Nonuniform ferro-elastic domain switching for the interfacial crack

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Abstract

Existing theoretical researches about interfacial crack of bimaterial piezoelectric composites are confined to linear piezoelectric constitutive relation, neglecting the nonlinear part driven by domain switching. This paper attempts to extend the research of mode III interfacial crack from linear piezoelectricity to nonlinear ferroelectricity. The analysis focuses on the variation of stress intensity factor caused by domain switching, with an arbitrary three-dimensional initial poling orientation. Due to the mismatch of material properties, an asymmetric nonuniform domain switching zone is achieved around the interfacial crack under the nonuniform domain switching criterion. By employing the weight function method, analytic forms of mono-domain and multi-domain toughening effects about stationary and quasi-static steady-state crack are obtained, respectively. The conclusions come to that domain switching of mode III quasi-static steady-state growing interfacial crack has a positive effect to toughen the material. The research can provide some guidance for material selection to maximize the effect of ferro-elastic switch toughening.

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1. Introduction

Due to strong electro-mechanical coupling effects, piezoelectric materials have been widely used in various aspects (Scott, 2007). Specifically, multilayered actuators highlight the low driving voltage and quick response time. Their low fracture toughness, however, has increasingly become a barrier to the wide applications of piezoelectrics. Consequently, the researches about interfacial cracks, especially the fracture of bimaterial composites, have attracted lots of attention in the past few decades. Despite the low fracture toughness of ferroelectrics, fortunately, ferroelectric composites can increase the toughness via domain switching process.

This paper deals with a mode III interfacial crack while considering the effect of domain switching. A novel nonuniform switching criterion, proposed by Cui and Zhong (2012b), is adopted. Domain switching analysis for interfacial crack is carried on in section 2 with an asymmetric domain zone obtained. In section 3, analytic forms of mono-domain toughening about stationary and quasi-static growing steady-state cracks are calculated respectively. Then the results are extended to multi-domain by orientation distribution function and Reuss type approximation. Finally, conclusions are summarized in section 4.

2. Domain switching analysis

2.1. Domain switching induced by crack tip field

In this work, attention is concentrated on a semi-infinite mode III interfacial crack problem, as schematically illustrated in Fig. 1(a). Two dissimilar ferro-electric materials (denoted by the superscripts of I and II) occupy the upper and lower half planes, with anti-plane mechanical loads applied in the infinity. Two coordinate systems are involved. A global Cartesian coordinate system \((x_1, x_2, x_3)\) is attached to the cracked solid. A local Cartesian coordinate system \((x'_1, x'_2, x'_3)\) is attached to the mono-tetragonal crystal, as depicted in Fig. 1(b).

First, one obtains the asymptotic expansion of the mode III semi-infinite interfacial crack tip stress field,

\[
\sigma_{31} = -\frac{K_{app}}{\sqrt{2\pi r}} \sin \frac{\varphi}{2}, \quad \sigma_{32} = \frac{K_{app}}{\sqrt{2\pi r}} \cos \frac{\varphi}{2},
\]

(1)

![Fig. 1. (a) A mode III semi-infinite interfacial crack; (b) Schematic of domain switching of tetragonal crystal in the local coordinate.](image)

Then, we calculate the switch-induced strain. Each mono-domain owns six types of orientations, as shown in Fig. 1(a). The domain switching processes are categorized into two kinds, i.e. switching of \(180^\circ\) and \(90^\circ\). Only \(90^\circ\) switching needs to be considered, because \(180^\circ\) switching can be divided into two procedures of \(90^\circ\) switching (Hwang et al., 1995). \(90^\circ\) switch-induced strain in the local coordinate can be described as follows,

\[
[\Delta \varepsilon_{ij}^{\alpha}] = \varepsilon_{sp} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \quad [\Delta \varepsilon_{ij}^{\beta}] = \varepsilon_{sp} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix},
\]

(2)
where $\Delta \tilde{e}_{ij}^\alpha$ represents the strain when the poling orientation changes from $x_3'$ axis to $x_1'$ axis, $\Delta \tilde{e}_{ij}^\beta$ the strain when the poling orientation changes from $x_3'$ axis to $x_2'$ axis and $\varepsilon_{sp} = (c-a)/a$ the spontaneous polarization strain, where $c$ and $a$ are lattice parameters of tetragonal crystal.

