A Model of electric fracture and fatigue of ferroelectric material under electromechanical loading

D.N. Fang and G.Z. Mao
Department of Engineering Mechanics, Tsinghua University, Beijing 100084, China

ABSTRACT
The fracture and fatigue of ferroelectric ceramics under an electric field or a combined electric and mechanical loading are investigated in this paper. Domain switching is generally regarded as the cause for nonlinearity of ferroelectrics. A group of integrity expressions for the domain switching regions near the crack tip are given to distinguish the different regions of 90°domain switching and 180°domain switching under various electromechanical coupling loads, as well as under different initial poling directions. Based on the two-step switching criteria, another method is additionally developed to discuss the domain switching zones. The toughness variation of ferroelectric ceramics due to the domain switching is analyzed, showing that a positive electric field enhances the propagation of an insulating crack perpendicular to the poling direction, while a negative field impedes it. The problem of electric-field-induced fatigue failure in ferroelectric ceramics is theoretically and numerically studied by modifying the small-scale domain switching model[1][2]. In the modified analytical model presented in this paper, both the effect of anisotropy of the material and the effect of the electromechanical coupling of loading are considered. The fatigue crack growth under various coupling loads and the effects of the stress field and electric field on toughness variation are analyzed. The prediction of the crack growth versus cyclic electric field agrees well with experimental measurements.
KEYWORDS: domain switching; fracture toughness; fatigue; ferroelectric

INTRODUCTION

The intrinsic electromechanical properties and quick time response to external exactions make ferroelectrics ceramics ideal materials for the fabrications of electromechanical sensors, transducers, and adaptive (smart) structures[3]. Ferroelectric ceramics, as one of the most important functional ceramics, call for a better understanding of their failure mechanisms.

A small-scale domain switching model[1][2] based on nonlinear fracture mechanics was proposed. By employing the model, toughness variation of ferroelectrics induced by domain switching under uniform, non-uniform, or cyclic electric loading was evaluated. The mechanism of fatigue crack growth was revealed as the following recurrent processes of initiation, growth, arrest and re-initiation[4]. However, in this model, the coupling of electric and mechanical fields, as well as the anisotropy of the material properties, was neglected.

X Zeng and R K N D Rajapakse(2001)[5] first considered the two problems, electromechanical coupling and material anisotropic. Domain switching zone was numerically analyzed. And the toughness variation was evaluated by a scheme similar to that used in the study of transformation toughening of ceramics[6]. But the numerically results showed that a positive electric field impeded the propagation of an insulating crack perpendicular to the poling direction, while a negative field enhanced it. Such results are opposite to experimental observations. This problem, as well as fatigue crack growth under coupling loadings considering material anisotropic, motivates the present study.

A new domain-switching criterion for ferroelectric ceramics is proposed, in which each 180° switching is divided into two successive 90° switchings[7]. The general electroelastic solution in terms of complex potentials, which was performed on a piezoelectric material containing elliptical hole[8][9], is applied to investigate a ferroelectrics ceramic with an infinite crack in this paper.

In this paper, the failure mechanisms of electric fracture and fatigue are revealed by modifying the small-scale domain switching model. In the modified analytical model, both the effect of anisotropy of the material and the effect of the electromechanical coupling of loading are considered. A group of expressions for the domain switching regions near the crack tip are revealed. A more reasonable $\Delta K/K_E - \phi$ curve is given to analyze the toughness variation of ferroelectric ceramics due to the domain switching. The fatigue crack growth under alternative electromechanical coupling loadings is investigated. And the numerically results are studied and compared with available experimental observations.

DOMAIN SWITCHING ZONE 1

Consider the case of plane strain with domain switching in x_1 - x_2 plane. As shown in Fig.1, the poling axis of the medium makes an angel ϕ with x_1 axis.

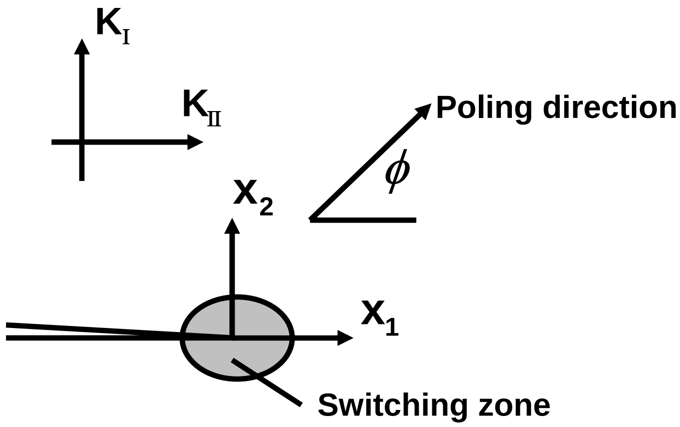

Fig.1 Switching zone near the tip of a crack

The general solution for two-dimensional piezoelectricity, the expressions for stress field and electric field near the crack tip considering the coupling loadings are adopted[10].

