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ORIGINAL PAPER

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Nanoscale anti-plane cracking of materials with consideration of bulk and surface piezoelectricity effects

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Abstract The influence of surface effect, including surface elasticity and surface piezoelectricity, on the fracture behavior of piezoelectric materials with an anti-plane crack is studied. Based on the coupled surface and interface elasticity model, the solutions to the problem are obtained by applying the singular integral method. By comparing the solutions influenced by the surface piezoelectricity with those affected by the surface elasticity, it is found that the influence of the surface piezoelectricity on the crack opening displacement, the crack electric potential jump across the crack center, the crack tip stress and electric displacement intensity factors cannot be ignored. Under various electrical boundary conditions, the influence of surface piezoelectricity on the sliding displacement, crack tip stress and electric displacement intensity factors exhibits the same tendency. Besides, the influence of surface piezoelectricity on the electric displacement intensity factor is independent of the electrical boundary conditions, which is different from the results where only the surface elasticity is considered.

1 Introduction

Owing to their unique mechanical and physical properties, piezoelectric nanostructured materials have found wide applications in engineering such as powering nanodevices and sensors in the field of medical science, defense technology and environment/infrastructure monitoring. There are increasing demands for studying the mechanic behaviors and properties of piezoelectric nanostructures for their reliability applications [1–4]. Investigation of fracture behavior of piezoelectric nanostructures is very significant for the design and safety analysis of these structures.

However, for piezoelectric nanomaterials, the surface effect becomes more evident due to the larger surface-to-volume ratio. To study the surface effect, the surface model [5] has been widely used by many researchers in predicting the strength of nanostructures and characterizing the effective properties of nanosized structural elements [6–9]. For piezoelectric nanomaterials, surface piezoelectricity may become essential at small scale which is pointed out earlier by Tagantsev [10]. Therefore, it is significant to incorporate electric field dependent surface effects when investigating the fracture behavior of the nanoscale piezoelectric structures. To deal with the surface effect on electro-mechanical properties of piezoelectric nanostructures, this surface model [5] was developed for the piezoelectric nanostructures [11–13]. In this coupling surface model, the surface elasticity, the residual surface stress and electric displacement are both considered to analyze the surface effect. This model was proposed and widely used to study the response of piezoelectric nanostructures. The pioneering

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work was done by Huang and Yu [14] to study the surface piezoelectricity on the electromechanical behavior of a piezoelectric ring. In their work a considerable effect of surface piezoelectricity on the stress and electric fields when the ring size reduced to nanometers was observed. Using the electro-elastic surface theory, Fang et al. [15] carried out the size-dependent effect on electro-mechanical behavior of a multilayer piezoelectric nanocylinder under electro-elastic waves.

Recently, adopting the continuum-based surface model, there has been a growing interest in studying the crack problems at nanoscale and it has proved that when considering fracture behaviors of nanomaterials, the surface effect is inevitable (see for example [16–19]). However, the works listed above did not give the analysis of surface piezoelectricity on the fracture of piezoelectric nanomaterials. Moreover, as a parameter to measure the fracture behavior of the materials, the crack tip field intensity factors play a significant role in assessing the structural safety and the residual life of the structures. For the future applications of fracture in micro/nanoscale material, it is vital to incorporate the influence of surface piezoelectricity in the crack tip field quantities (such as the stress and electric displacement intensity factors). Therefore, researches on an infinite piezoelectric matrix containing nanoscale cracks are relatively limited.

In the present paper, the problem of an anti-plane crack located within a nanoscale piezoelectric material is studied. To analyze the surface piezoelectricity effect, on the crack tip field of an anti-plane crack, the electro-elastic surface/interface theory is adopted. Using Fourier integrals and singular integral methods, the solutions to the problem are derived. The solutions to the sliding displacement, electric potential jump along the crack faces, stress and electric displacement intensity factors are obtained, and some useful conclusions are drawn.

