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Dislocation simulation of domain switching toughening in ferroelectric ceramics

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ABSTRACT

The method of dislocation simulation of domain switching toughening is extended to the piezoelectric coupling field. As a typical example, domain switching toughening in the ferroelectric ceramic with a semi-infinite crack being perpendicular to spontaneous polarization direction subjected to negative electric field is evaluated by using dislocation simulation. The transformed strain nucleus simulated by an assembly of four different edge dislocations is constructed first, then the generalized stress intensity factor generated by four dislocations in strain nucleus is used to simulate the transformed particle toughening. Based on this solution, the formulations for toughening arising from ferroelectric domain switching are derived by the Green's function method. Taking $BaTiO_3$ ferroelectric ceramic for example, the exact expression of generalized stress intensity factor is obtained, and it is discovered that the crack propagation can be promoted by domain switching induced by negative electrical load when crack surface is parallel to the isotropic plane, this result meets experimental phenomenon well. This method can also be used to evaluate domain switching toughening in ferroelectric ceramics under some other load and polarization types and those with some other cracks or holes.

1. Introduction

Since the end of 20th century, the rapid development of information industry has made the rise of techniques of microelectromechanical systems, microelectronic elements and microelectronic encapsulation, actuators, sensors, transducers, and so on. The multi-field coupling of function materials and mesoscopic or microscopic information structure mechanics has been proposed. When the interaction between stress, strain or heat and electromagnetic behavior is very strong, the mechanical mechanism is very important for designs of MEMS.

The earliest experimental investigations about strength and fracture toughness of ferroelectric ceramics should go back to the eighties of 20th century. Winzer et al. (1989) reported the fracture phenomenon of cofired multiplayer electrostrictive actuators at the earliest. Chung et al. (1989) observed the intergranular cracking and damage of barium titanate and lead zirconate titanate induced by electric field. McHenry and Koepke (1983) observed phenomena which were explained qualitatively by certain microstructural features, in particular internal stresses (Freiman and Pohanka, 1989) and energy dissipation (Mehta and Virkar, 1990) by domain switching processes. At the beginning of nineties of 20th century, Pak (1990, 1991) made a lot of investigations on fracture mechanism of piezoelectric and ferroelectric materials. Furuta and Uchino (1993) observed the process of crack nucleation and propagation in internal electrode of ferroelectric detent. Recently, electric-field-induced fatigue crack growth in ferroelectric ceramics was studied by Fang et al. (2010). Domain switching criterion differentiating 90 degree switching and 180 degree switching was proposed (Sun and Jiang, 1998), the corresponding domain switching and criterion of domain switching in ferroelectric crystal subjected to increasing electric field was observed and discussed by Jiang and Fang (2007a,b) and Engert et al. (2011) who combined experimental observations and theoretical analysis.

These experimental and theoretical investigations on fracture toughness and crack propagation of ferroelectric ceramics subjected to mechanical or electrical or electromechanical load showed that the toughness of ferroelectric ceramics can be substantially enhanced or reduced through domain switching. There are three analytical methods to study domain switching toughening. One is an energy balance, the fracture toughness of ferroelectric ceramics subjected to electromechanical load was analyzed by the balance of energy supplied by the driving forces (Kreher, 2002). Another is an Eshelby-type approach (Rice, 1972), Beom and Atluri (2003) investigated the disciplines of style, size and shape of domain switching zone around crack tip in ferroelectric ceramics subjected to electrical load and discussed fracture toughness variation of ferroelectrics under combined electric and mechanical loading by using Eshelby-type approach, and moreover, Landis and Chad (2003) studied the domain switching toughening of crack tip in ferroelectric ceramics subjected to mechanical load by using

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Eshelby-type approach, but this method is not convenient when multiple transformed zones are involved. The third approach is a Green's function method, which is based on the following works. Rose (1987) represented both dilatants and deviatoric transformed strain components with a set of fundamental singular solutions such as a force-doublet, similar to the work of Love (1927). His methodology is rigorous, but not straightforward and inconvenient for application. Ma (2011) applied dislocations to simulate the transformed strain nucleus and carried out a thorough and systematic study on the Green's function method for formulating problems of transformation toughening to enable more powerful tools for that application. In this method, the infinitesimal element with transformation strain can be represented by an assembly of four dislocations, and the different Burgers of four dislocations can simulate different local strains. Then, the generalized SIF generated by four dislocations in strain nucleus is used to simulate the transformed particle toughening. At last, the whole domain switching toughening can be derived by using the Green function integration.

