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Strain-Induced Morphotropic Phase Boundary in Multiferroic BiFeO3 Thin Films

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Abstract

A morphotropic phase boundary driven by epitaxial strain has been observed in a lead-free multiferroic BiFeO3 thin films and the strain-driven phase transitions were widely reported to be iso-symmetric Cc-Cc ones by recent works. We suggest that the tetragonal-like BiFeO3 phase identified in epitaxial films on (001) LaAlO3 single crystal substrates is monoclinic MC. This MC phase is different from MA type monoclinic phase reported in BiFeO3 films grown on low mismatch substrates, such as SrTiO3. Our recent results also demonstrate that the mixed-phase regions are mainly made up of two highly tilted triclinic ferroelectric phases. The first principles studies reveal that the piezoelectric responses of these two lowest-symmetry phases are not significantly large, and further suggest that the ease of phase transition between these two energetically close triclinic phases is responsible for the large piezoelectric response in the BiFeO3 films near its MPB observed by recent experimental works such as: R. J. Zeches et al., Science 326, 977 (2009) and J. X. Zhang et al., Nat Nano 6, 98 (2011). Our findings not only enrich the understandings on the lattice and domain structure of epitaxial BiFeO3 films but also may shed light on the origin of enhanced piezoelectric response near MPB.

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