APPENDIX A –
Landau Free-Energy Coefficients

Long-Qing Chen

Department of Materials Science and Engineering,
The Pennsylvania State University, University Park, Pennsylvania 16802 USA

The thermodynamics of ferroelectrics is usually described by the phenomenological Landau–Devonshire theory. Using the free energy for the unpolarized and unstrained crystal as the reference, the free energy of a ferroelectric crystal as a function of strain and polarization can be written as (see, e.g., [1])

$$F(\varepsilon, P) = \frac{1}{2}\alpha_{ij}P_iP_j + \frac{1}{3}\beta_{ijk}P_iP_jP_k + \frac{1}{4}\gamma_{ijkl}P_iP_jP_kP_l$$
$$+ \frac{1}{5}\delta_{ijklm}P_iP_jP_kP_lP_m + \frac{1}{6}\omega_{ijklmn}P_iP_jP_kP_lP_mP_n$$
$$+ \frac{1}{2}c_{ijkl}\varepsilon_{ij}\varepsilon_{kl} - a_{ijk}\varepsilon_{ij}P_k - \frac{1}{2}q_{ijkl}\varepsilon_{ij}P_kP_l + \cdots, \qquad (1)$$

where α_{ij}, β_{ijk}, γ_{ijkl}, δ_{ijklm}, and ω_{ijklmn} are the phenomenological Landau–Devonshire coefficients, and c_{ijkl}, a_{ijk}, and q_{ijkl} are the elastic, piezoelectric, and electrostrictive constant tensors, respectively. If the parent phase is centrosymmetrical, all odd terms are absent:

$$F(\varepsilon, P) = \frac{1}{2}\alpha_{ij}P_iP_j + \frac{1}{4}\gamma_{ijkl}P_iP_jP_kP_l + \frac{1}{6}\omega_{ijklmn}P_iP_jP_kP_lP_mP_n$$
$$+ \frac{1}{2}c_{ijkl}\varepsilon_{ij}\epsilon_{kl} - \frac{1}{2}q_{ijkl}\varepsilon_{ij}P_kP_l + \cdots. \qquad (2)$$

In (2), the set of coefficients, α, γ and ω, in the Helmholtz free energy correspond to those measured under a clamped boundary condition.

Under the stress-free boundary condition, the macroscopic shape change of a crystal due to the ferroelectric phase transition is described by the spontaneous strain that can be obtained through the derivative of the Helmholtz free energy (2) with respect to strain, i.e.,

$$\sigma_{ij} = c_{ijkl}\varepsilon^0_{kl} - \frac{1}{2}q_{ijkl}P_kP_l = 0. \qquad (3)$$

Solving (3) for strain, we have

$$\varepsilon^0_{kl} = \frac{1}{2}s_{ijkl}q_{klmn}P_mP_n = Q_{ijmn}P_mP_n, \qquad (4)$$

where s_{sijkl} is the elastic compliance tensor and

$$Q_{ijmn} = \frac{1}{2}s_{ijkl}q_{klmn}. \qquad (5)$$

Substituting the spontaneous strain (4) back into the free-energy expression (2), we have

$$G(P) = \frac{1}{2}\alpha_{ij}P_iP_j + \frac{1}{4}\left(\gamma_{ijkl} - \frac{1}{2}s_{mnor}q_{mnij}q_{orkl}\right)P_iP_jP_kP_l$$
$$+\frac{1}{6}\omega_{ijklmn}P_iP_jP_kP_lP_mP_n + \cdots, \tag{6}$$

or

$$G(P) = \frac{1}{2}\alpha_{ij}P_iP_j + \frac{1}{4}\left(\gamma_{ijkl} - 2c_{mnor}Q_{mnij}Q_{orkl}\right)P_iP_jP_kP_l$$
$$+\frac{1}{6}\omega_{ijklmn}P_iP_jP_kP_lP_mP_n + \cdots. \tag{7}$$

The fourth-order coefficients are different for the clamped (2) and stress-free (7) boundary conditions, and they are related by

$$\gamma'_{ijkl} = \gamma_{ijkl} - \frac{1}{2}s_{mnor}q_{mnij}q_{orkl} = \gamma_{ijkl} - 2c_{mnor}Q_{mnij}Q_{orkl}, \tag{8}$$

where γ'_{ijkl} is the fourth-order coefficient for the stress-free boundary condition. In general, experimentally determined coefficients correspond to γ' since it is usually easier to do measurements under stress-free boundary conditions.

