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A MICROMECHANICS METHOD TO STUDY THE EFFECT OF DOMAIN SWITCHING ON FRACTURE BEHAVIOR OF POLYCRYSTALLINE FERROELECTRIC CERAMICS *

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Abstract: *The effect of domain switching on anisotropic fracture behavior of polycrystalline ferroelectric ceramics was revealed on the basis of the micromechanics method. Firstly, the electroelastic field inside and outside an inclusion in an infinite ferroelectric ceramics is carried out by the way of Eshelby-Mori-Tanaka's theory and a statistical model, which accounts for the influence of domain switching. Further, the crack extension force (energy-release rate)* G_{ext} *for a penny-shape crack inside an effective polycrystalline ferroelectric ceramics is derived to estimate the averaged effect of domain switching on the fracture behavior of polycrystalline ferroelectric ceramics. The simulations of the crack extension force for a crack in a* $BaTiO_3$ *ceramics are shown that the effect of domain switching must be taken into consideration while analyzing the fracture behavior of polycrystalline ferroelectric ceramics. These results also demonstrate that the influence of the applied electric field on the crack propagation is more profound at smaller mechanical loading and the applied electric field may enhqnce the crack extension in a sense, which are consistent with the experimental results.*

Key words: ferroelectrics; domain switching; fracture behavior
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Introduction

Recently, the ferroelectric ceramics has such excellent characteristics of piezoelectricity and pyroelectricity *etc*. that it becomes one of the most important functional materials. For instance, the widely applied sensors, transducers and actuators *etc*. are made of the ferroelectric ceramics due to their good piezoelectric and pyroelectric properties[1]. Since these ferroelectric components are always subjected to the alternative and strong mechanical loading or electric field, it is crucially important to characterize the effective macroscopic electroelastic properties of the polycrystalline ferroelectric ceramics and analyze their reliability, such as the ferroelectric

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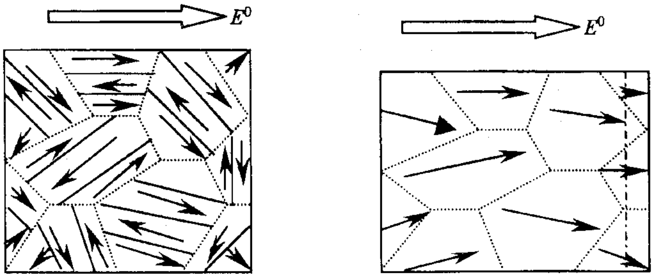
ceramics' fracture and failure. As is well-known, a commercial ferroelectric ceramics is a polycrystalline material and an individual crystal is composed of many domains with the spontaneous polarization and strains[2,3]. Moreover, all the experimental results had revealed that the spontaneous electrical polarization inside one domain can be reversed in a complicated way of new domain nucleation and domain-wall motion by means of a realizable electric or mechanical field, which is so-called domain switching, as shown in Fig.1. An electric field can cause both



(a) (b)

Fig.1 An illustration diagram shows the microstructure and its evolution in a polycrystalline ferroelectric ceramics

90° and 180° domain switching, buta mechanic loading can only reorient 90° domain. Only 90° domain switching can affect the spontaneous strains of a crystal. As the result of domain switching, the effective polarization and strains of an individual crystal treated as the vector sum of all the domains in will vary in the magnitude and the direction so as to minimize the body energy. Cao and Evans[4], Ansgar *et al*.[5] and Zhang *et al*.[6] demonstrated the fact that domain switching determines the macroscopic electroelastic properties of ferroelectric directly by the different experimental test method. In theory, Hwang *et al*.[7,8], Cheng *et al*.[9], Li and Weng[10] employed the different models to lighten the effect of domain switching and study the overall electroelastic properties of the ferroelectric ceramics with considering an evolving microstructure. Additionally, many experiments had been conducted to bring the intrinsic quality of fracture characteristics of polycrystalline ferroelectric ceramics into light and then found that the internal stress redistributed around the new-switchedly crystal was the inherent source of generating microcrack even leading to ferroelectric ceramics failure[2-5, 11-14]. All the studies made sure that the fracture behavior of ferroelectric ceramics is mainly associated with themselves inherent special microstructure-domain and microstructure-level phenomena-domain switching, and domain switching can prevent a crack parallel to the poling direction from propagating but promote a crack perpendicular to the poling direction to grow. Simultaneously, many theoretical works[15-20] had been proposed to investigate the electric-mechanic combined fracture characteristics of the linear piezoelectric ceramics in the light of the linear elastic fracture mechanic method. In spite of these theoretical studies for the linear piezoelectric ceramics has been achieved, these theoretical predictions differed from the experimental results without considering the influence of domain switching on the fracture toughness. Recently Yang and Zhu[21] studied the switching-toughening of ferroelectrics by a model of stress-assisted 90° polarization switching to quantify the toughening process based on the Reuss approximation.

Since the practical failure of polycrystalline ferroelectric ceramics is caused by the extension of the internal defects, such as voids and microcracks, it is feasible to establish a simply micromechanics model to solve the electroelastic field inside and outside an ellipsoidal inclusion in ferroelectric ceramics in terms of Eshelby-Mori-Tanaka's method; and then the crack extension force (energy-release rate) G_{ext} derived by a micromechanics model for a penny-shape crack inside an effective ferroelectric ceramics is utilized to analyze the averaged influence of domain switching on ferroelectrics fracture characteristics.

