

Structural phase relations and ferroic properties of (x)BiFeO₃-(1-x)BaTiO₃ multiferroics ceramics

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Abstract – BiFeO₃ is a ferroelectric antiferromagnetic multiferroic material below ~ 370 °C. Its magnetic spiral structure leads to cancellation of net macroscopic magnetization and therefore a linear magnetoelectric effect can not be observed. However this macroscopic magnetization can be released by chemical substitutions. Structural and ferroic studies on solid solutions and ceramics of the(x) BiFeO₃ - (1-x) BaTiO₃ system, prepared by mechanosynthesis, were performed. The results point to the formation of perovskite structured materials with coexistence of R3c and Cm phases. A intrinsic correlation between the ferroic properties and structural parameters are observed.

Materials that are ferroelectric and present some kind of magnetic order in the same phase are called multiferroic magnetoelectric materials [1]. Due to they properties of switchable polarization and magnetization, they have become the focus of research with intuit of developing multifunctional devices. Although very few of these materials exist, once that ferroelectric and magnetic ordering are mutually exclusive, generally the ferroelectric order requires empty d orbitals for the off-center displacement of the B site in the perovskite structure and the magnetic order arise from partially filled d orbitals [1,2].

One of the most studied multiferroic material is the perovskite structured BiFeO₃ compound. Its ferroelectric and antiferromagnetic phase transition temperatures are well above room temperature, with a T_C nearby 750 °C [3] and a T_N around 370 C° [3, 4], which create possibilities for room temperature multifunctional devices. BiFeO₃ present a rhombohedrally distorted perovskite structure in the R3c space group, where ferroelectricity arises from the Bi 6s lone pair [1,2], while partially filled d orbitals of Fe lead to a G-type antiferromagnetic spin configuration showing an incommensurate cycloidal spin structure [4,5]. This magnetic structure leads to the cancelation of net macroscopic magnetization and also inhibits the linear magnetoelectric effect [2]. However chemical substitutions can release this macroscopic magnetization. In this work we present studies on BaTiO₃ substituted BiFeO₃ compositions, (x)BiFeO₃-(1-x)BaTiO₃, where the structure, Fig. 1, electrical and magnetic properties, Fig. 2, of the system were investigated as a function of the BaTiO₃ concentration. Our results point to the formation of perovskite structured materials with coexistence of rhombohedral (R3c) and monoclinic (Cm) space groups, which are directly related to the ferroic properties of solid solutions. A phase diagram based on the structural, magnetic and electrical properties is proposed for this system.

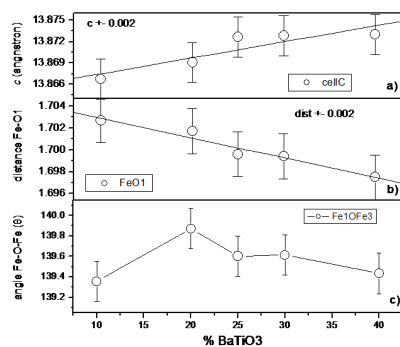


Figure 1 Calculated (Rietveld) structural parameters for (x)BiFeO₃ – (1-x)BaTiO₃ solid solutions as a function of the BaTiO₃ concentration. a) “c” lattice parameter b) Fe-O1 distance and c) Fe-O1-Fe angle.

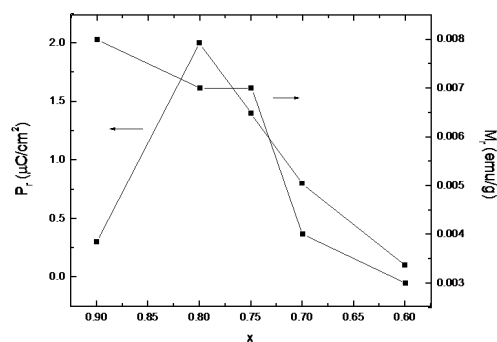


Figure 2 Remanent polarization, P_R, and remanent magnetization, M_R, for (x)BiFeO₃ – (1-x)BaTiO₃ solid solutions, as a function of BiFeO₃ concentration.

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