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Altered Phase Transitions in Strained Films of $SrTiO_3$

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Beamline(s): X22A

Introduction: Strains induced in thin films often cause to the nature of the phases present as well as the types of phase transitions. We have studied the strained films of $SrTiO_3$ (STO). This material is important for microwave applications as it has a large and tunable dielectric constant, though such properties are usually inferior in film structures. Bulk STO has a well-known cubic to tetragonal phase transition near 110 K. This phase transition is characterized by a change in lattice constant, as the sample becomes tetragonal and also new diffraction peaks connected with a rotation of TiO_6 octahedra. Thin films samples still have a transition with new diffraction peaks, though the transition temperature rises with amount of strain and any change in lattice constant is suppressed.

Methods and Materials: The samples were grown at Penn State University using pulsed laser deposition onto heated substrates. We have studied $SrTiO_3$ films in two types of structures; $SrTiO_3$ on a $LaAlO_3$ with a $SrRuO_3$ buffer layer (STO/SRO/LAO), $SrTiO_3$ on $LaAlO_3$ with no buffer layer (STO/LAO). X-ray diffraction measurements were conducted at beamline X22A. Particular attention was paid toward measurement of the lattice constants using grazing incidence diffraction and the intensity of the tetragonal superlattice peak.

Results: Samples with a thick SRO buffer layer have tensile strain, i.e. the in-plane lattice constant is larger than in the bulk. Samples without a buffer layer are compressively strained; the in-plane lattice constant is smaller than in the bulk. All of the samples showed a phase transition characterized by the appearance of a low temperature superlattice peak at half integer **q** values with respect to the perovskite high-temperature structure. The new peaks are the same as those that occur for the tetragonal phase in the bulk and are associated with a rotation of TiO_6 octahedra. The transition is not cubic to tetragonal since even at high temperature the structure is tetragonal due to substrate-induced strain. Figure 1 indicates the intensity of the superlattice peak with respect to temperature for samples of different thickness, and thus different amounts of strain. Very thick samples have little strain and a transition temperature very close to that in bulk STO. For thinner films, the strain increases to as much as 0.25% and show an increase in transition temperature of about 15 K. We find general agreement in the rise in transition temperature as a function of strain with theoretically predicted behavior by Pertsev et al. [1]. Several aspects of this phase transition are strange. For example, there appears to be no change in the temperature evolution of the lattice constants at the transition. Figure 2 shows this temperature evolution. This is a consequence of the clamping effect from the substrate, and remarkably endures even for films of thickness up to a micron.

Conclusions: The STO phase transition associated with a rotation of TiO_6 octahedra is substantially altered due to strains induced in thin films. The temperature of the phase transition is raised under either compressive or tensile strain, and there is no discontinuity in the temperature evolution of the lattice parameters.

References: N.A. Pertsev, A.K. Tagantsev, and N. Setter, Phys. Rev. B, **61**, R825, 2000

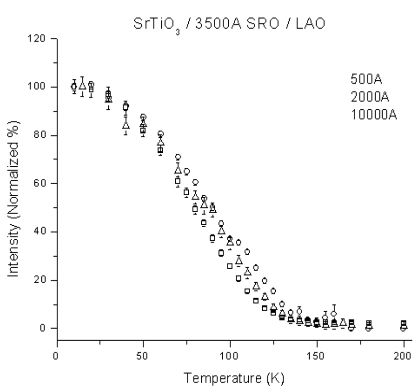

Fig. 1. Temperature dependence of the tetragonal superlattice peak for lightly strained films of $SrTiO_3$.

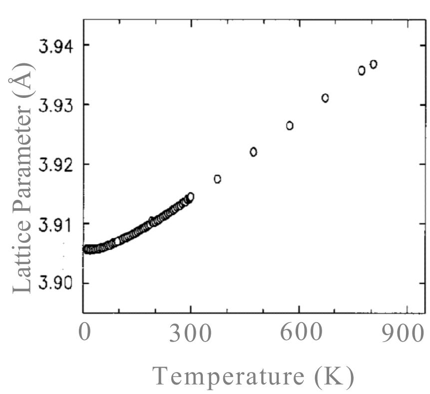

Fig. 2. Temperature dependence of the **c**-lattice parameter. The evolution is smooth through the phase transition near 120 K.