In the following, the Landau–Devonshire coefficients are presented for a number of oxides, including the well-studied systems BaTiO$_3$, SrTiO$_3$ and PZT, collected from the open literature. All the data were provided for the stress-free boundary conditions unless noted otherwise. They are all in SI units with the temperature in K.

1 BaTiO$_3$

For BaTiO$_3$, a Landau–Devonshire potential up to eighth order has been employed,

$$G(P_x, P_y, P_z) = \alpha_1\left(P_x^2 + P_y^2 + P_z^2\right) + \alpha_{11}\left(P_x^4 + P_y^4 + P_z^4\right)$$
$$+\alpha_{12}\left(P_x^2P_y^2 + P_y^2P_z^2 + P_x^2P_z^2\right) + \alpha_{111}\left(P_x^6 + P_y^6 + P_z^6\right)$$
$$+\alpha_{112}\left[P_x^2\left(P_y^4 + P_z^4\right) + P_y^2\left(P_x^4 + P_z^4\right) + P_z^2\left(P_x^4 + P_y^4\right)\right]$$
$$+\alpha_{123}P_x^2P_y^2P_z^2 + \alpha_{1111}\left(P_x^8 + P_y^8 + P_z^8\right)$$
$$+\alpha_{1112}\left[P_x^6\left(P_y^2 + P_z^2\right) + P_y^6\left(P_x^2 + P_z^2\right) + P_z^6\left(P_x^2 + P_y^2\right)\right]$$
$$+\alpha_{1122}\left(P_x^4P_y^4 + P_y^4P_z^4 + P_x^4P_z^4\right)$$
$$+\alpha_{1123}\left(P_x^4P_y^2P_z^2 + P_y^4P_z^2P_x^2 + P_z^4P_x^2P_y^2\right). \tag{9}$$

Two sets of coefficients for (9) are given in Table 1. The elastic and electrostrictive coefficients are listed separately in Table 2. The free energy under

Table 1. Landau–Devonshire potential coefficients for BaTiO$_3$ (SI units and T in K)

Coefficients	Sixth order [2, 3]	Eight-order [4]
$\alpha_1(10^5\,\mathrm{C}^{-2}\cdot\mathrm{m}^2\cdot\mathrm{N})$	$3.34(T-381)$	$4.124(T-388)$
$\alpha_{11}(10^6\,\mathrm{C}^{-4}\cdot\mathrm{m}^6\cdot\mathrm{N})$	$4.69(T-393)-202$	-209.7
$\alpha_{12}(10^8\,\mathrm{C}^{-4}\cdot\mathrm{m}^6\cdot\mathrm{N})$	3.23	7.974
$\alpha_{111}(10^7\,\mathrm{C}^{-6}\cdot\mathrm{m}^{10}\cdot\mathrm{N})$	$-5.52(T-120)+276$	129.4
$\alpha_{112}(10^9\,\mathrm{C}^{-6}\cdot\mathrm{m}^{10}\cdot\mathrm{N})$	4.47	-1.950
$\alpha_{123}(10^9\,\mathrm{C}^{-6}\cdot\mathrm{m}^{10}\cdot\mathrm{N})$	4.919	-2.5009
$\alpha_{1111}(10^{10}\mathrm{C}^{-8}\cdot\mathrm{m}^{14}\cdot\mathrm{N})$	0.0	3.863
$\alpha_{1112}(10^{10}\mathrm{C}^{-8}\cdot\mathrm{m}^{14}\cdot\mathrm{N})$	0.0	2.529
$\alpha_{1122}(10^{10}\mathrm{C}^{-8}\cdot\mathrm{m}^{14}\cdot\mathrm{N})$	0.0	1.637
$\alpha_{1123}(10^{10}\mathrm{C}^{-8}\cdot\mathrm{m}^{14}\cdot\mathrm{N})$	0.0	1.367