1 General Formulation

If the free charges and body forces do not exist in a piezoelectric body, the static elastic and electric field equation can be written in terms of Gauss's law and static equilibrium conditon as

Divergence equations

$$\sigma_{ij,j} = 0, \quad D_{i,i} = 0. \tag{1}$$

Gradient equations

$$\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}), \quad E_i = -\phi_{,i}. \tag{2}$$

Constitutive equations

$$\sigma_{ij} = C_{ijmn}\varepsilon_{mn} + e_{nij}\phi_{,n}, \quad D_i = e_{imn}\varepsilon_{mn} - k_{in}\phi_{,n}. \tag{3}$$

The shorthand notions used by Barnett and Lothe[22] are introduced to describe above equations as the following compact formation:

$$Z_{Mn} = \begin{cases} \varepsilon_{mn} & (M = 1,2,3), \\ \phi_{,n} & (M = 4) \end{cases} \tag{4}$$

and

$$U_M = \begin{cases} u_m & (M = 1,2,3), \\ \phi & (M = 4). \end{cases} \tag{5}$$

Similarly the stress and electric displacement are represented as

$$\Sigma_{iJ} = \begin{cases} \sigma_{ij} & (J = 1,2,3), \\ D_i & (J = 4). \end{cases} \tag{6}$$

In the same manner, the compact notation of electroelastic material coefficient tensor can be obtained

$$\boldsymbol{E}_{iJMn} = \begin{cases} \boldsymbol{C}_{ijmn} & (J, M = 1,2,3), \\ \boldsymbol{e}_{nij} & (J = 1,2,3; M = 4), \\ \boldsymbol{e}_{imn} & (J = 4; M = 1,2,3), \\ -\boldsymbol{k}_{in} & (J, M = 4). \end{cases} \tag{7}$$

It is noted that the "inverse" of $\boldsymbol{E}_{iJMn}$ is defined as $\boldsymbol{F}_{AbiJ}$, evidently $\boldsymbol{E}_{iJMn}$ and $\boldsymbol{F}_{AbiJ}$ are diagonally symmetric.

In order to be convenient to derive in next section, the above equations can be represented in the following matrix form:

$$\boldsymbol{\Sigma}_{9\times1} = \boldsymbol{E}_{9\times9}\boldsymbol{Z}_{9\times1}, \quad \boldsymbol{Z}_{9\times1} = \boldsymbol{F}_{9\times9}\boldsymbol{\Sigma}_{9\times1}, \tag{8}$$

where the mapping of adjacent indices is used as follows:

$$(11) \to 1, \quad (22) \to 2, \quad (33) \to 3, \quad (23) \to 4, \quad (13) \to 5,$$

$(12) \to 6, \quad (14) \to 7, \quad (24) \to 8, \quad (34) \to 9.$

2 A Theroetical Model

For an unpoled ferroelectric ceramics, the effective polarization of an individual crystal randomly distributes as shown in Fig. 1(a). When the ferroelectric ceramics is subjected to an electric field, the new domain will nucleate and the domain wall will move (two mechanisms of domain switching) so as to reorient the effective polarization of an individual crystal. Thus, the effective polarization will be closest to local electric field in order to minimize the body free energy, as shown in Fig. 1(b). Therefore based on the microstructure characteristic of polycrystalline ferroelectric ceramics, we can establish a statistical model to carry out the averaged effect of domain switching on the macroscopic electroelastic properties in the light of Eshelby-Mori-Tanaka's method. As mentioned by Mura[23], we can further employ a micromechanic model for a penny-shape crack inside an effective piezoelectric media to estimate the average influence of domain switching on the crack extension, as shown in Fig. 2. Therefore, we can only calculate the interaction energy between the external combined electric/mechanical field and the crack as the crack extension force if considering the crack as an inclusion inside the effective ferroelectric ceramics.

Therefore, it is of importance to analyze the eigenfield inside the new-switching crystal and crack firstly which are denoted by $\boldsymbol{Z}^{**}$ and $\boldsymbol{Z}_c^*$. In the course of solution for electroelastic field inside an inclusion, the effect of the penny-crack is not considered for obtaining $\boldsymbol{Z}^{**}$, but the interactions among the inclusions and the crack in taken into account by the back stress and electric displacement analysis, which is reasonable[24]. Once $\boldsymbol{Z}^{**}$ and $\boldsymbol{Z}_c^*$ are solved, we can compute the crack extension force (energy-release rate) G_{ext} for a penny-shape crack in an effective medium. For later convenience, the regions of the matrix, the new-swichedly crystal and the microcrack are denoted by Ω_m, Ω_f and Ω_c respectively. The electroelastic tensor coefficients of the matrix and the crystal are expressed as $\boldsymbol{E}_m$, $\boldsymbol{F}_m$ and $\boldsymbol{E}_f$, $\boldsymbol{F}_f$.

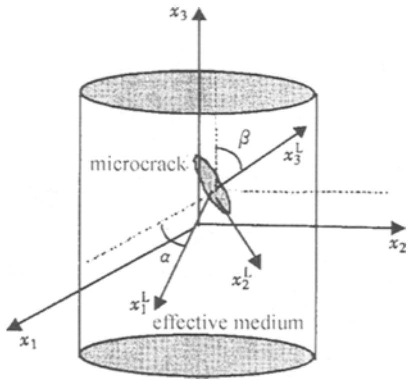


Fig. 2 A theoretical model of a penny-shape microcrack inside an effective polycrystalline ferroelectric ceramics