The domain switching process is discussed under three-dimensional initial poling orientation. Euler angles $(\theta, \phi, \psi)$ are used to describe the relationship between the local Cartesian coordinate and the global Cartesian coordinate, as depicted in Fig. 2(a). The coordinate transformation tensor $M_{ij}$ between the global coordinate and the local coordinate is listed as follows:

$$ [M_{ij}] = \begin{bmatrix} \cos \theta \cos \phi \cos \psi - \sin \phi \sin \psi & -\cos \psi \sin \phi - \cos \theta \cos \phi \sin \psi & \cos \phi \sin \theta \\ \\ \cos \theta \cos \phi \sin \psi + \cos \phi \sin \psi & \cos \phi \cos \psi - \cos \theta \sin \phi \sin \psi & \sin \theta \sin \phi \\ \\ -\cos \psi \sin \theta & \sin \theta \sin \psi & \cos \theta \end{bmatrix}. \quad (3) $$

Then we obtain two forms of switch-induced strains in the global coordinate,

$$ \Delta e_{ij}^\alpha = M_{ik} \Delta e_{kl}^{\alpha \alpha} M_{jl}, \quad \Delta e_{ij}^\beta = M_{ik} \Delta e_{kl}^{\beta \beta} M_{jl}, \quad (4) $$

and the corresponding work released by domain switching,

$$ W_\alpha = \sigma_{ij} \Delta e_{ij}^\alpha = \frac{K_{app}}{\sqrt{2\pi r}} \varepsilon_{sp} [3m + m \cos 2\psi - n \sin 2\psi], W_\beta = \sigma_{ij} \Delta e_{ij}^\beta = \frac{K_{app}}{\sqrt{2\pi r}} \varepsilon_{sp} [3m - m \cos 2\psi + n \sin 2\psi]. \quad (5) $$

where $m = \sin \theta \cos \theta \sin (\phi/2 - \phi)$, $n = \sin \theta \cos (\phi/2 - \phi)$.

Next, the actual domain switching work needs to be determined. Following analysis of Yang et al. (2001) about the out-of-plane poling problem, domain switching should proceed in the process to release the maximum of work. One obtains the actual domain switching work,

$$ W_{actual} = \max_{\psi \in [0, 2\pi]} [W_\alpha, W_\beta] = \frac{K_{app}}{\sqrt{2\pi r}} \varepsilon_{sp} [3m + \sqrt{m^2 + n^2}]. \quad (6) $$

In these two forms of domain switching processes, the actual switch-induced strains are identical.

Fig. 2. (a) Transformation between the local and global coordinate; (b) The contours of a nonuniform domain switching zone.

2.2. Domain switching zone

In this section, domain switching zone is determined via a nonuniform domain switching criterion. A nonuniform switching criterion is proposed by Cui and Zhong (2012) with the following piecewise function:

$$ V_{90} = \begin{cases} 0 & \sigma_{DS} < \sigma_{th}^I \\ V_{th} + k_1 (\sigma_{DS} - \sigma_{th}^I) & \sigma_{th}^I \leq \sigma_{DS} \leq \sigma_{sat}^I \text{ in I} \\ V_{sat} & \sigma_{DS} > \sigma_{sat}^I \end{cases} \quad , \quad V_{90} = \begin{cases} 0 & \sigma_{DS} < \sigma_{th}^II \\ V_{th} + k_1 (\sigma_{DS} - \sigma_{th}^II) & \sigma_{th}^II \leq \sigma_{DS} \leq \sigma_{sat}^II \text{ in II} \\ V_{sat} & \sigma_{DS} > \sigma_{sat}^II \end{cases} \quad (7) $$
where \( V_{90} \) denotes the volume fraction of the part that experiences 90° domain switching, \( \sigma_{th} \) and \( \sigma_{sat} \) show the threshold stress to trigger domain reorientation and to saturate switching respectively, \( V_{90}^{th} \) and \( V_{90}^{sat} \) are the corresponding volume fractions, \( k \) denotes the coefficient of proportionality. \( \sigma_{DS} = \sigma_{ij} \Delta \varepsilon_{ij} / 2 \varepsilon_{sp} \) is the unique control variable of the criterion, measuring the actual work during domain switching.

