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Perovskite Thin Films Under Strain

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SrTiO₃ nanoscale films were studied as a model oxide film system. Highly strained films were grown on different substrates, resulting in either compressive or tensile strain. The measured strain-temperature phase diagram is qualitatively consistent with theory; however, the change in transition temperature is much larger than predicted. Further, the film is constrained because it is epitaxially clamped to the substrate, which causes the SrTiO₃ to be tetragonal at all temperatures. Therefore, the phase transition involves only a lowering of symmetry. This leads to the unique situation in which the low temperature phase under tensile strain has an orthorhombic Cmc space group but a tetragonal lattice, a situation not possible for bulk materials.

In epitaxial films only several nanometers thick, the film atoms tend to align with the underlying substrate atoms. If the lattice parameters of the film and substrate material are different, the film will be strained from its natural bulk atomic spacing. An important area of research in recent years has focused on understanding exactly why the properties of strained films differ from related bulk materials. An ultimate goal is to learn how to use these differences to enhance the performance of devices, or as a tool to probe the fundamental physics of materials with strong electron interactions.

The many fascinating properties of perovskite-related materials, such as ferroelectricity and high-temperature superconductivity, are particularly sensitive to strain. Our experiments used synchrotron x-ray scattering to investigate the structural phase transitions in very highly strained films of various perovskite-based film materials. Our main model system has been $SrTiO_3$, which has a well-known structural phase transition involving rotations of the internal TiO_6 octahedral, as shown in **Figure 1(a)**. In this case, the transition is from a high symmetry cubic phase at a high temperature to a lower symmetry tetragonal phase below the transition temperature. The structural phase transition in $SrTiO_3$ is monitored through the superlattice diffraction peaks associated with the low-temperature phase.

We produced $SrTiO_3$ films with different amounts and types (compressive or tensile) of strain by carefully growing them on different underlying crystals. Under compressive strain, the phase transitions in $SrTiO_3$ films go from a high-symmetry tetragonal structure to a low-symmetry tetragonal phase. Under tensile strain, the transition is from high-symmetry tetragonal to orthorhombic. The structural phase transition temperature T_s is enhanced under both compressive strain and tensile strain. The main difference between the two cases is that the orientation of the rotation axis is different for compressive strain and tensile strain, as illustrated in **Figure 1(b)**. A very similar effect happens to the spontaneous polarization in related ferroelectric films.

An interesting phenomenon in epitaxial films is that, although internally there are structural changes corresponding to the phase transitions, externally the dimensions of the unit cells do not change because of the strong bonding, or clamping, from the substrates. Therefore, the tetragonality of the unit cell,



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which is the secondary order parameter for bulk $SrTiO_3$, is no longer a good order parameter for phase transitions in films. The internal transitions without the external changes in the shapes of the unit cells create unique morphologies that are not possible in bulk materials. For example, the low-temperature phase in $SrTiO_3$ films under tensile strain has an orthorhombic space group ($Cmcm$) but a tetragonal lattice as a consequence of strain and substrate clamping.

The strain phase diagram based on our experimental data is compared with the theoretical calculations by Pertsev *et al*, shown in **Figure 2**. Many aspects of the strain-temperature phase diagram, such as the domain structures and the general trend of the phase boundary, are well described by current theory, though improvements are necessary to describe the magnitude of the increase in transition temperature.

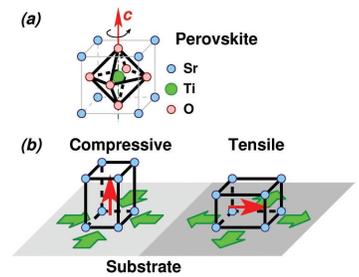


Figure 1. (a) Unit cell of $SrTiO_3$. The phase transition involves the rotation of internal TiO_6 octahedral. (b) The rotation axis of internal TiO_6 octahedral (red arrow) in $SrTiO_3$ oriented differently under compressive strain and tensile strain. The spontaneous polarizations in ferroelectric materials behave similarly.

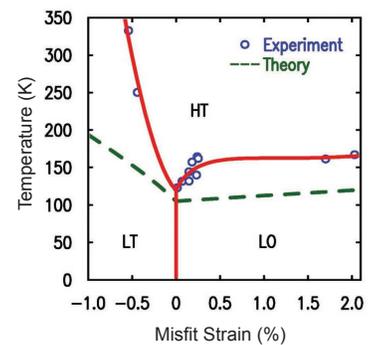


Figure 2. Strain-phase diagram for $SrTiO_3$ thin films. High-symmetry tetragonal, low-symmetry tetragonal, and orthorhombic phases are labeled HT, LT, and LO, respectively. For tensile strain, T_s increases rapidly over the small strain regime, then stabilizes at about 160–170 K for larger strain. Compressive strain induces a more dramatic effect. Only 0.5% compressive strain results in an increase in T_s of over 200 K versus the bulk value, nearing room temperature.