Abstract Submitted
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Phase Transitions in Epitaxial (-110) $BiFeO_3$ Films from First Principles*[1] SERGEY PROSANDEEV, University of Arkansas, IGOR KORNEV, Ecole Centrale Paris, LAURENT BELLAICHE, University of Arkansas — The effect of misfit strain on properties of epitaxial $BiFeO_3$ films that are grown along the pseudo-cubic $[\bar{1}10]$ direction, rather than along the "usual" [001] direction, is predicted from density functional theory. These films adopt the monoclinic Cc space group for compressive misfit strains smaller in magnitude than $\simeq$1.6% and for any investigated tensile strain. In this Cc phase, both polarization and the axis about which antiphase oxygen octahedra tilt rotate *within* the epitaxial plane as the strain varies. Surprisingly and unlike in (001) films, for compressive strain larger in magnitude than $\simeq$1.6%, the polarization vanishes and two orthorhombic phases of $Pnma$ and $P2_12_12_1$ symmetry successively emerge via strain-induced transitions. The $Pnma$-to-$P2_12_12_1$ transition is a rare example of a so-called pure "gyrotropic" phase transition, and the $P2_12_12_1$ phase exhibits original interpenetrated arrays of ferroelectric vortices and antivortices. This work is mostly supported by ONR Grants N00014-08-1-0915 and N00014-07-1-0825 (DURIP). *S. Prosandeev, Igor A. Kornev, and L. Bellaiche, Phys. Rev. Lett. 107, 117602 (2011).

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