The realistic switch-induced strain can be written as

\[
\Delta \varepsilon_{ij} = \Delta \varepsilon_{ij} V_{90} = \varepsilon_{sp} V_{90} \Delta \varepsilon_{ij}.
\]

Based on the nonuniform switching criterion (7), one gets the shape of switching zone for a certain initial poling orientation via setting \( \sigma_{DS} = \sigma_{th} \)

\[
\sqrt{R_{th}^2} = \frac{K_{app}}{2 \sqrt{2 \pi} \sigma_{th}^2} \left( 3m + m^2 + n^2 \right), \quad \varphi \in [0, \pi]; \quad \sqrt{R_{th}^2} = \frac{K_{app}}{2 \sqrt{2 \pi} \sigma_{th}^2} \left( 3m + m^2 + n^2 \right), \quad \varphi \in [-\pi, 0],
\]

Combining Eqs. (7) and (9), we can visualize the contours of volume fraction \( V_{90} \) around the tip of a mode III interfacial crack, as depicted in Fig. 2(b). In plotting the contour, a stationary crack is considered and we set \( K_{app} = 1 \text{MPa} \sqrt{\text{m}} \), \( \theta = \pi / 2 \), \( \phi = 0 \). Material constants are listed in Table 1. The domain switching zone is asymmetric due to the mismatch of bimaterial properties. The nonuniform switching zone can be divided into an asymmetric saturated core and an asymmetric transitional annulus.

<table>
<thead>
<tr>
<th>Table 1. Elastic and ferroelectric parameters of the materials.</th>
<th>( \varepsilon_{sp} )</th>
<th>( V_{90}^{th} )</th>
<th>( V_{90}^{sat} )</th>
<th>( \mu (\text{GPa}) )</th>
<th>( \sigma_{th} (\text{MPa}) )</th>
<th>( \sigma_{sat} (\text{MPa}) )</th>
<th>( k (10^{-3} \text{MPa}^{-1}) )</th>
</tr>
</thead>
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<tr>
<td>Material I</td>
<td>0.0154</td>
<td>0.027</td>
<td>0.51</td>
<td>22.39</td>
<td>11.5</td>
<td>100</td>
<td>5.438</td>
</tr>
<tr>
<td>Material II</td>
<td>0.013</td>
<td>0.105</td>
<td>0.54</td>
<td>12.41</td>
<td>10.3</td>
<td>95</td>
<td>5.136</td>
</tr>
</tbody>
</table>

3. Nonuniform switch toughening

3.1. Nonuniform switch toughening

Transformation strain induced by domain switching is the source of toughening (Yang, 2002). To quantify the interaction between transformation strain and interfacial crack, the weight function method is applied to evaluate the toughening effect induced by nonuniform ferro-elastic domain switching. According to the method given by Gao (1992), we calculate the weight function of a mode III semi-infinite interfacial crack between dissimilar isotropic bimaterial, to characterize the influence of switch-induced strain on the crack quantitatively,

\[
U_y^I = \frac{\mu_I}{2 \sqrt{2 \pi} (\mu_I + \mu_{II})^{3/2}} U_{ij}^{th}, \quad U_y^II = \frac{\mu_I}{2 \sqrt{2 \pi} (\mu_I + \mu_{II})^{3/2}} U_{ij}^{II},
\]