Table 2. Elastic and electrostrictive coefficients of BaTiO$_3$ [1, 3, 5–9]. (Note that additional data on the elastic constants of BaTiO$_3$ can be found in [1] and [8])

$c_{11}(10^{11}\,\mathrm{N}\cdot\mathrm{m}^{-2})$	1.78
$c_{12}(10^{11}\,\mathrm{N}\cdot\mathrm{m}^{-2})$	0.964
$c_{44}(10^{11}\,\mathrm{N}\cdot\mathrm{m}^{-2})$	1.22
$Q_{11}(\mathrm{C}^{-2}\cdot\mathrm{m}^4)$	$0.10,\ 0.11$
$Q_{12}(\mathrm{C}^{-2}\cdot\mathrm{m}^4)$	$-0.034,\ -0.045$
$Q_{44}(\mathrm{C}^{-2}\cdot\mathrm{m}^4)$	$0.029,\ 0.059$

a constant strain, ε, can be easily obtained from the above stress-free free energy through

$$F(P,\varepsilon) = G(P,\sigma=0) + \frac{1}{2}c_{ijkl}\left(\varepsilon_{ij}-\varepsilon_{ij}^0\right)\left(\varepsilon_{kl}-\varepsilon_{kl}^0\right), \tag{10}$$

where ε_{ij}^0 is given by (4).

2 SrTiO$_3$

To describe both the proper ferroelectric and the antiferroelastic distortion (AFD) structural transition in SrTiO$_3$ requires both the spontaneous polarization $P = (P_x, P_y, P_z)$ and the structural order parameter $\mathbf{q} = (q_1, q_2, q_3)$ as the order parameters.

The structural order parameter represents the linear oxygen displacement that corresponds to simultaneous out-of-phase rotations of oxygen octahedra around one of their four-fold symmetry axes. A fourth-order Landau polyno-

mial as a function of the polarization and structural order parameter is given by

$$G(P_i, q_i) = A_{ij}P_iP_j + A_{ijkl}P_iP_jP_kP_l + B_{ij}q_iq_j$$
$$+B_{ijkl}q_iq_jq_kq_l + C_{ijkl}P_iP_jq_kq_l \,, \tag{11}$$

where $i, j = x, y, z$, A_{ijkl}, B_{ijkl} and C_{ijkl} are constants and A_{ij} and B_{ij} are functions of temperature. Keeping only the terms allowed by the cubic symmetry of the $SrTiO_3$ crystal, one has

$$G = \alpha_1 \left(P_x^2 + P_y^2 + P_z^2 \right) + \alpha_{11} \left(P_x^4 + P_y^4 + P_z^4 \right)$$
$$+\alpha_{12} \left(P_x^2 P_y^2 + P_y^2 P_z^2 + P_x^2 P_z^2 \right) + \beta_1 \left(q_x^2 + q_y^2 + q_z^2 \right)$$
$$+\beta_{11} \left(q_x^4 + q_y^4 + q_z^4 \right) + \beta_{12} \left(q_x^2 q_y^2 + q_y^2 q_z^2 + q_x^2 q_z^2 \right)$$
$$-t_{11} \left(P_x^2 q_x^2 + P_y^2 q_y^4 + P_z^2 q_z^2 \right)$$
$$-t_{12} \left[P_x^2 \left(q_y^2 + q_z^2 \right) + P_y^2 \left(q_x^2 + q_z^2 \right) + P_z^2 \left(q_x^2 + q_y^2 \right) \right]$$
$$-t_{44} \left(P_x P_y q_x q_y + P_y P_z q_y q_z + P_z P_x q_z q_x \right), \tag{12}$$

where α_{ij}, β_{ij}, and t_{ij} are assumed to be constants and α_1 and β_1 depend on temperature.