3 Solution Procedure

3.1 The electroelastic field inside a new-switchedly crystal

As is well-known, domain switching is the inherent source of mainly affecting the macroscopic electroelastic properties of polycrystalline ferroelectric ceramics. Merz[25] made a conclusion by the experimental results that domain switching was mainly a problem of new domain nucleation under the action of an electric field. And an empirical expression of the nucleation (domain switching) probability P of an individual crystal was given by[9, 25]

$$P = P_0 \exp\left(-\frac{b}{E}\right), \tag{9}$$

where b is the threshold electrical field. For a $BaTiO_3$ ceramics, the threshold b is 470 kV/m. P_0 is the probability of nucleation (domain switching) for infinite field stregth E_∞. The probability of domain switching determined by Eq.(9) only depends on the applied electric field. Under the action of the external mechanical field, we can roughly "transfer" the applied mechanical field into the equal electric field applicable to Eq.(9) through the piezoelectric constitutive relationship. Since the experiential expression Eq.(9) was derived from a finite body, the actual electric field E in Eq.(9) applied to an individual crystal in an infinite ferroelectric ceramics must be replaced by the effective electric field considering the interactions among the crystals in this paper.

Thus, the volume fraction of the new-swithedly crystals V_f can be derived from the volume fraction V_f^0 of all the switchable crystals and the domain switching probability P

$$V_f = V_f^0 P. \tag{10}$$

In accordance with the theoretical model and Eshelby's equivalent inclusion theory, as the new-switchedly crystal caused by the external applied field is treated as an inclusion, the average field $\boldsymbol{\Sigma}_m$ of matrix with the electroelastic moduli $\boldsymbol{E}_m$ can be presented as

$$\boldsymbol{\Sigma}_m = \boldsymbol{\Sigma}^0 + \boldsymbol{\Sigma}_m^1 = \boldsymbol{E}_m(\boldsymbol{Z}^0 + \boldsymbol{Z}^1), \tag{11}$$

where $\boldsymbol{Z}^1$, $\boldsymbol{\Sigma}_m^1$ are the disturbed fields due to the inhomogeneous inclusion occupying a region Ω_f with the electroelastic moduli E_f and the interactions among the new-switchedly crystals. Inside the inclusion, the equivalent inclusion method yields the electroelastic field $\boldsymbol{\Sigma}_f$

$$\begin{aligned}\boldsymbol{\Sigma}_f &= \boldsymbol{\Sigma}^0 + \boldsymbol{\Sigma}_m^1 + \boldsymbol{\Sigma}_f^1 = \boldsymbol{E}_f(\boldsymbol{Z}^0 + \boldsymbol{Z}^1 + \boldsymbol{Z}^{pt} - \boldsymbol{Z}^*) = \\ &\boldsymbol{E}_m(\boldsymbol{Z}^0 + \boldsymbol{Z}^1 + \boldsymbol{Z}^{pt} - \boldsymbol{Z}^* - \boldsymbol{Z}^{**}),\end{aligned} \tag{12}$$

where $\boldsymbol{Z}^*$ is the eigenfield of the new-switchiedly crystal under the action of the external field. It is reasonable to assume that the effective polarization orientation of the new-switchedly crystal is parallel to the direction of the applied electrical field as a result of domain switching. $\boldsymbol{Z}^{**}$ is the fictitious eigenfield: strain and electric field due to the inhomogeneity. $\boldsymbol{Z}^{pt}$, the disturbed field, can be written as

$$\boldsymbol{Z}^{pt} = \boldsymbol{S}(\boldsymbol{Z}^* + \boldsymbol{Z}^{**}), \tag{13}$$

where $\boldsymbol{S}$ is the Eshelby's electroelastic tensor that is derived from Wang's[26] three-dimensional solution of an ellipsoidal inclusion in a piezoelectric material (see Appendix A).

When subjected to a far-field traction and electric displacement, $\boldsymbol{\Sigma}_{iJ}^0 \boldsymbol{n}_i$, on the boundary with outward unit normal vector $\boldsymbol{n}_i$, the average field of the throughout ceramics can be obtained in terms of Mori-Tanaka's mean field theory by

$$\langle \boldsymbol{\Sigma} \rangle = \frac{1}{V}\int_{D-\Omega_f} \boldsymbol{\Sigma}_m \mathrm{d}V + \frac{1}{V}\int_{\Omega_f} \boldsymbol{\Sigma}_f \mathrm{d}V = \boldsymbol{\Sigma}^0, \tag{14}$$

where $\langle \cdot \rangle$ means the volume average, V is the volume of the whole ferroelectric ceramics.

Substituting Eqs.(11), (12), (13) into Eq.(14) leads to

$$\boldsymbol{Z}^1 = -V_f(\boldsymbol{S} - \boldsymbol{I})(\boldsymbol{Z}^* + \boldsymbol{Z}^{**}), \tag{15}$$

where V_f is the volume fraction of the total new-switchedly crystals, as presented in Eq.(10).

