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Full Length Article

The effect of flexoelectricity on domain switching in the vicinity of a crack in ferroelectrics

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ABSTRACT

Ferroelectrics are widely used in the manufacture of transducers, actuators, and memory devices, due to their attractive electromechanical properties. However, the reliability and failure of devices is greatly dependent on their brittleness. In view of the fact that both the polarization distribution and elastic field are at nanoscale and vary greatly in the vicinity of the crack tip, flexoelectricity is expected to strongly affect the domain configuration. In this work, Ginzburg-Landau (TDGL) theory and the phase field method (PFM) are employed to analyze the influence of flexoelectric effect on the domain switching process in the vicinity of the crack tip of ferroelectric materials. The results obtained show that, the domain configuration would become asymmetric with increasing flexoelectric coefficients, and the flexoelectric effect has a larger influence on the polarization field than on the elastic field in the vicinity of the crack tip of ferroelectric materials.

1. Introduction

Ferroelectrics are widely used for the manufacture of sensors, actuators and high-speed memory devices [1] due to their attractive electromechanical coupling properties. However, the brittleness nature of ferroelectrics makes them susceptible to failure arising from the electroelastic mechanism. There have been extensive theoretical [2–6] and experimental [7–10] studies carried out to investigate the fracture behavior of ferroelectrics and related materials, and lots of previous works indicate that fracture behavior of ferroelectric materials is a complicated process, and greatly related to the domain switching in the vicinity of the crack tip.

Flexoelectric effect is the coupling between electric polarization and mechanical strain gradients in dielectrics. Owing to its universal nature, flexoelectricity attracts broad scientific interest. Recent experimental discovery of large flexoelectric coefficients in nanoscale ferroelectric ceramics [11–14] attracts great interest from both theoretical research and potential application perspectives [15,16]. It has been proven that the inhomogeneous strain becomes appreciable at the nanoscale and it acts like an applied electric field, capable of poling [17], switching [18], and rotation of polarization [13]. Since it is a known fact that the electric and elastic fields are concentrated in the vicinity of the crack tip in ferroelectrics, ferroelastic switching and flexoelectric effects are expected to interact and influence the polarization distribution.

In recent years, the phase field simulation technique has become an increasingly important approach in the study of nonlinear behavior of ferroelectric ceramics [19–24]. The said technique has been successfully employed to investigate the stability and evolution of domain microstructures as well as the ferroelectric and piezoelectric properties of materials. However, the flexoelectric coupling characteristics was not considered within the conventional Ginzburg-Landau framework. With the development of nanoscale technology, the measurement and utilization of the flexoelectric effects have fascinated many researchers [25–27], and remarkable progress has been achieved in the study of the flexoelectric effect of ferroelectric materials using the phase field simulation technique [28–31]. Nevertheless, to the best of the authors' knowledge, to-date, researchers have paid very little attention to the effect of flexoelectricity on the fracture behavior of ferroelectric materials. Thus, a systematic study of the said effect and its mechanism on fracture behavior is needed for achieving a better understanding of the influence of flexoelectric effects on the domain configuration and switching behavior in the vicinity of a crack tip in ferroelectrics, which will be carried out in the present study by employing TDGL theory and PFM.

2. Simulation methodology

In the present study, the domain evolution of ferroelectrics subjected to mechanical tensile loading is investigated. With the

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consideration of flexoelectric effect, the Helmholtz free energy of a ferroelectric material can be expressed as follows [32]:

$$F = \int_V (f_b + f_g + f_{el} + f_{es} + f_{fl})dV \tag{1}$$

where f_b, f_g, f_{el}, f_{es} and f_{fl} is the energy density of the bulk free energy, the gradient energy, the electric energy, the elastic energy and the flexoelecric energy, respectively.

Assuming that the boundary conditions are periodic, for a cubic system, the bulk free energy density can be expressed as follows [33]:

$$\begin{aligned} f_b = {} & a_1(P_1^2 + P_2^2 + P_3^2) + a_{11}(P_1^4 + P_2^4 + P_3^4) + a_{12}(P_1^2P_2^2 + P_2^2P_3^2 + P_1^2P_3^2) \\ & + a_{111}(P_1^6 + P_2^6 \\ & + P_3^6) + a_{112}[P_1^4(P_2^2 + P_3^2) + P_2^4(P_1^2 + P_3^2) + P_3^4(P_1^2 + P_2^2)] \\ & + a_{123}P_1^2P_2^2P_3^2 \end{aligned} \tag{2}$$

where P_i is the i-th component of the polarization vector $\boldsymbol{P}(\boldsymbol{r})$ at site $\boldsymbol{r}$, $\alpha_1 = \alpha_0(T - T_0) = (T - T_0)/\kappa_0 C$. T_0 and C denotes the Curie temperature and Curie-Weiss constant, respectively. The other α_i, α_{ij}, and α_{ijk} are the dielectric stiffness and higher-order stiffness coefficient at constant stress.