ε_{ij}^0 is the stress-free strain or the transformation strain as a result of the structural and/or ferroelectric transitions,

$$\varepsilon_{ij}^0 = Q_{ijkl}p_kp_l + \Lambda_{ijkl}q_kq_l \,, \tag{13}$$

in which Q_{ijkl} and Λ_{ijkl} represent, respectively, the electrostrictive coefficient and the linear–quadratic coupling coefficient between the strain and structural order parameter.

3 PbZr$_{1-x}$Ti$_x$O$_3$ (PZT)

Existing experimental measurements in PZT have been fitted to a sixth-order polynomial:

$$G(P_x, P_y, P_z) = \alpha_1 \left(P_x^2 + P_y^2 + P_z^2 \right) + \alpha_{11} \left(P_x^4 + P_y^4 + P_z^4 \right)$$
$$+\alpha_{12} \left(P_x^2 P_y^2 + P_y^2 P_z^2 + P_x^2 P_z^2 \right) + \alpha_{111} \left(P_x^6 + P_y^6 + P_z^6 \right)$$
$$+\alpha_{112} \left[P_x^2 \left(P_y^4 + P_z^4 \right) + P_y^2 \left(P_x^4 + P_z^4 \right) + P_z^2 \left(P_x^4 + P_y^4 \right) \right]$$
$$+\alpha_{123} P_x^2 P_y^2 P_z^2 \,. \tag{14}$$

Table 3. Landau–Devonshire coefficients for SrTiO$_3$ (SI units and T in K) [10–15]

$\alpha_1 (10^5 \, \mathrm{C}^{-2} \cdot \mathrm{m}^2 \cdot \mathrm{N})$	$405 \left[\coth(54/T) - \coth(54/30) \right]$
	$263.5 \left[\coth(42/T) - 0.90476 \right], T < 50 \, \mathrm{K}$
	$7.37(T - 28), T > 70 \, \mathrm{K}$
	$7.06(T - 35.5), T > 100 \, \mathrm{K}$
$\alpha_{11} (10^9 \, \mathrm{C}^{-4} \cdot \mathrm{m}^6 \cdot \mathrm{N})$	1.70
$\alpha_{12} (10^9 \, \mathrm{C}^{-4} \cdot \mathrm{m}^6 \cdot \mathrm{N})$	1.37
$Q_{11} \, (\mathrm{C}^{-2} \cdot \mathrm{m}^4)$	$0.0457, 0.08, 0.066$
$Q_{12} \, (\mathrm{C}^{-2} \cdot \mathrm{m}^4)$	$-0.0135, -0.015, -0.013$
$Q_{44} \, (\mathrm{C}^{-2} \cdot \mathrm{m}^4)$	0.00957
$c_{11} \, (10^{11} \, \mathrm{N} \cdot \mathrm{m}^{-2})$	$3.156, 3.181, 3.36, 3.48$
$c_{12} \, (10^{11} \, \mathrm{N} \cdot \mathrm{m}^{-2})$	$1.01, 1.025, 1.027, 1.07$
$c_{44} \, (10^{11} \, \mathrm{N} \cdot \mathrm{m}^{-2})$	$1.19, 1.215, 1.236, 1.27$
$\beta_1 \, (10^{29} \, \mathrm{N} \cdot \mathrm{m}^{-4})$	$1.32 \left[\coth(145/T) - \coth(145/105) \right]$
$\beta_{11} \, (10^{50} \, \mathrm{N} \cdot \mathrm{m}^{-4})$	$1.69, 1.58, 1.20, 0.996$
$\beta_{12} \, (10^{50} \, \mathrm{N} \cdot \mathrm{m}^{-6})$	$3.88, 3.78, 2.88, 2.73$
$\Lambda_{11} 10^{18} \, \mathrm{m}^{-2}$	$8.7, 14.7, 9.32, 8.35$
$\Lambda_{12} 10^{18} \, \mathrm{m}^{-2}$	$-7.8, -7.34, -6.4, -5.54$
$\Lambda_{44} 10^{18} \, \mathrm{m}^{-2}$	$-9.2, -9.88, -6.93, -7.56$
$t_{11} \, (10^{29} \, \mathrm{C}^{-2} \cdot \mathrm{N})$	$-1.74, -2.10$
$t_{12} \, (10^{29} \, \mathrm{C}^{-2} \cdot \mathrm{N})$	$-0.755, -0.845$
$t_{44} \, (10^{29} \, \mathrm{C}^{-2} \cdot \mathrm{N})$	5.85