2 Description of the problem

Consider a piezoelectric medium with an anti-plane crack of length $2a$ along the x direction as shown in Fig. 1, where (x, y) is a coordinate system. It is assumed that all the field variables are functions of x and y only, respectively. Let the medium be loaded by a remote uniform anti-plane stress τ_∞ and in-plane electric displacement D_∞ along the y direction. The solving technique employed in the remaining part of this section is not new. There are many references related to this technique. The displacements w along z axis and the electric potential ϕ will be derived from Fourier integrals and characteristic equations. Throughout the paper, for convenience the following notations are used:

$$\{b\} = \{b_1, b_2\}^{\mathrm{T}} = \left\{\tau_{yz}, D_y\right\}^{\mathrm{T}}, \tag{1.1}$$

$$\{b_\infty\} = \{b_{\infty 1}, b_{\infty 2}\}^{\mathrm{T}} = \{\tau_\infty, D_\infty\}^{\mathrm{T}}, \tag{1.2}$$

$$\{U\} = \{U_1, U_2\}^{\mathrm{T}} = \{w, \phi\}^{\mathrm{T}} \tag{1.3}$$

where τ_{yz} and D_y are the stresses and electric displacements, respectively.

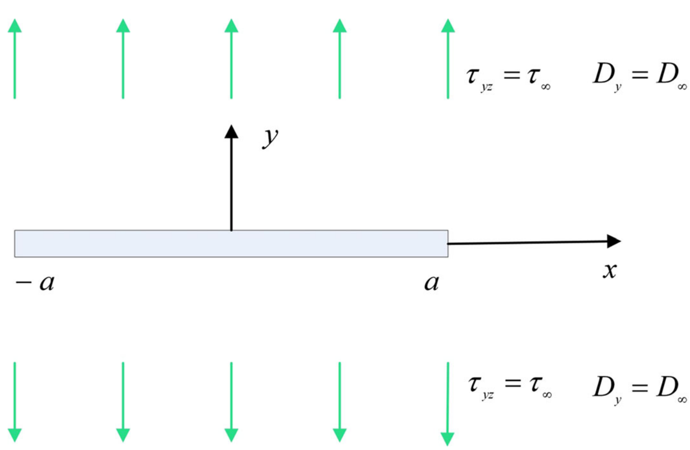

Fig. 1 A piezoelectric nanomaterial with a through-thickness crack, subjected to far-field anti-plane stress and in-plane electrical loads

After a series of solving strategies, the anti-plane stress and in-plane electric displacement can be expressed as [20]

$$\{b\,(x,0)\} = \frac{\Lambda}{2\pi}\int_{-a}^{a}\frac{1}{r-x}\,\{g\,(r)\}\mathrm{d}r + \{b_\infty\} \tag{2}$$

where Λ is the material parameter matrix, defined below,

$$\Lambda = \begin{bmatrix} c_{44} & e_{15} \\ e_{15} & -\in_{11} \end{bmatrix}, \tag{3}$$

and $\{g(x)\}$ is an auxiliary vector along the crack surface, which can be expressed as

$$g_J = 2\frac{\partial U_J\,(x,0)}{\partial x}, \quad J = 1,2. \tag{4}$$

The continuity condition requires that $\{g(x)\}$ vanishes for $|x| > a$.

Under the crack impermeable assumption, the mixed crack boundary condition considering the surface effect is written as follows [21]:

Inside the crack:

$$\tau_{yz}\,(x,0) = 0, \quad D_y\,(x,0) = 0, \quad |x| < a. \tag{5}$$

Along the anti-plane crack surface:

$$\tau_{yz}\,(x,0) + \frac{\partial \sigma_{yz}^{s}}{\partial y} = 0, \quad |x| < a, \tag{6.1}$$

$$D_y\,(x,0) + \frac{\partial D_y^{s}}{\partial y} = 0, \quad |x| < a. \tag{6.2}$$

Based on the coupling surface piezoelectric model, the surface stress and surface electric displacement on the crack surface can be expressed as [12]

$$\sigma_{yz}^{s} = \tau_0 + c_{44}^{s}\frac{\partial w}{\partial y} + e_{15}^{s}\frac{\partial \phi}{\partial y}, \tag{7.1}$$

$$D_y^{s} = D_0^{s} + e_{15}^{s}\frac{\partial w}{\partial y} - \in_{11}^{s}\frac{\partial \phi}{\partial y} \tag{7.2}$$

where τ_0 and D_0^{s} can be termed as the residual surface stress and surface electric displacement without applied strain and electric field; c_{44}^{s}, e_{15}^{s} and $\in_{11}^{s}$ are, respectively, the surface elastic constant, surface piezoelectric constant and surface dielectric constant, which are often determined by extensive atomistic simulations. Thus in the following formulation, the elastic stiffness, dielectric constant and piezoelectric constant of the surface are considered as known quantities.