Combining Eqs.(11) – (15) leads to

$$\begin{aligned}\boldsymbol{Z}^{**} &= [\boldsymbol{E}_m(\boldsymbol{S} - \boldsymbol{I}) - \boldsymbol{E}_f\boldsymbol{S} + V_f(\boldsymbol{E}_f - \boldsymbol{E}_m)(\boldsymbol{S} - \boldsymbol{I})]^{-1} \times \\ &(\boldsymbol{E}_f - \boldsymbol{E}_m)[\boldsymbol{Z}^0 + (1 - V_f)(\boldsymbol{S} - \boldsymbol{I})\boldsymbol{Z}^*].\end{aligned} \tag{16}$$

Therefore in the new-switchedly crystals, we have

$$\boldsymbol{\Sigma}_{\mathrm{f}}^{1} = \boldsymbol{E}_{\mathrm{m}}(\boldsymbol{S} - \boldsymbol{I})(\boldsymbol{Z}^{*} + \boldsymbol{Z}^{**}). \tag{17}$$

3.2 The general solution for the electroelastic field inside a void

Now let us consider a spatially distributed penny-shape crack occupying a region Ω_c in a ferroelectric ceramics to carry out the internal eigenfield. Based on the Eshelby's equivalent inclusion theory, we present the electroelastic field $\boldsymbol{\Sigma}_{\mathrm{c}}^{\mathrm{L}}$ inside a crack in the local coordinate system:

$$\boldsymbol{\Sigma}_{\mathrm{c}}^{\mathrm{L}} = \boldsymbol{\Sigma}^{0\mathrm{L}} + \boldsymbol{\Sigma}^{1\mathrm{L}} + \boldsymbol{\Sigma}_{\mathrm{c}}^{pt\mathrm{L}} = 0 = \boldsymbol{E}_{\mathrm{m}}(\boldsymbol{Z}^{0\mathrm{L}} + \boldsymbol{Z}^{1\mathrm{L}} + \boldsymbol{Z}_{\mathrm{c}}^{pt\mathrm{L}} - \boldsymbol{Z}_{\mathrm{c}}^{*\mathrm{L}}), \tag{18}$$

where superscript "L" denotes the local coordinate system (Fig.2). We can assume that the fixed coordinate system is denoted as (x_1, x_2, x_3), the local coordinate system can be established by $(x_1^{\mathrm{L}}, x_2^{\mathrm{L}}, x_3^{\mathrm{L}})$. The x_3^{L} is the symmetric axis like the fixed coordinate and let x_1^{L} lie in (x_1, x_2) plane with no loss in generality, then, we can obtain the transformation matrix $\boldsymbol{T}$ from the fixed one to the local one:

$$\boldsymbol{T} = \begin{bmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha\cos\beta & \cos\alpha\cos\beta & \sin\beta \\ \sin\alpha\sin\beta & -\sin\beta\cos\alpha & \cos\beta \end{bmatrix},$$

then

$$\varepsilon_{ij}^{L} = T_{im}T_{jn}\varepsilon_{mn}, \quad E_i^L = T_{in}E_n \tag{19}$$

Based on the Eshelby's electroelastic tensor $\boldsymbol{S}$, $\boldsymbol{Z}_{\mathrm{c}}^{*L}$ can be given from Eq.(18) as

$$\boldsymbol{Z}_{\mathrm{c}}^{*L} = -(\boldsymbol{S}_{\mathrm{c}} - \boldsymbol{I})^{-1}(\boldsymbol{Z}^{0L} + \boldsymbol{Z}^{1L}). \tag{20}$$

Then using the coordinate transformation matrix $\boldsymbol{A}$ (see Appendix B), we can obtain

$$\boldsymbol{Z}_{\mathrm{c}}^{*} = -\boldsymbol{A}^{-1}(\boldsymbol{S}_{\mathrm{c}} - \boldsymbol{I})^{-1}\boldsymbol{A}(\boldsymbol{Z}^{0} + \boldsymbol{Z}^{1}). \tag{21}$$

3.3 The crack extension force for a crack inside a ferroelectric ceramics

Similar to the micromechanics definition of the strain energy release-rate for an crack as an inclusion in the effective elastic medium, the interaction energy ΔW between the external electric/mechanic combined field and an inclusion in a ferroelectric ceramics can be defined as the change of total elastic and electric energy (the Gibbs free energy) due to the presence of inclusion[19]

$$\Delta W = \frac{1}{2}\int_{\Omega}(\boldsymbol{\Sigma}^{0} + \boldsymbol{\Sigma}^{1})(\boldsymbol{Z}^{0} + \boldsymbol{Z}^{1})\mathrm{d}V - \int_{|D|}(\boldsymbol{\Sigma}^{0}\boldsymbol{n}_i)(\boldsymbol{U}^{0} + \boldsymbol{U}^{1})\mathrm{d}V - \left[\frac{1}{2}\int_{\Omega}\boldsymbol{\Sigma}^{0}\boldsymbol{Z}^{0}\mathrm{d}V - \int_{|D|}(\boldsymbol{\Sigma}^{0}\boldsymbol{n}_i)\boldsymbol{U}^{0}\mathrm{d}V\right], \tag{22}$$

where in the matrix $\boldsymbol{\Sigma}^{1}$ is equal to $\boldsymbol{\Sigma}_{\mathrm{m}}^{1}$ and in the inclusion $\boldsymbol{\Sigma}^{1}$ is equal to $\boldsymbol{\Sigma}_{\mathrm{m}}^{1} + \boldsymbol{\Sigma}_{\mathrm{f}}^{1}$.

Applying Gauss's theorem to Eq.(22) and considering a crack as the inclusion inside an effective electroelastic medium can yield

$$\Delta W = -\frac{1}{2}\int_{\Omega_c}\boldsymbol{\Sigma}^{0}\boldsymbol{Z}_{\mathrm{c}}^{*}\,\mathrm{d}V = -\frac{1}{2}V_{\mathrm{c}}\boldsymbol{\Sigma}^{0}\boldsymbol{Z}_{\mathrm{c}}^{*}, \tag{23}$$

where $V_{\mathrm{c}} = (4\pi/3)c^2 t$ is the volume of a penny-shape crack. c and t denotes the size of the principal axes of a penny-shaped crack.