The corresponding Landau–Devonshire and electrostrictive coefficients are given by [16–20]

$$\alpha_1 = (T - T_0)/2\varepsilon_0 C_0, \varepsilon = 8.85 \times 10^{-12},$$

$$\alpha_{11} = (10.612 - 22.655x + 10.955x^2) \times 10^{13}/C_0,$$

$$\alpha_{111} = (12.026 - 17.296x + 9.179x^2) \times 10^{13}/C_0,$$

$$\alpha_{112} = (4.2904 - 3.3754x + 58.804e^{-29.397x}) \times 10^{14}/C_0,$$

$$\alpha_{12} = \eta_1/3 - \alpha_{11}, \alpha_{123} = \eta_2 - 3\alpha_{111} - 6\alpha_{112},$$

$$\eta_1 = \left[2.6213 + 0.42743x - (9.6 + 0.012501x) \, e^{-12.6x} \right] \times 10^{14}/C_0,$$

$$\eta_2 = \left[0.887 - 0.76973x + (16.225 - 0.088651x) \, e^{-21.255x} \right] \times 10^{15}/C_0,$$

$$T_0 = 462.63 + 843.4x - 2105.5x^2 + 4041.8x^3 - 3828.3x^4 + 1337.8x^5,$$

$$C_0 = \left(\frac{2.1716}{1 + 500.05(x - 0.5)^2} + 0.131x + 2.01 \right) \times 10^5, \text{ when } 0.0 \leq x \leq 0.5,$$

$$C_0 = \left(\frac{2.8339}{1 + 126.56(x - 0.5)^2} + 1.4132 \right) \times 10^5, \text{ when } 0.5 \leq x \leq 1.0,$$

$$Q_{11} = \frac{0.029578}{1 + 200(x - 0.5)^2} + 0.042796x + 0.045624,$$

$$Q_{12} = \frac{0.026568}{1 + 200(x - 0.5)^2} + 0.012093x - 0.013386,$$

$$Q_{44} = \frac{1}{2} \left(\frac{0.025325}{1 + 200(x - 0.5)^2} + 0.020857x + 0.046147 \right),$$

Table 4. The compliance tensor was estimated for a number of compositions [21]

Ti content x	0.4	0.5	0.6	0.7	0.8	0.9
s_{11} $(10^{-12}\,\mathrm{m}^2/\mathrm{N})$	8.8	10.5	8.6	8.4	8.2	8.1
s_{12} $(10^{-12}\,\mathrm{m}^2/\mathrm{N})$	-2.9	-3.7	-2.8	-2.7	-2.6	-2.5
s_{44} $(10^{-12}\,\mathrm{m}^2/\mathrm{N})$	24.6	28.7	21.2	17.5	14.4	12

Table 5. Landau–Devonshire potential coefficients for $\mathrm{PbTiO_3}$ (SI units and T in K) [16, 22]