Without resorting to the details of non-equilibrium thermodynamic process of domain switching, Hwang et al[8] proposed the following energy-based criterion to determine the critical loading level at which domain switching occurs:

$$\sigma_{ij}\Delta\varepsilon_{ij} + E_i\Delta P_i \geq 2P_sE_c \tag{1}$$

In despite of the different expressions of spontaneous strain and polarization between 90° and 180° domain switching, a uniform express of the boundary of a domain switching zone with a given ϕ can be drawn in terms of the radius $r(\theta)$ as

$$\sqrt{r} = \frac{1}{2\sqrt{2\pi}\,P_sE_c}\,\mathrm{Re}\sum_{k=1}^{3}\frac{h_k(\phi)(\Lambda_{k1}K_I + \Lambda_{k2}K_{II} + \Lambda_{k3}K_D)}{\sqrt{\cos\theta + \mu_k\sin\theta}} \tag{2}$$

where ϕ is initial poling direction. $h_k(\phi)$ are only determined by material properties and ϕ, different between 90° and 180° switching. For 90° domain switching,

$$h_k(\phi) = \gamma_s\left[(1-\mu_k^2)\cos 2\phi + 2\mu_k\sin 2\phi\right] - \sqrt{2}P_s\left[s_k\cos(\phi \pm \frac{3}{4}\pi) + t_k\sin(\phi \pm \frac{3}{4}\pi)\right] \tag{3}$$

while for 180° domain switching

$$h_k(\phi) = 2P_s(s_k\cos\phi + t_k\sin\phi) \tag{4}$$

Equations (2), (3) and (4) show that domain switching zone is determined by electromechanical coupling loading, material properties and initial poling direction. If both 90° and 180° domain switching meet the switching criterion, the actual switching zone near tip occurs in the direction with the higher value of radius $r(\theta)$ as.

In this paper, PZT-5H is used in numerical study. Domain switching zone under various electromechanical coupling loadings, as well as under different initial poling directions, can be given by numerically computing based on equations (2), (3) and (4).

As shown in Fig.2, a stationary crack under an applied electric field intensity factor ($K_E = 0.16 MPa\sqrt{m}$) is firstly considered. The crack tip locates the grid origin. Curve 1 and curve 2 in Fig.2 show the shape of 90° , 180° domain switching zones corresponding to the initial poling direction $\phi = 0^\circ$ respectively. Curve 3 shows that 90° domain switching is the only one near the crack tip under the initial poling direction $\phi = 90^\circ$.

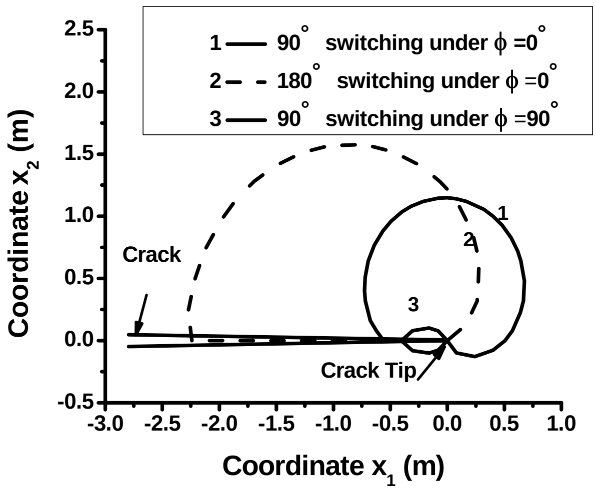

Fig.2 Domain switchings under $K_E = 0.16 MPa\sqrt{m}$

DOMAIN SWITCHING ZONE 2

A sufficiently spindly ellipse can be similarly regarded as a slit crack. To gain the expressions of coupling fields near the crack tip, the electroelastic solution in terms of complex potentials to a piezoelectric material containing elliptical hole[8][9] is applied in this paper.

