

Supplementary Information: Strain-engineered divergent electrostriction in KTaO_3

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THERMODYNAMICS OF INDIRECT ELECTROSTRICTIVE EFFECT

Electrostriction as stress/strain derivative of permittivity/dielectric susceptibility

To confirm the thermodynamic validity of the methodology we propose, we will derive it for the coefficients Q_{ijkl} . Start by considering the elastic Gibbs free energy for a bulk material:

$$G_1 = u - T.s - Xx \quad (1)$$

$$dG_1 = -s.dT - x_{kl}.dX_{kl} + E_i.dP_i \quad (2)$$

where u is the internal energy per unit volume (J/m^3), T the temperature (K), s the volume density of entropy (J/m^3), E the electric field (V/m), and P the polarisation (C/m^2). Taking first derivatives, and considering only electromechanical deformations, in linear dielectrics, we have:

$$\frac{\partial G_1}{\partial X_{ij}} = -x_{kl}; \quad x_{ij} = g_{ijk}P_k + Q_{ijkl}P_kP_l \quad (3)$$

$$\frac{\partial G_1}{\partial P_i} = -E_i; \quad E_i = \eta_{ij}P_j \quad (4)$$

Where η_{ij} is the dielectric stiffness. Now proceed to third derivatives by differentiating Eq. (3) by P_i followed by P_j :

$$\frac{\partial^3 G_1}{\partial P_j \partial P_i \partial X_{kl}} = -\frac{\partial^2 x_{kl}}{\partial P_j \partial P_i} = -2Q_{ijkl} \quad (5)$$

and differentiating Eq. (4) by P_j and X_{kl} :

$$\frac{\partial^3 G_1}{\partial X_{kl} \partial P_j \partial P_i} = \frac{\partial^3 G_1}{\partial X_{kl} \partial P_j \partial P_i} = \frac{\partial \eta_{ij}}{\partial X_{kl}} \quad (6)$$

G_1 being \mathcal{C}^∞ , by Schwarz's theorem, we have that Eq. (5)=Eq. (6) and the desired result, defining the converse electrostrictive effect:

$$-\frac{1}{2} \frac{\partial \eta_{ij}}{\partial X_{kl}} = Q_{ijkl} \quad (7)$$

The expressions for the other electrostrictive coefficients, q_{ijkl} , m_{ijkl} , and M_{ijkl} may be derived in a similar manner, but starting from the Helmholtz free energy, the electric Gibbs free energy, and Gibbs free energy, respectively.

Electrostriction from piezoelectric tensor and spontaneous polarisation

In a non-piezoelectric material at equilibrium, a strain will develop due to stresses, according to the elastic compliance, and due to polarisations, according to the electrostrictive Q tensor:

$$x_i = -s_{ij}X_j + Q_{ijmn}P_mP_n, \quad (8)$$

where Voigt notation has been used to simplify the tensors. Taking the derivative of this equation:

$$\frac{\partial x_i}{\partial P_m} = 2Q_{ijmn}P_n. \quad (9)$$

The left hand side of this equation defines the piezoelectric coefficient g_{mi} , meaning that a material which normally has zero piezoelectric coefficients will have finite ones if a polarisation is induced, which, in the case of this paper, by straining to the ferroelectric phase.



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