

CAN EPITAXIAL STRAIN STABILIZE A FERROELECTRIC SnTiO_3 ?

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INTRODUCTION

PbTiO_3 and its derivative compounds play a vital role as sensors, capacitors, actuators and transducers in a wide array of electronic devices because of their ferroelectric polarization. However, the toxicity of lead has motivated an active search for isovalent ferroelectric oxides free of these elements (1-4). Attempts to produce a SnTiO_3 substitute for PbTiO_3 have failed in bulk (1) and, in thin film by pulsed laser deposition, resulted in a nonpolar tin titanate of unclear stoichiometry (4). Calculations using quantum mechanics to predict crystalline properties (first-principles) of SnTiO_3 have focused on the perovskite structure of polar PbTiO_3 (1-3). The uncertainty cast on the nature of the ground state of SnTiO_3 by both calculations (5-6) and experiment (4) motivate a thorough investigation of potential crystalline polymorphs and the potential to stabilize a polar phase with epitaxy.

METHODOLOGY

Density functional theory with the local-density approximation for exchange and correlation calculates crystal phase properties. Plane-wave functions represent the electron density, and ultrasoft pseudopotentials replace the core-valence electron interaction.

RESULTS

After surveying Sn(II) titanates SnTiO_3 stoichiometry, we predict a tetragonal perovskite $P4mm$ phase with a large axial ratio ($c/a = 1.134$) and ferroelectric polarization (1.27 C/m^2) to be the ground state equilibrium structure. We also show that heteroepitaxial thin films of perovskite SnTiO_3 promote the stereochemical lone-pair activity and simultaneously enable control over the direction of the net electric polarization (see Figure 1) and magnitude of the electronic band gap. Finally, we examine the consequence of anisite defects on the polar cation displacements by studying the substitution of Sn on Ti-sites. We demonstrate that local metallic screening that results from site-substitution diminishes the magnitude of

the polar distortions but does not completely quench it. Based on these calculations, we suggest that polar perovskite SnTiO_3 ferroelectrics are viable thin film alternatives to Pb-containing oxides.

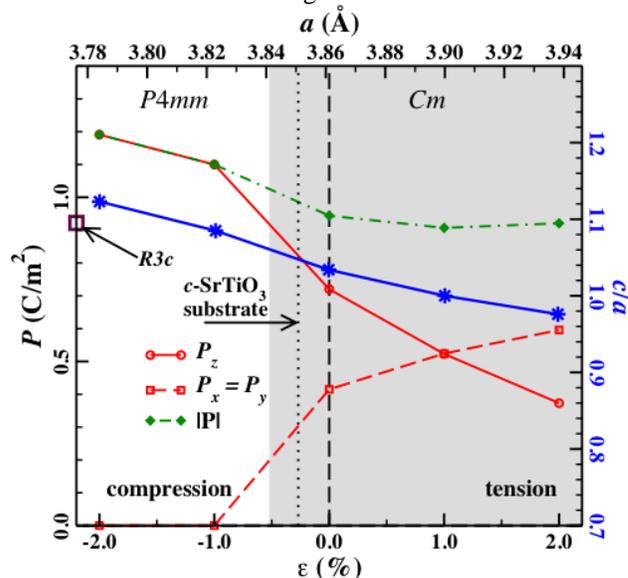


Figure 1: Polarization (P) and tetragonality (c/a) of SnTiO_3 under epitaxial strain (ϵ). In-plane (x-y) components of polarization appear under tension.

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