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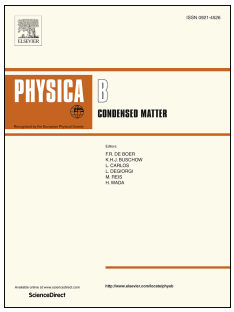

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Variation in Phase Diagrams of Strained (011) Epitaxial $BaTiO_3$ Thin Films

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Abstract

Phenomenological theory based on sixth-order and eighth-order potentials are used to investigate the effect of variation in free energy coefficients and material constants on phase stability of single-domain (011)-oriented epitaxial $BaTiO_3$ subject to both biaxial and uniaxial substrate constraints. Relative size of a variety of ferroelectric regions in the computed misfit strain phase diagrams is systematically examined. The computed Curie phase transition and subsequent polarization rotation and formation of low-symmetry monoclinic structures are dependent on the selection of potentials and variation in electrostrictive and elastic constants, and such dependence is found to be closely associated with in-plane strain anisotropy.

Keywords: phenomenological theory, ferroelectric thin films, phase transition, epitaxial strain

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