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Elastic anomalies accompanying phase transitions in (Ca,Sr)TiO_3 perovskites: Part I. Landau theory and a calibration for $SrTiO_3$

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ABSTRACT

Landau theory has been used to develop expressions for the elastic anomalies that accompany octahedral tilting transitions in perovskites that are associated with the M and R points of the Brillouin zone. The master equation is a 246 Landau potential with saturation terms that provides phenomenological descriptions of transition sequences from a parent cubic structure through tetragonal or rhombohedral intermediates to orthorhombic or monoclinic product structures. Data from the literature have been used to determine values for all the coefficients required to generate a quantitative description of the $Pm\bar{3}m \leftrightarrow I4/mcm$ transition in $SrTiO_3$, which is taken as a model system. Solutions to the Landau expansion have been adapted to include the general influence of hydrostatic pressure and non-hydrostatic stress on transition temperature and the evolution of the order parameter. Critical examination of elastic constant data from the literature reveals inconsistencies between the results of measurements on tetragonal samples using ultrasonic rather than Brillouin scattering methods. An internally consistent data set has, nevertheless, been assembled. Good qualitative agreement was obtained between the general pattern of calculated and observed variations of all the single crystal elastic constants, and semi-quantitative agreement was obtained for C_{11}, C_{33}, C_{12}, and C_{13}. Some inconsistencies remain in relation to the temperature dependence of the square of the soft mode frequencies in the tetragonal phase, which follow the square of the order parameter rather than its inverse susceptibility, but the 246 potential seems to provide a good description of the structural evolution of $SrTiO_3$ over a wide temperature interval up to the cubic-tetragonal transition point.

Keywords: Phase transitions, Landau theory, perovskite, $SrTiO_3$