koehler, et. al., *Acta Cryst*, **16**, 957 (1963).
- [3] M. Isobe et al., *Acta Cryst.* **C47**, 423 (1991).
- [4] S.C. Abrahams, *Acta Cryst.* **B57**, 485(2001).
- [5] B. B. Van Aken, A. Meetsma, and T. T. M. Palstra, *Acta Cryst*, **C57**, 230 (2001).
- [6] H.L. Yakel, *Acta Cryst*, **8**, 394(1955).