

Tilt transitions in Compressively Strained $\text{AgTa}_{0.5}\text{Nb}_{0.5}\text{O}_3$ Thin Films

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Abstract: Phase transitions in coherently strained epitaxial $\text{AgTa}_{0.5}\text{Nb}_{0.5}\text{O}_3$ films grown on SrTiO_3 (001) substrates were characterized by high-resolution x-ray diffraction and transmission electron microscopy. Coherently strained films were found to undergo the same phase transition sequence as bulk materials: cubic (C) \leftrightarrow tetragonal (T) \leftrightarrow orthorhombic (O) \leftrightarrow orthorhombic (M(3)). However, the compressive in-plane strain stabilized the tetragonal and orthorhombic phases, expanding these phase fields by approximate to 280 degrees C. The compressive strain state also favors c-axis domain texture. Consequently, unit cell quadrupling in the M(3) phase and the in-phase tilt of the T phase both occur around the out-of-plane direction. In contrast, bulk materials and relaxed films are polydomain, with the complex tilt system occurring along all three of the orthogonal axes. Compressively strained films are in the M(3) phase at room temperature rather than in the M(2) phase as is observed in bulk. This suggests that strain not only modifies octahedral rotations but may also disrupt the ordering of local cation displacements. These results demonstrate unambiguously that strain engineering in systems with complex tilt sequences such as $\text{AgTa}_{0.5}\text{Nb}_{0.5}\text{O}_3$ is feasible and open up the possibility of modifying properties by manipulation of the pertinent octahedral tilt transition temperature in a wide range of functional ceramics.

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