Substituting the expressions of surface stress and surface electric displacement into Eq. (6) yield

$$\begin{Bmatrix} \tau_{yz}\,(x,0) \\ D_y\,(x,0) \end{Bmatrix} = -\Lambda^{s}\begin{Bmatrix} \frac{\partial^2 w}{\partial y^2} \\ \frac{\partial^2 \phi}{\partial y^2} \end{Bmatrix} \tag{8}$$

where Λ^{s} is a surface parameter matrix, which can be expressed as:

$$\Lambda^{s} = \begin{bmatrix} c_{44}^{s} & e_{15}^{s} \\ e_{15}^{s} & -\in_{11}^{s} \end{bmatrix}. \tag{9}$$

In the piezoelectric material, the governing equations for the bulk are expressed, in the absence of body force and body charge, as:

$$c_{44}\nabla^2 w + e_{15}\nabla^2\phi = 0, \quad e_{15}\nabla^2 w - \in_{11}\nabla^2\phi = 0 \tag{10}$$

where c_{44}, e_{15} and $\in_{11}$ are the elastic, piezoelectric and dielectric coefficients, respectively.

With conventional materials, $c_{44} \in_{11} + e_{15}^2 \neq 0$ [22], thus the above equations can be simplified to two independent biharmonic equations,

$$\nabla^2 w = 0, \quad \nabla^2 \phi = 0. \tag{11}$$

Then considering the surface effect, the boundary conditions along the crack surface of piezoelectric nanomaterial can be expressed as

$$\{b(x,0)\} = \frac{\Lambda^{\mathrm{s}}}{2}\left\{g'(x)\right\}. \tag{12}$$

3 Solution to the problem

Inserting the anti-plane stresses and in-plane electric displacements into the mixed boundary conditions Eq. (12) at $y = 0$ gives

$$\frac{\Lambda}{2\pi}\int_{-a}^{a}\frac{1}{r-x}\{g(r)\}\,\mathrm{d}r + \{b_\infty\} = \frac{\Lambda^{\mathrm{s}}}{2}\left\{g'(x)\right\}. \tag{13}$$

It can be seen that the residual surface stress τ_0 and surface electric displacement D_0^{s} have no influence on mechanical and electric fields. As a result, surface piezoelectricity and surface elasticity contribute to this anti-plane crack problem. That is, in this problem, the surface effect includes only the surface piezoelectricity and surface elasticity. Equation (13) is a system of singular integral equations which has Cauchy-type integral kernel $1/(r-x)$. Let $\bar{r} = r/a$ and $\bar{x} = x/a$, then, under the theory of the integral equation, the solution to $\{g(x)\}$ can be expressed as [23,24]

$$\{g(x)\} = \begin{Bmatrix} g_1(a\bar{r}) \\ g_2(a\bar{r}) \end{Bmatrix} = \sum_{m=1}^{\infty}\begin{Bmatrix} C_{wm} \\ C_{\phi m} \end{Bmatrix}\frac{T_m(\bar{r})}{\sqrt{1-\bar{r}^2}} \tag{14}$$

where $T_m(\bar{r}) = \cos(m\arccos(\bar{r}))$ are the Chebyshev polynomials of the first kind, and C_{wm}, $C_{\phi m}$ are unknown constants to be determined.

