Sample Ferroelectric Document

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1 Free Energy Analysis

The phase transistions of a bulk crystal of $BaTiO_3$ can be analyzed by studying the free energy and its successive derivatives. The equilibrium conditions can be determined by setting the first derivative equal to zero for each order parameter.

2 Equations Studied

2.1 Orthorhombic $BaTiO_3$

The Free Energy can be broken down into various subsections:

$$F_{Polar} = a_1 \sum_i P_i^2 + a_{11} \sum_i P_i^4 + a_{12} \sum_{i<j} P_i^2 P_j^2 \tag{1}$$

$$F_{Elastic} = \frac{1}{2} c_{11} \sum_i u_{ii} + c_{12} \sum_{i<j} u_{\mathrm{ii}} u_{jj} + + \frac{1}{2} c_{44} \sum_{ij} u_{\mathrm{ij}} \tag{2}$$

$$F_{Electrostriction} = -q_{11} \sum_i P_i^2 u_{\mathrm{ii}} - q_{12} \sum_{i \neq j \neq k} u_{\mathrm{ii}} \left(P_j^2 + P_k^2 \right) - q_{44} \sum_{i<j} P_i u_{\mathrm{ij}} P_j \tag{3}$$

$$F_{Gradient} = \frac{1}{2} g_{11} \sum_i P_{i,i}^2 + g_{12} \sum_{i<j} P_{i,i} P_{j,j} + \frac{1}{2} g_{44} \sum_{i<j} \left(P_{i,j} + P_{j,i} \right)^2 \tag{4}$$

The solutions for the orthorhombic phase of barium titanate have the following equlibrium solutions for the strain order parameter.

$$2 + 2 = 4 \tag{5}$$

Lets reference our first equation denoted by (5)

3 Conclusion