$\alpha_1(10^5\,\mathrm{C}^{-2}\cdot\mathrm{m}^2\mathrm{N})$	$3.8(T-752)$	Q_{11} $(\mathrm{C}^{-2}\cdot\mathrm{m}^4)$	0.089
$\alpha_{11}(10^8\,\mathrm{C}^{-4}\cdot\mathrm{m}^6\mathrm{N})$	-0.73	Q_{12} $(\mathrm{C}^{-2}\cdot\mathrm{m}^4)$	-0.026
$\alpha_{12}(10^8\,\mathrm{C}^{-4}\cdot\mathrm{m}^6\mathrm{N})$	7.5	Q_{44} $(\mathrm{C}^{-2}\cdot\mathrm{m}^4)$	0.0675
$\alpha_{111}(10^8\,\mathrm{C}^{-6}\cdot\mathrm{m}^{10}\mathrm{N})$	2.6	s_{11} $(\mathrm{C}^{-12}\cdot\mathrm{m}^2/\mathrm{N})$	8.0
$\alpha_{112}(10^8\,\mathrm{C}^{-6}\cdot\mathrm{m}^{10}\mathrm{N})$	6.1	s_{12} $(\mathrm{C}^{-12}\cdot\mathrm{m}^2/\mathrm{N})$	-2.5
$\alpha_{123}(10^8\,\mathrm{C}^{-6}\cdot\mathrm{m}^{10}\mathrm{N})$	-37	s_{44} $(\mathrm{C}^{-12}\cdot\mathrm{m}^2/\mathrm{N})$	9.0

where x is the mole fraction of $\mathrm{PbTiO_3}$ in PZT. The units are SI with the temperature in K. The elastic compliance values for a number of selected compositions were provided in [21] (Table 4).

4 PbTiO$_3$

For pure $\mathrm{PbTiO_3}$, the free-energy coefficients are given in Table 5.

5 LiTaO$_3$ and LiNbO$_3$

$\mathrm{LiNbO_3}$ and $\mathrm{LiTaO_3}$ belong to the $\bar{3}m$ point group. Denoting the crystallographic uniaxial directions as the z-axis, the free-energy expansion is given by [23]

$$
\begin{aligned}
F = &-\frac{\alpha_1}{2}P_z^2 + \frac{\alpha_2}{4}P_z^4 + \frac{\alpha_3}{2}\left(P_x^2 + P_y^2\right) + \beta_1\varepsilon_3^2 + \beta_2\left(\varepsilon_1 + \varepsilon_2\right)^2 \\
&+\beta_3\left[\left(\varepsilon_1 - \varepsilon_2\right)^2 + \varepsilon_6^2\right] + \beta_4\varepsilon_3\left(\varepsilon_1 + \varepsilon_2\right) + \beta_5\left(\varepsilon_4^2 + \varepsilon_5^2\right) \\
&+\beta_6\left[\left(\varepsilon_1 - \varepsilon_2\right)\varepsilon_4 + \varepsilon_5\varepsilon_6\right] + \gamma_1\left(\varepsilon_1 + \varepsilon_2\right)P_z^2 + \gamma_2\varepsilon_3P_z^2 \\
&+\gamma_3\left[\left(\varepsilon_1 - \varepsilon_2\right)P_yP_z + \varepsilon_6P_xP_z\right] + \gamma_4\left(\varepsilon_5P_xP_z + \varepsilon_4P_yP_z\right),
\end{aligned} \tag{15}
$$

where electrostriction terms that do not involve the primary z component of polarization have been ignored. The corresponding coefficients are given in Table 6 (noted that in this example, α_i are determined at constant zero strain rather than constant zero stress).

