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Elastic anomalies accompanying phase transitions in (Ca,Sr)TiO_3 perovskites: Part III. Experimental investigation of polycrystalline samples

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Abstract

Bulk and shear moduli of polycrystalline samples of perovskites with different compositions across the $CaTiO_3$-$SrTiO_3$ solid solution have been measured at ambient conditions and in-situ at high pressures by pulse-echo ultrasonic methods. The samples were prepared as dense pellets by hot pressing synthetic powders at ~7.5 GPa and ~1000 °C. Any variations of bulk modulus due to phase transitions are small, but significant anomalies have been observed in the shear modulus at ambient conditions. These are associated with a sequence of symmetry changes $Pm\bar{3}m \rightarrow I4/mcm \rightarrow Pbcm \rightarrow Pnma$ with increasing $CaTiO_3$ content. Comparison with variations in elastic properties predicted using Landau theory suggests that a substantial part of the elastic softening observed in tetragonal samples could be due to anelastic contributions from transformation twin walls. This additional softening does not occur in orthorhombic samples, and the transition from tetragonal to orthorhombic symmetry results in a stiffening of the shear modulus. No overt evidence was found for a phase transition $I4/mcm \leftrightarrow Pnma$ at high pressures in $Ca_{0.35}Sr_{0.65}TiO_3$ but small changes in the trends of both bulk and shear moduli in the range 2.5–3 GPa could be due either to a different transition or a change in compression mechanism. A $Pm\bar{3}m \leftrightarrow I4/mcm$ transition at ~2 GPa in $Ca_{0.05}Sr_{0.95}TiO_3$ shows the same form of softening as observed for the transition as a function of composition. A simple model of twin wall contributions to the compliance of tetragonal samples failed to match the observed variations that, alternatively, seem to follow $\Delta G \propto q_4$ where ΔG is the change in shear modulus and q_4 the driving order parameter for the $Pm\bar{3}m \leftrightarrow I4/mcm$ transition. Analogous elastic behavior is expected to occur in (Mg,Fe)SiO_3 and $CaSiO_3$ perovskites at high pressures and temperatures.

Keywords: Elastic constants, phase transitions, $CaTiO_3$-$SrTiO_3$ solid solution, anelasticity