However, in the past works of domain switching toughening, the piezoelectric coupling effect was neglected, additionally, the local internal stresses must be obtained first in the evaluations of the stress intensity factor at crack tip if we use Eshelby technique. Those will lead that the results are not precise enough in piezoelectric anisotropic field. The spontaneous strain generated by domain switching can be simulated directly by dislocations (Ma, 2011), the method which applies the generalized stress filed of dislocations to evaluate the toughening of ferroelectric material could be the most intuitive and effective approach.

In this paper, we firstly obtain the solution of finite crack which can be regarded as the fundamental one, the solution of semi-infinite crack can be obtained by approximation technique from this fundamental solution. Actually, the solutions of other types of cracks and holes can also be obtained by using mapping or approximation technique, so it is a widely applicable solution procedure.

2. Statement of problem

When displacements, electric potential, stresses and electric displacements are independent of x_3 axis in rectangular Cartesian coordinates (x_1,x_2,x_3), the problem can be called plane problem. Linear constitutive relation for electro-elastic material possessing transversal isotropy with respect to all three groups of properties (elastic stiffness, piezoelectric coupling and dielectric permeabilities), with x_2 axis being the axis of symmetry for each, forms

$$\begin{bmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{21}\\ D_1\\ D_2\end{bmatrix} = \begin{bmatrix} c_{11} & c_{13} & 0\\ c_{13} & c_{33} & 0\\ 0 & 0 & c_{44}\\ 0 & 0 & e_{15}\\ e_{31} & e_{33} & 0\end{bmatrix}\begin{bmatrix}u_{1,1}\\ u_{2,2}\\ u_{1,2}+u_{1,3}\end{bmatrix} + \begin{bmatrix}0 & e_{31}\\ 0 & e_{33}\\ e_{14} & 0\\ -\kappa_{11} & 0\\ 0 & -\kappa_{33}\end{bmatrix}\begin{bmatrix}\varphi_{,1}\\ \varphi_{,2}\end{bmatrix} \tag{1}$$

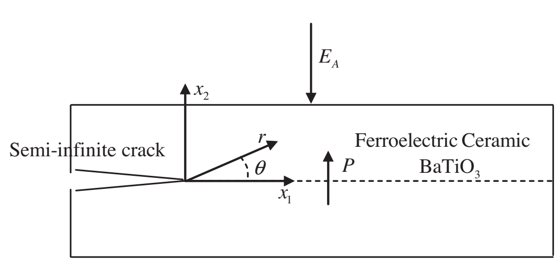

Fig. 1. A semi-infinite crack being perpendicular to spontaneous polarization direction in the ferroelectric ceramic subjected to negative electric field load.

In order to investigate the switching toughening in ferroelectric ceramics with the dislocation simulation method, a typical example of a semi-infinite crack being perpendicular to spontaneous polarization direction in the ferroelectric ceramic subjected to negative electric field load E_A is proposed and shown in Fig. 1. Possessing x_1–x_3 plane being the isotropic plane and crack surface being traction free, the remote load vector can be denoted by $\mathbf{t}_2^\infty = [0 \quad 0 \quad D_2^\infty]^T$.

