Crystal Structure and Physical Property of Tetragonal-like Epitaxial Bismuth Ferrites Film

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Basically, the lattice mismatch between film and substrate can make those $BiFeO_3$(BFO) films distorted with strain structure. BFO phase can be stabilized on $LaAlO_3$(LAO) represents the example of a multiferroic with giant axial ratio. Its crystal structure is not strictly tetragonal, but tetragonal with a slight monoclinic distortion and related to the rotation of the oxygen octahedra. In this study, we show that phases with a tetragonal-like epitaxial BFO films can indeed be ferroelectric and also can be stabilized via epitaxial growth onto LAO.

Recent reports on epitaxial BFO films show that the crystal structure changes from nearly rhombohedral ("R-like") to nearly tetragonal("T-like") at strains exceeding approximately -4.5%, with the "T-like" structure being characterized by a highly enhanced c/a ratio. While both the "R-like" and the "T-like" phases are monoclinic, our detailed x-ray diffraction results reveal asymmetry change from MA and MC type, respectively. By applying additional strain or by modifying the unit cell volume of the film by substituting Ba for Bi, the monoclinic distortion in the "T-like" MC phase is reduced, i.e. the system approaches a true tetragonal symmetry.

There are two different M-H loops for $Bi_{1-x}Ba_xFeO_{3-\delta}$(BBFO) and BFO films on $SrTiO_3$(STO) & LAO substrates. Along with the ferroelectric characterization, these magnetic data indicate that the BFO phase stabilized on LAO represents the first example of a multiferroic with giant axial ratio. However, there is a significant difference between this phase and other predicted ferroelectrics with a giant axial ratio: its crystal structure is not strictly tetragonal, but tetragonal with a slight monoclinic distortion. Therefore, in going from bulk to highly-strained films, a phase sequence of rhombohedral(R)-to-monoclinic ["R-like" M_A-to-monoclinic, "T-like" M_C-to-tetragonal (T)] is observed.

This sequence is otherwise seen only near morphotropic phase boundaries in lead-based solid-solution perovskites (i.e. near a compositionally induced phase instability), where it can be controlled by electric field, temperature, or composition. Our results show that this evolution can occur in a lead-free, stoichiometric material and can be induced by stress alone. Those major results are summarized as follows ; 1) Ba-doping increases the unit cell volume, 2) BBFO on LAO can be fully strained up to x=0.08 as a strain limit (Fig. 1), 3) P(E) & M(H) properties can be tuned by the variation of composition, strain, and film thickness.

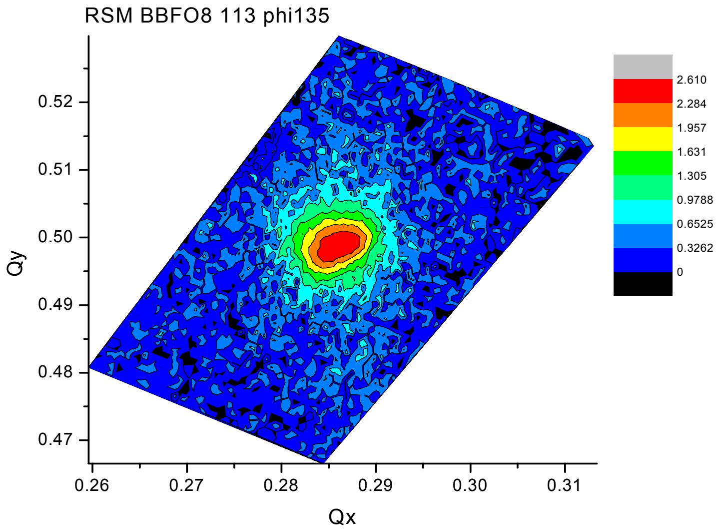

Fig. 1. Reciprocal space mapping of Bi1-xBaxFeO3-δ(x=0.08) film on LAO showing almost fully tetragonal structure.