

## BASIC EQUATIONS FOR FERROELECTRICS

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### ABSTRACT

A set of new formula of energy functions for ferroelectrics was proposed, and then the new basic equations were derived in this paper. The finite element formulation based on the new basic equations was improved to avoid the equivalent nodal load produced by remnant polarization. With regard to the fundamentals of mathematics and physics, the new energy functions and basic equations are reasonable for the material element of ferroelectrics in finite element analysis.

**Key Words:** Ferroelectrics; Basic equations; Energy functions; FEM

### INTRODUCTION

Ferroelectrics have been used in smart structures such as sensors and actuators for their electromechanical behaviors. Experimental and theoretical studies have been devoted to their nonlinear constitutive behaviors due to domain switching. The theoretical models can fall into two classes-micromechanical and phenomenological [1,2]. The electromechanically coupled nonlinear behaviors have been simulated by the finite element method [3,4]. In the finite element calculation, the equivalent load induced by remnant polarization is too large to accomplish the calculation and must be omitted. Later, Li and Rajapakse [5] gave the detailed physical arguments. The depolarization field induced by polarization gradient is completely compensated by free charges for the charge-screening effect in real ceramics. The free charges are trapped by unbalanced polarization and turn into space charges, which cannot be driven by the applied loads unless the polarization switches. The space charges are released and move to the surface of the material when domain switching occurs. Furthermore, some current energy functions for ferroelectrics have been described and analyzed. It shows the energy functions should not be mathematically desirable.

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A set of new formula of energy function is proposed for ferroelectrics. The new basic equations derived by the new energy functions can successfully resolve the hurdle in the current finite element analysis of ferroelectrics.

## CURRENT BASIC EQUATIONS AND ENERGY FUNCTIONS

Using the current basic equations, one gives the following variational equation

$$\int_V \sigma_{ij} \delta \gamma_{ij} dV - \int_V D_k \delta E_k dV - \int_{S_a} \bar{t}_i \delta u_i dS + \int_{S_a} \bar{\omega} \delta \phi dS = 0 \quad (1)$$

where  $\sigma_{ij}$ ,  $\gamma_{ij}$ ,  $E_k$ ,  $D_k$ ,  $\bar{t}_i$  and  $\bar{\omega}$  are the stress tensor, strain tensor, electric field vector, electric displacement vector, prescribed traction and surface charge respectively.

Thus, the finite element formulation which is of displacement-electric potential type can be carried out. The generalized displacement  $\mathbf{u}$  can be interpolated from the generalized nodal displacement  $\mathbf{u}^N$  and the generalized interpolation matrix  $\mathbf{N}$

$$\mathbf{u} = [u_1 \ u_2 \ u_3 \ \phi]^T = \mathbf{N} \mathbf{u}^N \quad (2)$$

In the same way, the generalized strain and stress can be expressed as respectively

$$\boldsymbol{\Gamma} = [\gamma_{11} \ \gamma_{22} \ \gamma_{33} \ 2\gamma_{23} \ 2\gamma_{31} \ 2\gamma_{12} \ -E_1 \ -E_2 \ -E_3]^T = \mathbf{B} \mathbf{u}^N \quad (3)$$

$$\boldsymbol{\Sigma} = [\sigma_{11} \ \sigma_{22} \ \sigma_{33} \ \sigma_{23} \ \sigma_{31} \ \sigma_{12} \ D_1 \ D_2 \ D_3]^T = \mathbf{C} (\boldsymbol{\Gamma} - \boldsymbol{\Gamma}^s) + \mathbf{D}^s \quad (4)$$

where  $\mathbf{B}$ ,  $\mathbf{C}$ ,  $\boldsymbol{\Gamma}^s$  and  $\mathbf{D}^s$  are the generalized strain gradient matrix, stiffness matrix, remnant strain tensor and electric displacement tensor. Substituting Eq.(3) and (4) into (1), and we can get the following finite element equation in a discretized form

$$\int_V \mathbf{B}^T \mathbf{C} \mathbf{B} \mathbf{u}^N dV = \int_V \mathbf{B}^T \mathbf{C} \boldsymbol{\Gamma}^s dV - \int_V \mathbf{B}^T \mathbf{D}^s dV + \int_{S_a} \mathbf{N}^T \bar{\mathbf{T}} dS - \int_{S_a} \mathbf{N}^T \bar{\omega} dS \quad (5)$$

The second term on the right-hand side of Eq.(5) is the additional nodal load due to remnant polarization, represented by  $\mathbf{F}^s$ . One can carry out the finite element calculation based on Eq.(5). Unfortunately it is difficult to process the computation and the computation results are remarkably deviating from the experimental results. Li and Fang [4] neglect this term in their calculation because they believe that there could be some free charges to balance this term in real ceramics.