3. Stroh solution of transversely isotropic piezoelectric field

Generalized displacement, generalized stress function and generalized stress components (Sosa, 1991; Chung and Ting, 1996; Ting, 1996) are shown as

$$\mathbf{u} = [u_1 \quad u_2 \quad \varphi]^T = 2\,\mathrm{Re}\,\mathbf{Af}(z) \tag{2}$$

$$\mathbf{\Phi} = [\phi_1 \quad \phi_2 \quad \phi_3]^T = 2\,\mathrm{Re}\,\mathbf{Bf}(z) \tag{3}$$

$$\mathbf{t}_1 = [\sigma_{11} \quad \sigma_{12} \quad D_1]^T = -\mathbf{\Phi}_{,2} \tag{4}$$

$$\mathbf{t}_2 = [\sigma_{21} \quad \sigma_{22} \quad D_2]^T = \mathbf{\Phi}_{,1} \tag{5}$$

Here $\mathbf{A} = \begin{bmatrix} a_1(p_1) & a_1(p_2) & a_1(p_3)\\ a_2(p_1) & a_2(p_2) & a_2(p_3)\\ a_3(p_1) & a_3(p_2) & a_3(p_3)\end{bmatrix}$, and $\mathbf{B} = \begin{bmatrix} b_1(p_1) & b_1(p_2) & b_1(p_3)\\ b_2(p_1) & b_2(p_2) & b_2(p_3)\\ b_3(p_1) & b_3(p_2) & b_3(p_3)\end{bmatrix}$ are 3×3 complex matrices, and $\mathbf{f}(z) = [f(z_1) \ f(z_2) \ f(z_3)]^T$ is the vector of arbitrary function to be determined.

Matrices **A** and **B** should meet the following normalized orthogonality and closed relations,

Orthogonality relation

$$\begin{bmatrix}\mathbf{B}^T & \mathbf{A}^T\\ \bar{\mathbf{B}}^T & \bar{\mathbf{A}}^T\end{bmatrix}\begin{bmatrix}\mathbf{A} & \bar{\mathbf{A}}\\ \mathbf{B} & \bar{\mathbf{B}}\end{bmatrix} = \begin{bmatrix}\mathbf{I} & \mathbf{0}\\ \mathbf{0} & \mathbf{I}\end{bmatrix} \tag{6}$$

Closed relation

$$\begin{bmatrix}\mathbf{A} & \bar{\mathbf{A}}\\ \mathbf{B} & \bar{\mathbf{B}}\end{bmatrix}\begin{bmatrix}\mathbf{B}^T & \mathbf{A}^T\\ \bar{\mathbf{B}}^T & \bar{\mathbf{A}}^T\end{bmatrix} = \begin{bmatrix}\mathbf{I} & \mathbf{0}\\ \mathbf{0} & \mathbf{I}\end{bmatrix} \tag{7}$$

The corresponding intrinsic equation is shown as

$$\begin{bmatrix} c_{11}+c_{44}p^2 & c_s p & e_s p\\ c_s p & c_{44}+c_{33}p^2 & e_{15}+e_{33}p^2\\ e_s p & e_{15}+e_{33}p^2 & -(\kappa_{11}+\kappa_{33}p^2)\end{bmatrix}\begin{bmatrix}a_1\\ a_2\\ a_3\end{bmatrix} = \begin{bmatrix}0\\0\\0\end{bmatrix} \tag{8}$$

If the determinant of coefficient matrix equals to zero, the following algebraic equation is obtained

$$d_3p^6 + d_2p^4 + d_1p^2 + d_0 = 0 \tag{9}$$

where

$$\begin{aligned}
d_0 &= c_{11}(c_{44}\kappa_{11} + e_{15}^2)\\
d_1 &= c_{44}(c_{11}\kappa_{33} + e_{15}^2) + \kappa_{11}(c_{11}c_{33} + c_{44}^2 - c_s^2)\\
&\quad + 2e_{15}(c_{11}e_{33} - c_se_s) + c_{44}e_s^2\\
d_2 &= c_{33}(c_{44}\kappa_{11} + e_s^2) + \kappa_{33}(c_{11}c_{33} + c_{44}^2 - c_s^2)\\
&\quad + 2e_{33}(c_{44}e_{15} - c_se_s) + c_{11}e_{33}^2\\
d_3 &= c_{44}(c_{33}\kappa_{33} + e_{33}^2)\\
c_s &= (c_{13} + c_{44})\\
e_s &= (e_{15} + e_{31})
\end{aligned}$$

Possessing three complex roots which imaginary parts are greater than zero, the eigenvector **A** corresponding each p_α can be obtained, namely