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Elastic anomalies accompanying phase transitions in $(Ca,Sr)TiO_3$ perovskites: Part II. Calibration for the effects of composition and pressure

MICHAEL A. CARPENTER*

Department of Earth Sciences, University of Cambridge, Downing Street, Cambridge CB2 3EQ, U.K.

ABSTRACT

A Landau free energy expansion has been developed in a first attempt to describe the $Pm\bar{3}m \leftrightarrow I4/mcm$ octahedral tilting transition in perovskite across a complete binary solid solution, $CaTiO_3$-$SrTiO_3$ (CST). Only two parameters, the critical temperature and the coefficient, λ_4, for coupling between the order parameter and the tetragonal strain are given a composition-dependence. The best match between observed and calculated variations of the tetragonal strain as a function of temperature in $CaTiO_3$ (CST0) and as a function of composition at room temperature is found for a model of the solid solution in which the transition is close to tricritical for the composition range CST0 to ~CST90. The change in transition character from second order (246 potential) to tricritical is accounted for by an increase in $|\lambda_4|$ between $SrTiO_3$ (CST100) and ~CST90. The Landau potential is used to calculate the variations of single-crystal and bulk elastic constants through the $Pm\bar{3}m \leftrightarrow I4/mcm$ transition as functions of both pressure and composition. This model for the CST solid solution permits the classical softening effects of strain/order parameter coupling to be separated quantitatively from the much larger superelastic softening observed for twinned crystals of tetragonal $SrTiO_3$ and CST. Data from the literature for relative changes of elastic properties measured at low frequencies have been rescaled to absolute values for comparison with calculated values of Young's modulus. These appear to show that, below the temperature for domain wall pinning, some 5–10% of softening of the isotropic Young's modulus could still be due to the effects of twin wall movements.

Keywords: Landau theory, elastic constants, phase transitions, $CaTiO_3$-$SrTiO_3$ solid solution