In the new domain-switching criterion for ferroelectric ceramics, to explain the phenomenon that a suddenly poled ferroelectric ceramic have significantly larger remnant polarization and strain than the corresponding values of a gradually poled one, an assumption that each 180° switching is divided into two successive 90° switchings is proposed. An electric field can result in a single 90° switching or two successive 90° switchings, so-called the first 90° switching and the second 90° switching to form a 180° domain reorientation.

According to the Gibbs free energy-based domain-switching criterion developed by Lu, W. and Fang, D. N, et al[12], the first 90° switching as well as a single 90° domain switching occurs when

$$\Delta g \geq P_s E_c \tag{5}$$

where Δg denotes the variation of Gibbs free energy due to domain switching, while the second 90° switching criterion is given as

$$\Delta g \geq 2 P_s E_c \tag{6}$$

Numerical computation is also carried out to analyze the domain switching zones in this paper. Fig.3 shows the shape of the switching zones corresponding to the initial poling direction $\phi = 90^0$ (perpendicular to the crack) and a positive electric field loading. The coordinates in Fig.3 are normalized by $r_0 = [K_E / 2\sqrt{\pi}\, E_c]^2$.

Unlike traditional domain switching zones predictions, the 180° switching zone is inside the first 90° domain switching zones, which is decided by the switching criterion.

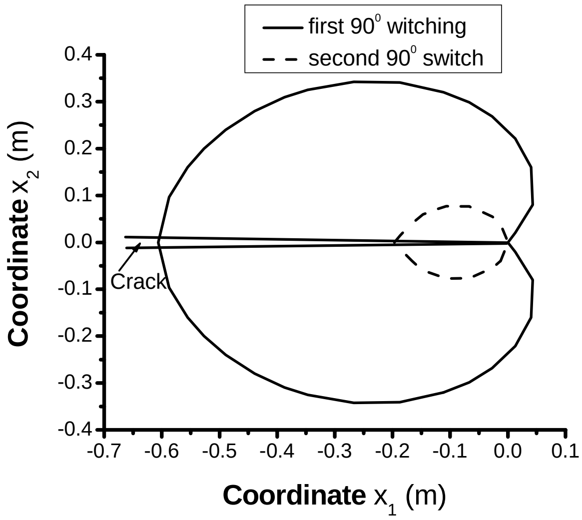

Fig.3 Domain Switchings zones induced by an positive electric field

FRACTURE TOUGHNESS VARIATION

In the present study, attention is focused on a mode I crack. Near the crack tip the stress approaches a level characterized by a local stress intensity factor K_{tip}. By the method of inclusion, Xu and Rajapakse (1999)[10] gave the change in mode I fracture toughness ΔK as

$$\Delta K = \frac{1}{\sqrt{8\pi}} \int_{\Omega} (\mathrm{Re} \sum_{k=1}^{3} \frac{G_k (1+\mu_k^2)}{(\cos\theta + \mu_k \sin\theta)^{3/2}}) r^{-1/2} dr d\theta \tag{7}$$

where complex parameter G_k is solely determined by material properties.

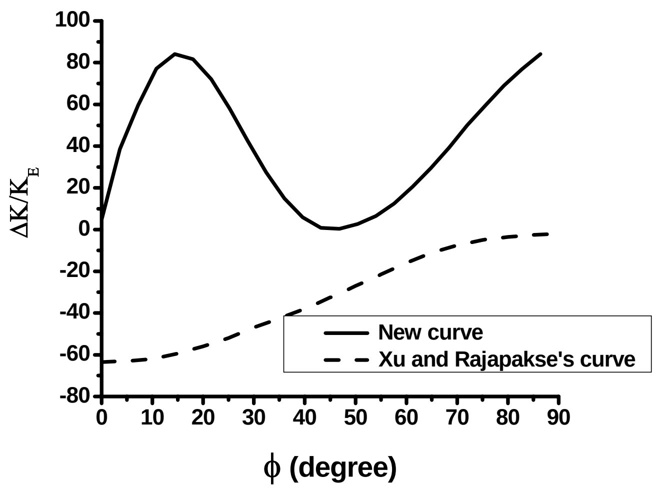

Fig.4 $\Delta K/K_E - \phi$ *relation curve*

By numerical integration based on equation (7), fracture toughness variation ΔK induced by the domain switching zone is evaluated. Using the similar method, Xu and Rajapakse[10] gave the relation curve about initial poling directions to fracture toughness variation ΔK, as shown in Fig.4. It shows that a positive electric field induces negative ΔK, while a negative one induces positive ΔK. That means a positive electric field impedes the growth of a crack, while a negative field enhances it. And such results are opposite to experimental observations. This problem does not exist in the new $\Delta K/K_E - \phi$ curve given in this paper, as shown in Fig.4. That $\Delta K/K_E$ reaches its maximum value when $\phi = 14.400^\circ$ and the minimum zero when $\phi = 45^\circ$ is another numerical result.