where \( U_{13} = -\sin 3\theta / 2, U_{23} = \cos 3\theta / 2, U_{33} = 0 \) and \( \mu_I, \mu_{II} \) denote the shear moduluses of the bimaterial. Then, the formula of switch toughening can be achieved,

\[
\Delta K = \Delta K^I + \Delta K^{II} = 2 \mu_I \int_{A_{th}} U_{ij}^{th} \Delta \varepsilon_{ij} \text{d}A + 2 \mu_{II} \int_{A_{th}} U_{ij}^{II} \Delta \varepsilon_{ij} \text{d}A = \Delta K_{uni} + \Delta K_{uni}^{II} + \Delta K_{tran} + \Delta K_{tran}^{II} + \Delta K_{sat} + \Delta K_{sat}^{II}
\]

where \( A_{th} \) denotes the upper zone of domain switching and \( A_{II} \) denotes the lower one. Due to the piecewise function of \( V_{90} \), it is convenient to divide the toughness increment \( \Delta K \) into three fractions: the uniform switching fraction, the transitional switching fraction, and the saturated fraction.

3.2. Switch toughening effect of a stationary growing crack

Our calculation begins with a stationary crack. The restriction of \( \theta = \pi / 2 \) is removed in this subsection. First, we concentrate on the uniform fraction of material I. Substituting \( V_{90} = V_{90}^{th} \) and Eq. (9) into Eq. (11), toughening from uniform domain switching can be obtained,

\[
\Delta K_{uni}^{I} = \frac{\mu_I \mu_{II} \varepsilon_{sp}^{th}}{2 \sqrt{2 \pi} (\mu_I + \mu_{II})} \int_{\phi_k}^{\pi/2} \frac{1}{V_{90}^{th} U_{ij} \Delta \varepsilon_{ij} \frac{1}{2} \text{d} \varphi} = \frac{\mu_I \mu_{II} \varepsilon_{sp}^{th}}{2 \pi (\mu_I + \mu_{II})} \int_{\phi_k}^{\pi/2} \frac{\Theta(\phi_k) - \Theta(\phi)}{\sigma_{th}^{th}} K_{app},
\]

where 90\(^{\circ}\) denotes the volume fraction of the part that experiences 90° domain switching, \( \sigma_{th} \) and \( \sigma_{sat} \) show the threshold stress to trigger domain reorientation and to saturate switching respectively, \( V_{90}^{th} \) and \( V_{90}^{sat} \) are the corresponding volume fractions, \( k \) denotes the coefficient of proportionality. \( \sigma_{DS} = \sigma_{ij} \Delta \varepsilon_{ij} / 2 \varepsilon_{sp} \) is the unique control variable of the criterion, measuring the actual work during domain switching.
where \( \Theta(\phi) = \frac{1}{4} \sin^2 \phi \left[ (4 + 5 \cos 2\theta) \sin(2\phi - 2\theta) + 2 (6 + 5 \cos 2\theta - 6 \cos \theta \sin(\phi - \frac{\phi}{2}) \sqrt{1 + 3 \cos 2\theta + 2 \cos (2\phi - \phi) \sin^2 \theta}) \sin \phi \right]. \)

Then, we get the saturated and transitional fraction from non-uniform switching,

\[
K_{\text{sat}}^i = \frac{2 \mu_i \mu_{\text{eff}}}{\sqrt{2 \pi} (\mu_i + \mu_{\text{eff}})} \int_\phi^\pi \int_{\phi_{\text{th}}}^{\phi_{\text{eff}}} \int_{\phi_{\text{th}}}^{\phi_{\text{eff}}} \frac{d\phi}{\sin \phi} \left[ 1 - \frac{1}{\sigma_{\text{th}}} \right] \Theta(\phi^+) - \Theta(\phi^-) \right] K_{\text{app}},
\]