With regard to dielectric physics, the state of homogeneous elastic dielectrics can be described by three pairs of variables, strain  $\boldsymbol{\gamma}$  and stress  $\boldsymbol{\sigma}$ , electric displacement  $\mathbf{D}$  and electric field  $\mathbf{E}$  and entropy  $S$  and temperature  $T$ , then the internal energy density, electric enthalpy density and Gibbs free energy density of the system are respectively denoted by  $U$ ,  $W$  and  $G$ , which are given by [7]

$$U = \int TdS + \sigma_{ij}d\gamma_{ij} + E_k dD_k \quad (6)$$

$$W = U - E_k D_k \quad (7)$$

$$G = U - TS - \sigma_{ij}\gamma_{ij} - E_k D_k \quad (8)$$

The energy functions for ferroelectrics are the same as those for the dielectrics in the physical and mechanical communications. Neglecting heat effects, some energy functions for ferroelectrics can be described as

$$U = \frac{1}{2}\sigma_{ij}(\gamma_{ij} - \gamma'_{ij}) + \frac{1}{2}E_k(D_k - D'_k) \quad (9)$$

$$W = \frac{1}{2}\sigma_{ij}(\gamma_{ij} - \gamma'_{ij}) - \frac{1}{2}E_k(D_k + D'_k) \quad (10)$$

$$G = -\frac{1}{2}\sigma_{ij}(\gamma_{ij} + \gamma'_{ij}) - \frac{1}{2}E_k(D_k + D'_k) \quad (11)$$

The first term on the right-hand side of Eq.(10) includes  $\gamma_{ij} - \gamma'_{ij}$ , but the second includes  $D_k + D'_k$ . Apparently, the expression (10) for  $W$  is not symmetric in terms of mathematics. Likewise, the expression (11) for  $G$  is not desirable due to two terms  $\gamma_{ij} + \gamma'_{ij}$  and  $D_k + D'_k$ .

## NEW ENERGY FUNCTIONS AND BASIC EQUATIONS

When cooling through the Curie point, ferroelectrics undergo a phase transition. It results in a spontaneous polarization and spontaneous strain. Hence, without heat effects, the electric enthalpy density  $W$  and Gibbs free energy density  $G$  should be respectively defined by

$$W = U - E_k(D_k - D'_k) = \frac{1}{2}\sigma_{ij}(\gamma_{ij} - \gamma'_{ij}) - \frac{1}{2}E_k(D_k - D'_k) \quad (12)$$

$$G = U - \sigma_{ij}(\gamma_{ij} - \gamma'_{ij}) - E_k(D_k - D'_k) = -\frac{1}{2}\sigma_{ij}(\gamma_{ij} - \gamma'_{ij}) - \frac{1}{2}E_k(D_k - D'_k) \quad (13)$$

Eq.(12) and (13) satisfy the mathematical symmetric principle. Eq.(13) is the same as the one described by Elhadrouz et al.[8]. Without considering the body force and the free body charges, the potential energy  $\Psi$  can be modified as

$$\Psi = \int_V W dV - \int_{S_\sigma} \bar{t}_i u_i dS + \int_{S_\omega} \bar{\omega} \phi dS \quad (14)$$

Based on the principle of stationary potential energy, one can obtain the following new field equations and boundary conditions

$$\sigma_{0,j} = 0, \quad (D_i - D'_i)_j = 0 \quad (15)$$

$$\sigma_{ij} n_j = \bar{t}_i, \quad (D_i - D'_i) n_i = -\bar{\omega} \quad (16)$$

With regard to the constitutive law and Eq.(12), Eq.(14) can be written in a discrete form according to  $\delta\Psi = 0$ , then one can obtain the finite element equation is the same as Eq.(5) without  $\mathbf{F}'$ . It can mathematically confirm that the effect of remnant polarization doesn't exist really in the finite element formulation.

## CONCLUSIONS

This paper has carefully examined the problem in the finite element modeling of nonlinear behaviors of ferroelectrics and then has analyzed the cause of the problem according to the mathematical formula of the energy functions and basic equations. Therefore, this paper has proposed a set of new formula of energy functions based on the mathematical principle of symmetry and then has derived the corresponding basic equations. The new energy functions and basic equations can mathematically provide a reasonable interpretation.

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