FATIGUE CRACK GROWTH

The mechanism of fatigue crack growth was revealed by Zhu and Yang as the following recurrent processes of initiation, growth, arrest and re-initiation[4]. In this paper, the effects of electromechanical coupling loadings and material anisotropy property are both considered. The method of numerical simulation is used in the study.

A stationary crack whose initial half-length a is 0.01m is considered in the sample calculation. The initial poling direction is 90° . The crack undergoes a cyclic electric field whose peak value is $E_c/2$ ($E_c = 0.9MVm^{-1}$), that is, $K_E = 0.08MV/m^{1/2}$ is constant. Fig.5 shows the $K_{tip}(\Delta a)$ versus the crack growth length Δa curve.

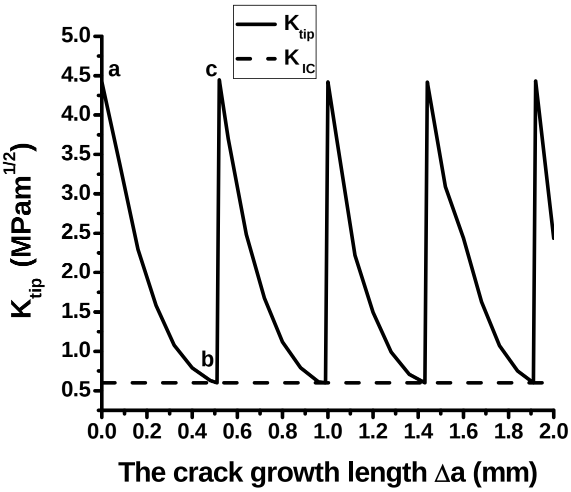

Fig.5 $K_{tip}(\Delta a)$ at the crack tip vs. the crack growth Δa

The induced initial stress intensity factor K_{tip} is beyond K_{IC}, see point a in Fig. 5. So the crack starts to grow. And as the crack grows, K_{tip} decreases monotonically. The crack arrests at $K_{tip}(\Delta a) = K_{IC}$, see point b. Upon the reversal of the electric field, the polarization directions of domains near the arrested crack tip with the electric field are changed, and domain switching reactivates. As shown in Fig.5, K_{tip} jumps from point b, corresponding to the arrested state, to point c, indicating that the newly switched domains re-initiate the crack. The process of initiation, growth, arrest and re-initiation repeats itself, leading to cyclic crack growth.