\[
\Delta K_{\text{tran}}^i = \frac{\mu_i \mu_{\text{eff}}}{\sqrt{2 \pi} (\mu_i + \mu_{\text{eff}})} \int_{\phi_{\text{th}}}^{\phi_{\text{eff}}} \int_{\phi_{\text{th}}}^{\phi_{\text{eff}}} \int_{\phi_{\text{th}}}^{\phi_{\text{eff}}} \frac{d\phi}{\sin \phi} \left[ 1 - \frac{1}{\sigma_{\text{th}}} \right] \Theta(\phi^+) - \Theta(\phi^-) \right] K_{\text{app}}.
\]

Similar conclusion can be obtained for material II. Substituting Eqs. (12), (13) and (14) into Eq. (11), we obtain the whole switch toughening effect,

\[
\Delta K = \mu_i \left[ \Theta(\phi^+) - \Theta(\phi^-) \right] + N_{\text{th}} \left[ \Theta(\phi^+) - \Theta(\phi^-) \right] K_{\text{app}},
\]

where \( \mu_{\text{eff}} = \frac{2 \mu_i \mu_{\text{th}}}{\mu_i + \mu_{\text{th}}} \), \( N_{\text{th}} = \frac{\phi_{\text{th}}}{4\pi} \left[ 1 - \sigma_{\text{th}} \right] \), and \( \phi_1 \) and \( \phi_2 \) are the initial and final values of the poling angle for switching zone. In Eq. (15), three coupling parameters, \( \mu_{\text{eff}} \), \( N_{\text{th}} \) and \( N_{\text{th}} \), are defined to evaluate the influence of bimaterial constants.

Substituting the switching zone into Eq. (15), we get the toughening effect of mode III stationary interfacial crack,

\[
\Delta K = \mu_i \left[ \Theta(\phi^+) - \Theta(\phi^-) \right] + N_{\text{th}} \left[ \Theta(\phi^+) - \Theta(\phi^-) \right] K_{\text{app}} = 0.
\]

It is concluded that in spite of the involvement of interface, transformation toughening effect is zero for a stationary crack, which is corresponding to results of the homogenous material (Yang et al., 2001).

3.3. Switch toughening effect of a quasi-static steady-state growing crack

In this subsection, concentration is centered on the toughening of a quasi-static steady-state growing crack. We assume that the crack is growing along the interface. Restriction of \( \theta = \pi / 2 \) is set for simplicity, so that \( \phi^+ = \phi^- = 0 \). It is convenient to divide the domain switching zone into two parts: the front zone and the wake zone,

\[
\Delta K = \Delta K_{\text{front}} + \Delta K_{\text{wake}}.
\]

The front zone can be regarded as a part of a stationary crack. Substituting the initial and final values of the poling angle into Eq. (26), we obtain the toughening effect of the front zone,

\[
\Delta K_{\text{front}} = \mu_i \left[ \Theta(\phi^+) - \Theta(\phi^-) \right] K_{\text{app}}.
\]

Then, the contribution of the wake zone is explored. Similar to the settlement of the stationary crack, we also divide the wake zone into three fractions: the uniform one, the transitional one and the saturated one,

\[
\Delta K_{\text{wake}} = \lim_{h/\Delta z \to 0} \left( \Delta K_{\text{uni}}^{\text{wake}} + \Delta K_{\text{tran}}^{\text{wake}} + \Delta K_{\text{sat}}^{\text{wake}} \right),
\]

where \( h \) denotes the height of the wake zone, and \( \Delta z \) the increment length of the crack. The area of the wake fraction is an infinite horizontal strip with a finite height. And the corresponding area elements are expressed as

\[
r = r / \sin \phi, \quad dd = r dr d\phi = r / \sin^2 \phi d\phi dh.
\]

