1 Formulation of Problem

$$\frac{\partial \Phi}{\partial u_{ij}} = 0 \to u_{ij}[P] \to \frac{\partial \Phi}{\partial P_i} = 0 \to P_i[T] \tag{1}$$

The Free Energy is given below using a sixth order expansion of the polarization order parameter.

$$\begin{aligned}\Phi = {} & a_1\left(P_1^2+P_2^2+P_3^2\right)+a_{11}\left(P_1^4+P_2^4+P_3^4\right)+a_{12}\left(P_1^2P_2^2+P_3^2P_2^2+P_1^2P_3^2\right)+\\ & a_{111}\left(P_1^6+P_2^6+P_3^6\right)+a_{112}\left(P_1^4\left(P_2^2+P_3^2\right)+P_2^4\left(P_1^2+P_3^2\right)+P_3^4\left(P_2^2+P_1^2\right)\right)+a_{123}P_1^2P_2^2P_3^2+\\ & \frac{1}{2}c_{11}\left(u_1^2+u_2^2+u_3^2\right)+c_{12}\left(u_1u_2+u_3u_2+u_1u_3\right)+\frac{1}{2}c_{44}\left(u_4^2+u_5^2+u_6^2\right)-\\ & q_{11}\left(P_1^2u_1+P_2^2u_2+P_3^2u_3\right)-q_{12}\left(P_1^2\left(u_2+u_3\right)+P_3^2\left(u_1+u_2\right)+P_2^2\left(u_1+u_3\right)\right)-\\ & q_{44}\left(P_2P_3u_4+P_1P_3u_5+P_1P_2u_6\right)\end{aligned} \tag{2}$$

2 Strain Relations

The first derivative of the free energy gives the strain equilbrium conditions.

2.1 Tetragonal Phase

$$u_1 = Q_{11}P_1^2 + Q_{12}(P_2^2 + P_3^2) \tag{3}$$
$$u_2 = Q_{11}P_2^2 + Q_{12}(P_1^2 + P_3^2) \tag{4}$$
$$u_3 = Q_{11}P_3^2 + Q_{12}(P_1^2 + P_2^2) \tag{5}$$
$$u_4 = Q_{44}P_2P_3, \quad u_5 = Q_{44}P_1P_3, \quad u_6 = Q_{44}P_1P_2 \tag{6}$$

Where $Q_{11} = 0.1, Q_{12} = -0.045, Q_{44} = 0.029$

The renormalized coefficient is then

$$a'_{11} = a_{11} - \frac{1}{6}\left(\frac{2(q_{11}-q_{12})^2}{c_{11}-c_{12}} + \frac{(q_{11}+2q_{12})^2}{c_{11}+2c_{12}}\right) \tag{7}$$

Using the parameters from Bell and Cross

$$2^{nd} \text{ Term Correction} \propto 4.260 \times 10^7$$
$$a_{11} = -2.02 * 10^8 - 4.69 * 10^6(-393 + T) \tag{8}$$
$$a'_{11} = -2.44601 * 10^8 - 4.69 * 10^6(-393 + T) \tag{9}$$

The Polarization is then

$$P_3 = \sqrt{\frac{\sqrt{(a'_{11})^2 - 3a_1a_{111}} - a'_{11}}{3a_{111}}} \tag{10}$$

$$P_3^2 = \frac{\sqrt{(a'_{11})^2 - 3a_1a_{111}} - a'_{11}}{3a_{111}} \tag{11}$$

The polarization can be expressed by means of the unstrained solution with some perturbation from the elastic subsystem.

$$P_3' = P_0 + \delta P$$

$$a_{11}' = a_{11} + \delta \mathrm{A}$$

$$P_3' = \sqrt{\frac{\sqrt{(a_{11}')^2 - 3a_1 a_{111}} - a_{11}'}{3a_{111}}} \tag{12}$$

$$P_0 = \sqrt{\frac{\sqrt{(a_{11})^2 - 3a_1 a_{111}} - a_{11}}{3a_{111}}} \tag{13}$$

$$\delta P = P_3' - P_0 \tag{14}$$

$$\delta P = \frac{P_0 \delta \mathrm{A}}{2\sqrt{a_{11}^2 - 3a_1 a_{111}}} - \frac{\left(a_{11}^2 - \sqrt{a_{11}^2 - 3a_1 a_{111}}\, a_{11} + 3a_1 a_{111}\right) \delta \mathrm{A}^2}{8\left(\sqrt{3} a_{111} \left(a_{11}^2 - 3a_1 a_{111}\right)^{3/2} \sqrt{\frac{\sqrt{a_{11}^2 - 3a_1 a_{111}} - a_{11}}{a_{111}}}\right)} + O\left(\delta \mathrm{A}^3\right) \tag{15}$$

For temperatures within the Tetragonal Phase $283 < T < 393$ the correction of the polarization is minimal

$$\delta P|_{T=300} = P_0 * 0.0255407 + O\left(\delta \mathrm{A}^2\right) \tag{16}$$