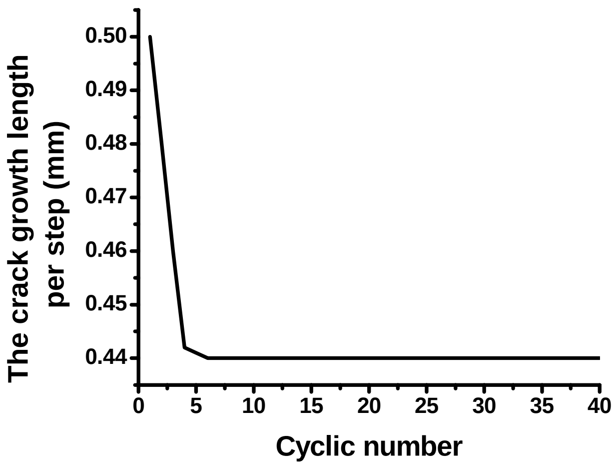

Fig.6 Crack growth per reversal vs. reversal number

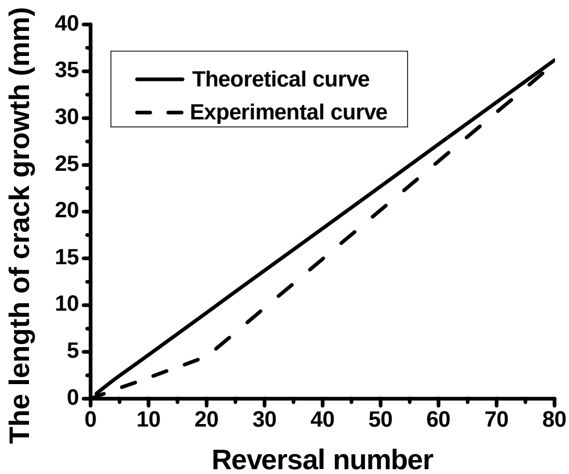

Fig.7 The crack growth vs the reversal number

Fig.6 shows the curve of the crack increment in each electric field reversal versus the reversals number. As shown in the figure, with the reversal, the crack extends rapidly, and then slows down, gradually entering a stabilized stage (The crack increment in each reversal reaches a constant, 0.44mm, in the sixth reversal. The constant has nothing to do with the crack length). This result agrees with the experiment observations by Cao and Evans (1994)[13] qualitatively. Fig.7 shows the theoretical and experimental curves of the crack growth versus the reversal number. The numerical result is in of accord with the experiment reservations.

CONCLUSION

The fracture and fatigue failure in ferroelectrics ceramic are theoretically and numerically studied in this paper, based on modifying the small-scale domain switching model, considering both electromechanical coupling loadings and anisotropy of the material. A group of expressions for the domain switching zones near the crack tip are given to distinguish the different regions of 90 ° domain switching and 180 ° domain switching under various electromechanical coupling loadings, as well as under different initial poling directions. The toughness variation induced by domain switching is investigated. An acceptable curve of $\Delta K/K_E$ versus ϕ shows a positive electric field enhances the propagation of a crack, while a negative electric field impedes it. In addition, the effects of a stress field and an electric field on toughness variation are also analyzed. Fatigue crack growth under various coupling loadings is numerically simulated. A cyclic electric field below the coercive electric field can also cause fatigue crack growth. The cyclic electric field is the primary factor to fatigue crack growth. The phenomenon that with the cyclic electric field reversal the crack increment per reversal gradually decreases to a constant having nothing to do with the crack length is theoretically explained.

REFERENCES

1. Zhu T and Yang W. Toughness variation of ferroelectrics by polarization switch under non-uniform electric field, *Acta. Mate,* 1997,45:4695-4702

2. Yang W and Zhu T. Switching-toughening of ferroelectrics subjected to electric field, *J. Mech. Phys. Solids*, 1998, 46:291-311

3. Loewy R G. Recent developments in smart structures with aeronautical applications, *Smart Mater. Struct*, 1997, 6:R11-42

4. Zhu T and Yang W. Fatigue crack growth in ferroelectrics driven by cyclic electric loading, *J. Mech. Phys. Solids*, 1999, 47:81-97

5. X Zeng and R K N D Rajapakse. Domain switching induced fracture toughness variation in ferroelectrics, *Smart.Mater.Struc*, 2001, 10:203~211

6. McMeeking R M and Evans A G. Mechanics of transformation-toughening in brittle materials, *Am. Ceram. Soc*, 1982, 65:242-246

7. Fa-Xin Li, Dai-Ning Fang and Ai-Kah Soh. An analytical axisymmetric model for the poling-history dependent behavior of ferroelectric ceramics. *Smart Mater. Struct*. 13 (2004) 1–8

8. Horacio Sosa. Plane problems in piezoelectric media with defects. *Int. J solids. Structure.* Vol 28, 1991,No.4: 491-505.

9. Horacio Sosa and Naun Khutoryansky. New developments concerning piezoelectric materials with defects. *Int. J solids. Structure.*1996, 33(23): 3399-3414.

10. X-L Xu and R K N D Rajapakse. Analytical solution for an arbitrarily oriented void/crack and fracture of piezoelectrics, *Acta Mater*, 1999, 47:1725~1747

11. Hwang S C, Lynch C S and McMeeking R M. Ferroelectric/ferroelastic interactions and a polarization switching model, *Acta Metall.Mater*, 1995, 43(5):2073~2084

12. Lu, W., Fang, D. N and Hwang, K. C. Numerical analysis of ferroelectric/ferroelastic domain switching in ferroelectric ceramics. *Computational Material Science.* 1997, 8: 291-308

13. Cao H C and Evans A G. Electric-field-induced fatigue crack growth in piezoelectrics. *J. Am. Ceram. Soc.* 77,1994:1783-1786