The Griffith fracture criterion can be written as

$$\delta G = \delta(\Delta W + 2s\gamma), \tag{24}$$

where G is the Gibbs free energy and γ is the surface energy per unit area of the crack surface.

Thus we can obtain the crack extension force G_{ext} as

$$G_{\text{ext}} = -\frac{\partial \Delta W}{2\partial s}, \tag{25}$$

where "s" is the surface area of the crack.

Once $G_{\text{ext}} \geqslant \gamma$, the crack extends to propagate. Since we aim at analyzing the averaged effects of domain switching on the crack extension force, we can adopt the mean field approach to consider the interactions among the new-switchedly crystals, in which the external field $\boldsymbol{\Sigma}^0$ in Eq. (23) should be replaced by the effective field which was given by Mori-Tanaka[24] as follows:

$$\boldsymbol{\Sigma}^{\text{eff}} = \boldsymbol{\Sigma}^0 - V_{\text{f}}\boldsymbol{E}_{\text{m}}(\boldsymbol{S} - \boldsymbol{I})(\langle \boldsymbol{Z}^* \rangle + \langle \boldsymbol{Z}^{**} \rangle).$$

Thus from Eq. (25), we have the crack extension force G_{ext} in the case of considering the effect of domain switching

$$G_{\text{ext}} = \frac{1}{3} c\rho \boldsymbol{\Sigma}^{\text{eff}} \boldsymbol{Z}_c^*, \tag{26}$$

where ρ is the aspect ratio t/c of the crack.

If the effect of domain switching is not taken into consideration, the crack extension force G_{ext} for the case of pure matrix surrounding a penny-shaped crack is set as G_0. The crack extension force G_0 can be obtained in the same produce as

$$G_0 = -\frac{\partial W_0}{\partial s} = \frac{1}{3} c\rho \boldsymbol{\Sigma}^0 \boldsymbol{Z}_{c0}^*, \tag{27}$$

where $\boldsymbol{Z}_{c0}^*$ can be obtained by the means of Eshelby's equivalent inclusion theory as

$$\boldsymbol{Z}_{c0}^* = -\boldsymbol{A}^{-1}(\boldsymbol{S}_c - \boldsymbol{I})^{-1}\boldsymbol{A}\boldsymbol{Z}^0. \tag{28}$$

Since the surface energy γ can be regarded as one of material constants for a given material, we can verify directly the effect of domain switching on the fracture behavior of polycrystalline ferroelectric ceramics through comparing the crack extension force G_{ext} with G_0 under the same condition.

4 Numerical Results and Discussions

In this section, the simulations for the crack extension force of a crack in a $BaTiO_3$ ceramics are taken as example. At the room temperature, the tetragonal phase of $BaTiO_3$ single crystal has the cell constants $a = 3.992$ Å and $c = 4.035$ Å and a spontaneous polarization $P_s = 0.26$ C/m^2. Thus, the eigenstrain and eigenelectric displacement of a single-crystal can be calculated in the local coordination as follows: $\varepsilon_{11}^* = \varepsilon_{22}^* = -0.005$, $\varepsilon_{33}^* = 0.01$, $D_3^* = 0.26$ C/m^2 and others are all zero. The relevant elastic, piezoelectric and dielectric coefficients for $BaTiO_3$ single-crystal and polycrystalline ceramics at 25°C are shown as follows:

Ceramics

$C_{11}^E = 166$ GPa, $C_{33}^E = 162$ GPa, $C_{44}^E = 43$ GPa,

$C_{12}^E = 77$ GPa, $C_{13}^E = 78$ GPa,

$e_{31} = -4.4$ C/m^2, $e_{33} = 18.6$C/m^2, $e_{15} = 11.6$ C/m^2,

$k_{11} = 11.2 \times 10^{-9}$ C^2/(Nm^2), $k_{33} = 12.6 \times 10^{-9}$ C^2/(Nm^2),

$d_{31} = -79 \times 10^{-12}$ C/N, $d_{33} = 191 \times 10^{-12}$ C/N, $d_{15} = 270 \times 10^{-12}$ C/N

Single crystal

$C_{11}^{E} = 275$ GPa, $C_{33}^{E} = 164.8$ GPa, $C_{44}^{E} = 54.3$ GPa,

$C_{12}^{E} = 178.9$ GPa, $C_{13}^{E} = 151.6$ GPa,

$e_{31} = -2.69$ C/m^2, $e_{33} = 3.65$ C/m^2, $e_{15} = 21.3$ C/m^2,

$k_{11} = 17.4 \times 10^{-9}$ C^2/(Nm^2), $k_{33} = 0.96 \times 10^{-9}$ C^2/(Nm^2),

$d_{31} = -34.5 \times 10^{-12}$ C/N, $d_{33} = 85.6 \times 10^{-12}$ C/N, $d_{15} = 392 \times 10^{-12}$ C/N