The gradient energy density is given by [33]

$$\begin{aligned} f_g = {} & \tfrac{G_{11}}{2}(P_{1,1}^2 + P_{2,2}^2 + P_{3,3}^2) + G_{12}(P_{1,1}P_{2,2} + P_{1,1}P_{3,3} + P_{2,2}P_{3,3}) + \tfrac{G_{44}}{2}[(P_{1,2} + P_{2,1})^2 + (P_{2,3} + P_{3,2})^2 + (P_{1,3} + P_{3,1})^2] \\ & + \tfrac{G'_{44}}{2}[(P_{1,2} - P_{2,1})^2 + (P_{2,3} - P_{3,2})^2 + (P_{1,3} - P_{3,1})^2] \end{aligned} \tag{3}$$

where G_{11}, G_{12}, G_{44} and G'_{44} are the gradient coefficients, and $P_{i,j}$ denotes $\partial P_i/\partial r_j$.

The electrical energy density, including the contribution from the external electric field $\boldsymbol{E}^a$ and the depolarization field $\boldsymbol{E}^d$, can be expressed as follows [34]:

$$f_{el} = -P_i\left(E_i^a + \frac{E_i^d}{2}\right) \tag{4}$$

The depolarization field could be expressed as follows [35]:

$$\begin{aligned} \mathbf{E}^d = {} & -\frac{1}{4\pi\kappa_0\chi}\int\left\{\frac{\mathbf{P}(\boldsymbol{r}_j)}{|\boldsymbol{r}_i - \boldsymbol{r}_j|^3} \right. \\ & \left. - \frac{3(\boldsymbol{r}_i - \boldsymbol{r}_j)[\mathbf{P}(\boldsymbol{r}_j)\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j)]}{|\boldsymbol{r}_i - \boldsymbol{r}_j|^5}\right\}d^3\mathbf{r}_j \\ = {} & -\tfrac{1}{4\pi\kappa_0\chi}\int\left\{\mathbf{P}(\boldsymbol{r}_j)\left[\tfrac{1}{|\boldsymbol{r}_i - \boldsymbol{r}_j|^3} - \tfrac{3(\boldsymbol{r}_i - \boldsymbol{r}_j)\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j)}{|\boldsymbol{r}_i - \boldsymbol{r}_j|^5}\right]\right\}d^3\mathbf{r}_j \end{aligned} \tag{5}$$

where κ_0 and χ is the electric permittivity of free space and relative permittivity of the dielectric material, respectively.

In the present study, the condition is satisfied for the material parameters shown in Table 1. Therefore the gradient terms $v_{ijklmn}(\partial\varepsilon_{ij}/\partial x_k)(\partial\varepsilon_{lm}/\partial x_n)$ in the elastic energy can be neglected [36], and the elastic energy density can be expressed as [33]

Table 1
Material Parameters of $BaTiO_3$.

Coefficients	Values (collected mainly from Ref. [40,41])
χ	1100 [42]
α_i (C^{-2} m J)	$\alpha_1 = 3.34 \times 10^5 \times (T - 108)$
α_{ij} (C^{-4} m^5 J)	$\alpha_{11} = 4.69 \times 10^6 \times (T - 163)$, $\alpha_{12} = 3.23 \times 10^8$
α_{ijk} (C^{-6} m^9 J)	$\alpha_{111} = -5.52 \times 10^7 \times (T - 443)$, $\alpha_{112} = 4.47 \times 10^9$, $\alpha_{123} = 4.91 \times 10^9$
G_{ij} (10^{-11} C^{-2} m^3 J)	$G_{11} = 51$, $G_{12} = -2$, $G_{44} = 2$
q_{ij} (10^9 C^{-2} m J)	$q_{11} = 14.20$, $q_{12} = -0.74$, $q_{44} = 1.57$
C_{ij} (10^{10} N m^{-2})	$C_{11} = 27.50$, $C_{12} = 17.90$, $C_{44} = 5.43$
f_{ij}^0 (J C^{-1})	$f_{11} = -0.5338$, $f_{12} = -2.5714$, $f_{44} = -0.5230$ (recalculated from Ref. [39])

