

ERRATUM

Elastic anomalies accompanying phase transitions in (Ca,Sr)TiO₃ perovskites: Part I. Landau theory and a calibration for SrTiO₃ by Michael A. Carpenter (vol. 92, p. 309–327, 2007: DOI 10.2138/am.2007.2295).

Carpenter (2007a, 2007b) and Carpenter et al. (2007) used Landau theory to develop a general treatment for variations of elastic moduli that are expected to accompany structural phase transitions due to octahedral tilting in perovskites. The well-established concept is, first, that an externally applied stress induces a strain according to Hooke's law. If a phase transition can also occur, there may be an additional relaxation that is due to coupling of that strain with the order parameter for the transition. As a consequence, lowering of symmetry can be marked by substantial elastic softening. Possible space groups for silicate perovskites in the Earth's lower mantle include *I4/mcm* and *Pnma*, which are related by the development of order parameters belonging to M₃⁺ and R₄⁺ special points of the Brillouin zone of the parent *Pm3m* structure. In Carpenter (2007a), a single Landau free energy expansion was presented to describe phase transitions to these structure types as well as to related *P4/mbm* and *Imma* structures. The elastic moduli were derived from this by applying a simplified form of the original expression from Slonczewski and Thomas (1970):

$$C_{ik} = C_{ik}^o - \sum_m \frac{\partial^2 G}{\partial e_i \partial q_m} \left(\frac{\partial^2 G}{\partial q_m^2} \right)^{-1} \cdot \frac{\partial^2 G}{\partial e_k \partial q_m}. \quad (1)$$

Here, C_{ik} are elastic moduli of the low symmetry phase, C_{ik}^o are moduli of the parent, cubic phase, G is the Landau excess free energy due to the phase transition, e_i , e_k ($i, k = 1 - 6$) are spontaneous strains and q_m ($m = 1 - 3$) are components of the order parameter. This simplified form is adequate for many phase transitions in minerals (e.g., Carpenter and Salje 1998) but is incomplete for certain cases where the middle term is a matrix with non-zero off-diagonal terms. The expressions given in Tables 3 and 5 of Carpenter (2007a) for *Imma* and *Pnma* structures are incorrect because these off-diagonal terms were not included. The purpose of this erratum is to draw attention to this error and direct readers to the correct expressions, which are now given in McKnight et al. (2009).

The full expression of Slonczewski and Thomas (1970) is

$$C_{ik} = C_{ik}^o - \sum_{l,m} \frac{\partial^2 G}{\partial e_i \partial q_l} R_{lm} \cdot \frac{\partial^2 G}{\partial e_k \partial q_m} \quad (2)$$

where the matrix R_{lm} is the inverse of the matrix, $(\partial^2 G)/(\partial q_l \partial q_m)$, i.e.,

$$\sum_m R_{lm} \frac{\partial^2 G}{\partial q_m \partial q_n} = \delta_{ln}. \quad (3)$$

Equations 1 and 2 give the same result if R_{lm} contains only diagonal terms but, if it contains off-diagonal terms, Equation 2 must be used. Table 4 of McKnight et al. (2009) for the *Imma* perovskite structure should be used in place of Table 3 of Carpenter et al. (2007a), therefore, and Table 6 of McKnight et al. (2009) in place of Table 5 of Carpenter (2007a) for the *Pnma* structure. This correction does not affect any of the other results or conclusions given in Carpenter (2007a, 2007b) and Carpenter et al. (2007).

Finally, a couple of typographical errors have also been detected in Carpenter (2007a). The expression for C_{11} in Table 2 should be

$$C_{11} = C_{22} = C_{11}^o - M^2 \chi_4 q_4^2 \quad (4)$$

and the expression for G_V in Table 4 should be

$$G_V = \frac{1}{5} (C_{11}^o - C_{12}^o + 3C_{44}^o) - \frac{2}{5} (8\lambda_3^2 \chi_2 - 3\lambda_6 - 2\lambda_7) q_2^2. \quad (5)$$

This erratum comes with the apologies of the author.

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