Based on the proposed model, the crack extension force (energy release rate) G_{ext} for a penny-shaped crack inside a ferroelectric ceramics is calculated to study the averaged effect of domain switching on the fracture behavior of polycrystalline ferroelectric ceramics. In the case of the aspect ratio $\rho = 1/100$ and the distribution angle $\alpha = \beta = 0$ of a crack, the simulations for the crack extension force are shown in Fig.3 as a function of the external applied field and the aspect ratio of a new-switchedly crystal. From Fig.3, it is obvious that the normalized crack extension force G_{ext}/G_0 increases to a maximum while $E_3 \approx 600$ kV/m, which is approximated to the coercive field of a $BaTiO_3$ ceramics, and then decreases to an asymptotic value about 50 as the applied electric field increasing. The results shown in Fig.3 also indicate that the influence of the applied electric field on the crack extension force will decrease while the applied mechanic loading increases. All the phenomena can be interpreted as a result of domain switching. Since both the applied electric field and mechanic field can cause domain swithing, more and more swithable crystals will reorient no matter which of either electric field or mechanic loading increases. Consequentially, the effective macroscopic properties of ferroelectric ceramics will be approximated to that of the single crystal and then the normalized crack extension force G_{ext}/G_0 will be approximated to a finite value, as stated in Eqs.(25) and (28). But, all the simulations confirm that the applied electric field can enhance the crack propagation, which means that the electric field may decrease the critical fracture stress in theory after domain switching is taken into consideration. The effect of the aspect ration of a new-switchedly crystal shown in Fig.4 indicates

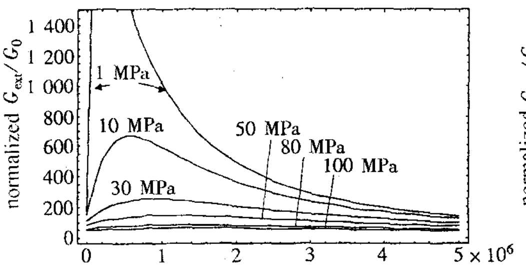


Fig.3 Influence of the applied electrical field E_3 and the mechanical field σ_{33} on the normalized crack extension force G_{ext}/G_0 in the case of $\alpha = \beta = 0°$ and $c = 10$ um

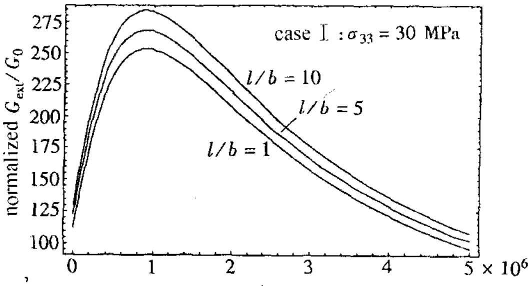


Fig.4 Influence of the aspect ratio l/b of the new-switchedly crystal on the normalized crack extension force G_{ext}/G_0 in a given mechanic loading

that the more the aspect ratio of the crystal, the larger is the normalized crack extension force G_{ext}/G_0. However compared to the effect of the applied electric field, the effect of the aspect ratio of a new-switchedly crystal on the crack ectension is not much obvious. On the other hand, Fig.5 gives the crack extension force (energy release rate) G_{ext} and G_0 as a function of the crack