$$f_{es} = \frac{1}{2}C_{ijkl}e_{ij}e_{kl} = \frac{1}{2}C_{ijkl}(\varepsilon_{ij} - \varepsilon_{ij}^0)(\varepsilon_{kl} - \varepsilon_{kl}^0) \tag{6}$$

where C_{ijkl}, e_{ij}, ε_{ij}, and ε_{ij}^0 are the elastic stiffness, elastic strain, total strain, and eigenstrain, respectively. For ferroelectric materials, the eigenstrains, ε_{ij}^p, resulted from polarization can be expressed as,

$$\begin{aligned} \varepsilon_{11}^p(\mathbf{r}) &= Q_{11}P_1(\mathbf{r})^2 + Q_{12}(P_2(\mathbf{r})^2 + P_3(\mathbf{r})^2) \\ \varepsilon_{22}^p(\mathbf{r}) &= Q_{11}P_2(\mathbf{r})^2 + Q_{12}(P_1(\mathbf{r})^2 + P_3(\mathbf{r})^2) \\ \varepsilon_{33}^p(\mathbf{r}) &= Q_{11}P_3(\mathbf{r})^2 + Q_{12}(P_1(\mathbf{r})^2 + P_2(\mathbf{r})^2) \\ \varepsilon_{12}^p(\mathbf{r}) &= Q_{44}P_1(\mathbf{r})P_2(\mathbf{r}) \\ \varepsilon_{23}^p(\mathbf{r}) &= Q_{44}P_2(\mathbf{r})P_3(\mathbf{r}) \\ \varepsilon_{13}^p(\mathbf{r}) &= Q_{44}P_1(\mathbf{r})P_3(\mathbf{r}) \end{aligned} \tag{7}$$

where Q_{11}, Q_{12} and Q_{44} are the electrostrictive coefficients. By employing the method used by Jin et al. [37], the influence of crack on the mechanical system of a structure can be treated as eigenstrain in the crack area ε_{ij}^c. Therefore, the sum of the eigenstrains is given by

$$\varepsilon_{ij}^0(\mathbf{r}) = \varepsilon_{ij}^p(\mathbf{r}) + \varepsilon_{ij}^c(\mathbf{r}) \tag{8}$$

The flexoelectric energy density can be expressed as [38],

$$f_{fl} = \frac{f_{ijkl}}{2}\left(\varepsilon_{ij}\frac{\partial P_k}{\partial x_l} - \frac{\partial\varepsilon_{ij}}{\partial x_l}P_k\right) \tag{9}$$

where f_{ijkl} is the flexoelectric tensor. Note that the flexoelectric effect consists of both mechanical and electrical effects on the system. The induced electric field is given by:

$$E_i^{fl} = -\frac{\delta F_{fl}}{\delta P_i} = f_{ijkl}\frac{\partial\varepsilon_{kl}}{\partial x_j} \tag{10}$$

Similarly, the stress field induced by flexoelectric effect is obtained as follows:

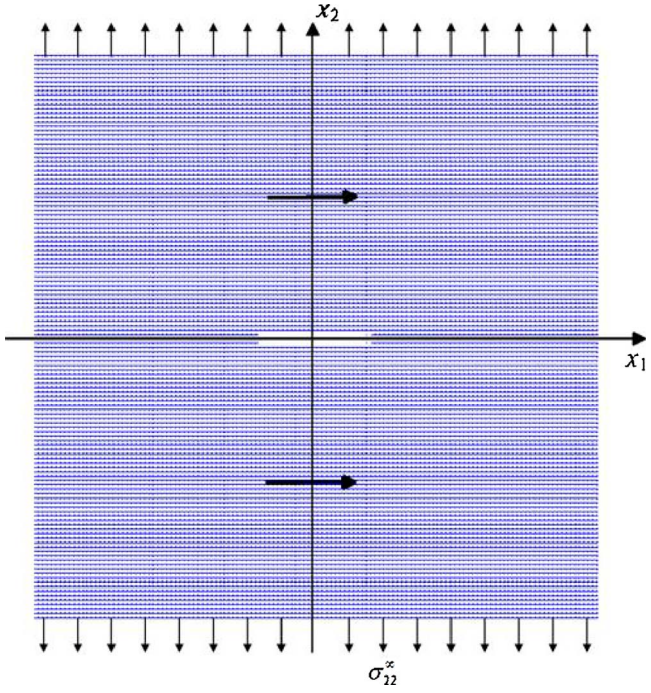

Fig. 1. Schematic illustration of the simulation model.