Substituting Eq. (20) into Eqs. (12), (13) and (14) yields that,

\[
\lim_{h/\Delta z \to 0} \Delta K_{\text{uni}}^{\text{wake}} = \mu_i \left[ \frac{\phi_{\text{th}}}{4\pi} \right] \left[ \frac{\psi(\phi^-) - \psi(\phi^+)}{\psi(\phi^+)} \right] K_{\text{app}}
\]

\[
\lim_{h/\Delta z \to 0} \Delta K_{\text{tran}}^{\text{wake}} = \mu_i \left[ \frac{\phi_{\text{th}}}{4\pi} \right] \left[ \frac{\psi(\phi^-) - \psi(\phi^+)}{\psi(\phi^+)} \right] K_{\text{app}}
\]

\[
\lim_{h/\Delta z \to 0} \Delta K_{\text{sat}}^{\text{wake}} = \mu_i \left[ \frac{\phi_{\text{th}}}{4\pi} \right] \left[ \frac{\psi(\phi^-) - \psi(\phi^+)}{\psi(\phi^+)} \right] K_{\text{app}}
\]

where \( \psi(\phi) = 2 \sin \phi \cos^2 (\phi - \phi / 2) \). Substituting Eqs. (21), (22) and (23) into Eq. (19) yields the switch toughening effect of the wake zone,
Finally, combining Eqs. (11), (17), (18) and (24), we obtain the switch toughening effect of a quasi-static steady-state growing crack analytically,

$$K_{\text{tip}} = \left(1 + \frac{1}{3} \left[ N_t \Omega(\phi_{\text{max}}^t) - N_t \Omega(\phi_{\text{max}}^s) \right] \right) K_{\text{app}},$$

where

$$\Omega(\phi) = \phi(\phi) - \Psi(\phi) - \Theta(0) = \frac{1}{4} \left[ 2 \sin \phi - \sin(2\phi - 2\Theta) \right] - 2 \sin \phi \cos^2(\phi - \frac{\phi}{2}) + \frac{1}{4} \sin 2\phi.$$  

The form of the crack tip stress intensity factor (SIF) in Eq. (25) is similar to the conclusion of Cui and Zhong (2012a).

3.4. Multi-domain solution

Now, we concentrate on the unpoled ferroelectrics consisting of domains in different orientations. A random orientation distribution function, $f(\phi) = 1/2\pi$, is introduced to describe the poling orientation of ferroelectrics. We obtain the analytic expression of switch toughening effect for unpoled ferroelectrics,

$$K_{\text{tip}}^{\text{unpoled}} = \int_0^{2\pi} f(\phi) K_{\text{tip}}(\phi) d\phi = \left[ 1 - \frac{\mu}{8\pi} \mu \left( N_t + N_{II} \right) \right] K_{\text{app}}^{\text{unpoled}}.$$

Reuss type approximation is used during the calculation. Since $\mu$, $N_t$, and $N_{II}$ are all positive parameters, $K_{\text{tip}}^{\text{unpoled}} > K_{\text{III}}$. Domain switching of mode III quasi-static growing interfacial crack can toughen the material.

4. Concluding remarks

This work deals with a mode III interfacial crack while considering the effect of domain switching. An asymmetric domain switching zone is obtained due to the mismatch of bimaterial properties. In addition, analytic forms of mono-domain toughening effect about stationary and quasi-static steady-state growing cracks are achieved, which are used to construct the solution for multi-domain. All the solutions are derived in closed forms. $\theta = \pi / 2$ is set for simplicity. The conclusions can be reached from the analysis above:

(1) The involvement of the interfacial crack leads to the asymmetry of the domain switching zone. Under the nonuniform switching criterion, domain switching zone can be divided into saturated cores and transitional annuluses, asymmetric with respect to the plane of $x_i = 0$. The asymmetric switching zone is reduced to a symmetric one when the constituents of bimaterial are identical.

(2) For a mode III stationary interfacial crack, no toughening effect exists despite the mismatch of bimaterial properties, the same to the result of a homogenous ferroelectric material. For a mode III quasi-static steady-state growing interfacial crack, domain switching can toughen the material.

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References