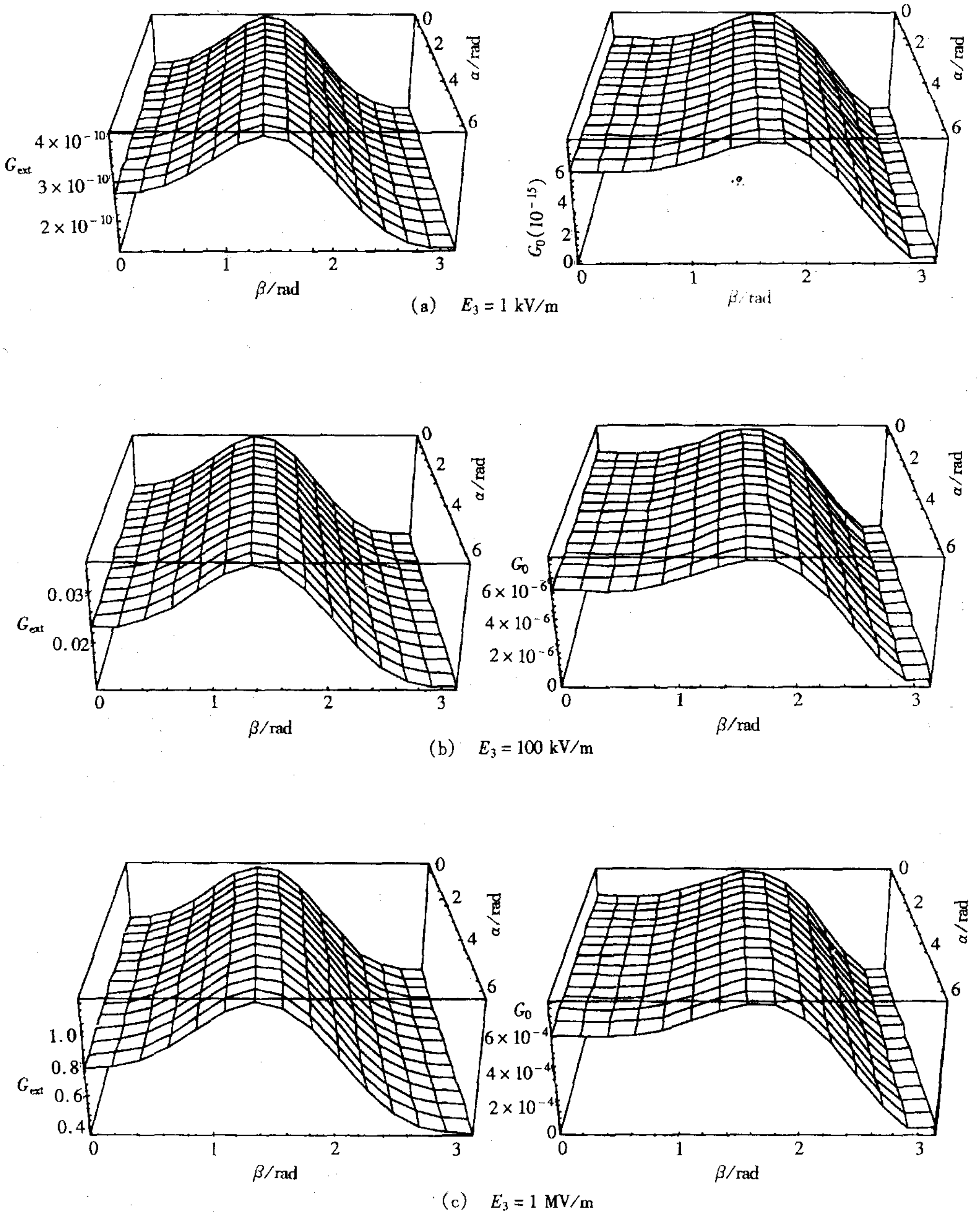


Fig.5 Effect of the crack orientation on the crack extension force G_{ext} and G_0 (unit: N/m) in the case of a given electrical filed and c = 10 um

orientation for a constant external electric field. It is obviously marked that the simulation G_{ext} shown in Fig.5 increases to a maximum at $\beta = 80° \sim 90°$ and then decreases to a minimum at $\beta = 180°$ in any case of $\alpha = 0° \sim 360°$ while the ferroelectric ceramics is subjectecd to an electric field. Obviously, the values of G_{ext} are much greater than G_0 due to take the effect of domain switching into consideration. These results also indicate that the crack in polarization plane will propagate more easily than that in the perpendicular plane, which are good in agreement with the observed phenomena[11-14].

5 Conclusion

According to the inherent microstructure and microstructure-level phenomenon of ferroelectric ceramics, we employ the Cheng's *et al*.[9] statistical model to study the effect of domain switching on the electroelastic field by the way of Eshelby-Mori-Tanaka method and Wang's[26] solution of an inclusion embedded by piezoelectric matrix firstly. Further, the crack extension force (energy release rate) G_{ext} of a penny-shape crack in an effective polycrystalline ferroelectric ceramics is carried out to analyze the effect of domain switching on the fracture behavior. The calculations of the crack extension force for a crack in a $BaTiO_3$ ceramics demonstrate that the applied electric field can enhance the crack extension in a ferroelectric ceramics, namely the applied electric field can decrease the fracture strength of ferroelectric ceramics, which are consistent with the experimental results[11-14].

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Appendix A

The non-zero components of Eshelby's electroelastic tensors $\boldsymbol{S}$ can be presented as following formation:

$$\boldsymbol{Z}^I = \boldsymbol{S}\boldsymbol{Z}^*,$$

where

$$S_{11} = \frac{1}{4\pi}(C_{11}^0 N_{1111}^1 + C_{12}^0 N_{1212}^1 + C_{31}^0 N_{1313}^1 + e_{31}^0 N_{113}^2),$$

$$S_{12} = \frac{1}{4\pi}(C_{12}^0 N_{1111}^1 + C_{22}^0 N_{1212}^1 + C_{32}^0 N_{1313}^1 + e_{32}^0 N_{113}^2),$$

$$S_{13} = \frac{1}{4\pi}(C_{13}^0 N_{1111}^1 + C_{23}^0 N_{1212}^1 + C_{33}^0 N_{1313}^1 + e_{33}^0 N_{113}^2),$$

$$S_{14} = \frac{1}{4\pi}e_{24}^0 N_{113}^2,$$

$$S_{15} = \frac{1}{4\pi}e_{15}^0 N_{113}^2,$$

$$S_{19} = -\frac{1}{4\pi}(e_{31}^0 N_{1111}^1 + e_{32}^0 N_{1212}^1 + e_{33}^0 N_{1313}^1 - k_{33}^0 N_{113}^2),$$

$$S_{21} = \frac{1}{4\pi}(C_{11}^0 N_{2121}^1 + C_{21}^0 N_{2222}^1 + C_{31}^0 N_{2323}^1 + e_{31}^0 N_{223}^2),$$

$$S_{22} = \frac{1}{4\pi}(C_{12}^0 N_{2121}^1 + C_{22}^0 N_{2222}^1 + C_{32}^0 N_{2323}^1 + e_{32}^0 N_{223}^2),$$

$$S_{23} = \frac{1}{4\pi}(C_{13}^0 N_{2121}^1 + C_{23}^0 N_{2222}^1 + C_{33}^0 N_{2323}^1 + e_{33}^0 N_{223}^2),$$

$$S_{24} = \frac{1}{4\pi} e_{24}^0 N_{223}^2, \quad S_{25} = \frac{1}{4\pi} e_{15}^0 N_{223}^2,$$

$$S_{29} = -\frac{1}{4\pi}(e_{31}^0 N_{2121}^1 + e_{32}^0 N_{2222}^1 + e_{33}^0 N_{2323}^1 - k_{33}^0 N_{223}^2),$$

$$S_{31} = \frac{1}{4\pi}(C_{11}^0 N_{3131}^1 + C_{21}^0 N_{3232}^1 + C_{31}^0 N_{3333}^1 + e_{31}^0 N_{333}^2),$$

$$S_{32} = \frac{1}{4\pi}(C_{12}^0 N_{3131}^1 + C_{22}^0 N_{3232}^1 + C_{32}^0 N_{3333}^1 + e_{32}^0 N_{333}^2),$$

$$S_{33} = \frac{1}{4\pi}(C_{13}^0 N_{3131}^1 + C_{23}^0 N_{3232}^1 + C_{33}^0 N_{3333}^1 + e_{33}^0 N_{333}^2),$$