Table 6. Landau-Devonshire potential coefficients for LiTaO$_3$ and LiNbO$_3$ [23]

Coefficients	LiTaO$_3$	LiNbO$_3$
$\alpha_1(10^9\,\text{C}^{-2}\cdot\text{N}\cdot\text{m}^2)$	1.256	2.012
$\alpha_2(10^9\,\text{C}^{-2}\cdot\text{N}\cdot\text{m}^2)$	5.043	3.608
$\alpha_3(10^9\,\text{C}^{-2}\cdot\text{N}\cdot\text{m}^2)$	2.22	1.345
$\beta_1(10^{10}\,\text{N}\cdot\text{m}^{-2})$	13.55	12.25
$\beta_2(10^{10}\,\text{N}\cdot\text{m}^{-2})$	6.475	6.4
$\beta_3(10^{10}\,\text{N}\cdot\text{m}^{-2})$	4.925	3.75
$\beta_4(10^{10}\,\text{N}\cdot\text{m}^{-2})$	7.4	7.5
$\beta_5(10^{10}\,\text{N}\cdot\text{m}^{-2})$	4.8	3
$\beta_6(10^{10}\,\text{N}\cdot\text{m}^{-2})$	-1.2	0.9
$\gamma_1(10^9\,\text{C}^{-2}\cdot\text{N}\cdot\text{m}^2)$	-0.202	0.216
$\gamma_2(10^9\,\text{C}^{-2}\cdot\text{N}\cdot\text{m}^2)$	1.317	1.848
$\gamma_3(10^9\,\text{C}^{-2}\cdot\text{N}\cdot\text{m}^2)$	-2.824	-0.33
$\gamma_4(10^9\,\text{C}^{-2}\cdot\text{N}\cdot\text{m}^2)$	4.992	3.9

Table 7. Landau-Devonshire potential coefficients for SrBi$_2$Nb$_2$O$_9$ (E is Young's modulus and ν is Poisson's ratio) [24]

$\alpha_1(10^6\,\text{C}^{-2}\cdot\text{m}^2\cdot\text{N})$	$1.03(T-663)$	$Q_{11}(10^{-3}\,\text{C}^{-2}\cdot\text{m}^4)$	0.385
$\alpha_{11}(10^8\,\text{C}^{-4}\cdot\text{m}^6\cdot\text{N})$	-0.94	$Q_{12}(10^{-3}\,\text{C}^{-2}\cdot\text{m}^4)$	-0.04
$\alpha_{12}(10^8\,\text{C}^{-4}\cdot\text{m}^6\cdot\text{N})$	9.38	$Q_{44}(10^{-3}\,\text{C}^{-2}\cdot\text{m}^4)$	0.05
$\alpha_{111}(10^8\,\text{C}^{-6}\cdot\text{m}^{10}\cdot\text{N})$	11.8	$E(10^{-12}\,\text{m}^2/\text{N})$	0.29
$\alpha_{112}(10^8\,\text{C}^{-6}\cdot\text{m}^{10}\cdot\text{N})$	23.6	$\nu(10^{-12}\,\text{m}^2/\text{N})$	0.31

6 Sr$_{0.8}$Bi$_{2.2}$Ta$_2$O$_9$

For Sr$_{0.8}$Bi$_{2.2}$Ta$_2$O$_9$, the only existing Landau free-energy description is a single double-well potential [25],

$$F = -2.03 \times 10^5 (T - 620)P^2 + 3.75 \times 10^9 P^4\,, \tag{16}$$

where T is in K and F and P are in SI units.

7 SrBi$_2$Nb$_2$O$_9$

The thermodynamics of SrBi$_2$Nb$_2$O$_9$ ferroelectrics was modeled using the following free-energy function,

$$\begin{aligned}
G(P_x, P_y) = \alpha_1\left(P_x^2 + P_y^2\right) + \alpha_{11}\left(P_x^4 + P_y^4\right) + \alpha_{12}P_x^2 P_y^2 \\
+ \alpha_{111}\left(P_x^6 + P_y^6\right) + \alpha_{112}\left(P_x^2 P_y^4 + P_y^2 P_x^4\right)\,.
\end{aligned} \tag{17}$$

Due to the lack of experimental data in this system, many of the coefficients were estimated (Table 7).

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