$$S_{34} = \frac{1}{4\pi} e_{24}^0 N_{333}^2, \quad S_{35} = \frac{1}{4\pi} e_{15}^0 N_{333}^2,$$

$$S_{39} = -\frac{1}{4\pi}(e_{31}^0 N_{3131}^1 + e_{32}^0 N_{3232}^1 + e_{33}^0 N_{3333}^1 - k_{33}^0 N_{333}^2),$$

$$S_{41} = \frac{1}{8\pi} e_{31}^0 N_{322}^2, \quad S_{42} = \frac{1}{8\pi} e_{32}^0 N_{322}^2, \quad S_{43} = \frac{1}{8\pi} e_{33}^0 N_{322}^2,$$

$$S_{44} = \frac{1}{4\pi}[C_{44}^0 (N_{3232}^1 + N_{3322}^1 + N_{2323}^1 + N_{2233}^1) + e_{24}^0 (N_{232}^2 + N_{322}^2)],$$

$$S_{45} = \frac{1}{4\pi} e_{15}^0 N_{322}^2,$$

$$S_{48} = -\frac{1}{8\pi}[e_{24}^0 (N_{3232}^1 + N_{3322}^1 + N_{2332}^1 + N_{2233}^1) - k_{22}^0 (N_{232}^2 + N_{322}^2)],$$

$$S_{51} = \frac{1}{8\pi} e_{31}^0 N_{311}^2, \quad S_{52} = \frac{1}{8\pi} e_{32}^0 N_{311}^2,$$

$$S_{53} = \frac{1}{8\pi} e_{33}^0 N_{311}^2, \quad S_{54} = \frac{1}{4\pi} e_{24}^0 N_{311}^2,$$

$$S_{55} = \frac{1}{4\pi}[C_{55}^0 (N_{1133}^1 + N_{1313}^1 + N_{3113}^1 + N_{3311}^1) + e_{15}^0 (N_{311}^2 + N_{131}^2)],$$

$$S_{57} = -\frac{1}{8\pi}[e_{15}^0 (N_{1133}^1 + N_{1331}^1 + N_{3113}^1 + N_{3311}^1) - k_{11}^0 (N_{311}^2 + N_{131}^2)],$$

$$S_{66} = \frac{1}{4\pi} C_{66}^0 (N_{1122}^1 + N_{1221}^1 + N_{2112}^1 + N_{2211}^1),$$

$$S_{75} = -\frac{1}{2\pi}[C_{13}^0 (N_{311}^2 + N_{131}^2) + e_{15}^0 N_{11}^3],$$

$$S_{77} = \frac{1}{4\pi}[e_{15}^0 (N_{311}^2 + N_{131}^2) - k_{11}^0 N_{11}^3],$$

$$S_{84} = -\frac{1}{2\pi}[C_{44}^0 (N_{322}^2 + N_{232}^2) + e_{24}^0 N_{22}^3],$$

$$S_{88} = \frac{1}{4\pi}[e_{24}^0 (N_{322}^2 + N_{232}^2) - k_{22}^0 N_{22}^3],$$

$$S_{91} = -\frac{1}{4\pi}(C_{11}^0 N_{113}^2 + C_{12}^0 N_{223}^2 + C_{31}^0 N_{333}^2 + e_{31}^0 N_{33}^3),$$

$$S_{92} = -\frac{1}{4\pi}(C_{12}^0 N_{113}^2 + C_{22}^0 N_{223}^2 + C_{32}^0 N_{333}^2 + e_{32}^0 N_{33}^3),$$

$$S_{93} = -\frac{1}{4\pi}(C_{13}^0 N_{113}^2 + C_{23}^0 N_{223}^2 + C_{33}^0 N_{333}^2 + e_{33}^0 N_{33}^3),$$

$$S_{99} = \frac{1}{4\pi}(e_{31}^0 N_{113}^2 + e_{32}^0 N_{223}^2 + e_{33}^0 N_{333}^2 - k_{33}^0 N_{33}^3)$$

Appendix B

The components of $\boldsymbol{A}$ matrix are shown as

$$\boldsymbol{f}_f = \begin{bmatrix} n^2 & m^2 & 0 & 0 & 0 & 2mn \\ m^2p^2 & n^2p^2 & q^2 & 2npq & -2mpq & -2nmp^2 \\ m^2q^2 & q^2n^2 & p^2 & -2npq & 2mpq & -2mnq^2 \\ pqm^2 & -pqn^2 & qp & np^2 - nq^2 & mq^2 - mp^2 & nmpq \\ nmq & -nmq & 0 & mp & np & qm^2 - qn^2 \\ -nmp & nmp & 0 & mq & nq & pn^2 - pm^2 \end{bmatrix},$$

$$\boldsymbol{f}_e = \begin{bmatrix} n & m & 0 \\ -mp & np & q \\ mq & -nq & p \end{bmatrix},$$

where $n = \cos\alpha$, $m = \sin\alpha$, $p = \cos\beta$, $q = \sin\beta$, $\boldsymbol{f}_f$ is 6×6 matrix and $\boldsymbol{f}_e$ is 3×3 matrix. Then,

$$\boldsymbol{A} = \begin{bmatrix} \boldsymbol{f}_f & \boldsymbol{0}_{6\times 3} \\ \boldsymbol{0}_{3\times 6} & \boldsymbol{f}_e \end{bmatrix}$$

and

$$\boldsymbol{A}^{\mathrm{T}} = \boldsymbol{A}^{-1},$$

where superscript "T" indicates the transpose of matrix and "-1" means the inverse of the matrix.