Equation (13) can be solved by truncating the first M terms of Eq. (14), i.e. $m = 1, \ldots, M$, and using the well-known integral $\int_{-1}^{1} T_m(\bar{r})/\left[(\bar{r}-\bar{x})\sqrt{1-\bar{r}^2}\right]\mathrm{d}\bar{r} = \pi U_{m-1}(\bar{x})$, where $U_{m-1}(\bar{x}) = \sin(m\arccos\bar{x})/\sqrt{1-\bar{x}^2}$ is the Chebyshev polynomial of the second kind. By adopting collocation techniques, Eq. (13) can be solved [23,24]. Let $x_k = \cos[(2k-1)\pi/(2M)]$, where $k \in [1, M]$, then $-1 \le x_k \le 1$. Substitution of x_k into Eq. (13) yields

$$\left\{\begin{bmatrix} G & 0 \\ 0 & G \end{bmatrix} - \frac{1}{a}\begin{bmatrix} n_{11}Q & n_{12}Q \\ n_{21}Q & n_{22}Q \end{bmatrix}\right\}\{C\} = 2[\Lambda_0]\{b_\infty\} \tag{15}$$

where $\{C\}$ is a column whose elements are C_{wm} and $C_{\phi m}$, respectively, $m = 1\ldots M$; Λ_0 is a $2M \times 2$ matrix whose first M elements are $\{-\bar{\Lambda}_{11}, -\bar{\Lambda}_{12}\}$ and the last M elements are $\left\{-\bar{\Lambda}_{21}, -\bar{\Lambda}_{22}\right\}$; $\bar{\Lambda}_{ij}$ is an element of matrix Λ^{-1}; n_{ij} is an element of matrix $\Lambda^{-1}\Lambda^{\mathrm{s}}$; Q and G are $M \times M$ matrices whose elements respectively are

$$(Q)_{mn} = \frac{n\sin(m\arccos x_m) + x_m\cos(n\arccos x_m)/\sqrt{1-x_m^2}}{1-x_m^2}, \tag{16}$$

and $(G)_{mn} = U_{n-1}(x_m)$. Then the solution of $\{g(x)\}$ can be obtained by $\{C\}$, which can be calculated by Eq. (15). Obviously, the crack sliding displacement δw, electric potential jump along the crack faces $\delta\phi$, stress intensity factor K_{III} and electric displacement intensity factor K_D can be calculated by $\{C\}$ as[22]

$$\delta w = 2w(0,0) = \left(2a\int_{-1}^{\bar{x}}\frac{g_1(a\bar{r})}{2}\mathrm{d}\bar{r}\right)_{\bar{x}=0} = -a\sum_{m=1}^{M}C_{wm}\frac{\sin(m\pi/2)}{m}, \tag{17.1}$$

$$\delta\phi = 2\phi(0,0) = \left(2a\int_{-1}^{\bar{x}}\frac{g_2(a\bar{r})}{2}\mathrm{d}\bar{r}\right)_{\bar{x}=0} = -a\sum_{m=1}^{M}C_{\phi m}\frac{\sin(m\pi/2)}{m}, \tag{17.2}$$

$$\{K_{\mathrm{III}}, K_D\}^{\mathrm{T}} = -\frac{\Lambda}{2}\sqrt{\pi a}\left\{\sum_{m=1}^{M}C_{wm}, \sum_{m=1}^{M}C_{\phi m}\right\}^{\mathrm{T}}. \tag{17.3}$$

As the increase in M, the solutions of Eq. (15) converge to the exact solutions and the correspondence results are shown graphically in the next section.

4 Numerical example

To illustrate the surface piezoelectric effect, PZT-5H piezoelectric medium is chosen, whose elastic and piezoelectric constants are [21]: $c_{44} = 3.53 \times 10^{10}\,\mathrm{Nm}^{-2}$, $e_{15} = 17\,\mathrm{Cm}^{-2}$, and the dielectric constant is: $\in_{11}= 150.3 \times 10^{10}$ C/Vm. For the purpose of this section is to depict the physics phenomenon which reveals the effect of surface piezoelectricity, a characteristic factor η is introduced to reflect the relation between the surface constants and piezoelectric constants, i.e.

$$c_{44}^{s} = \eta c_{44}, \quad e_{15}^{s} = \eta e_{15}, \quad \in_{11}^{s}= \eta \in_{11} . \tag{18}$$

Then Eq. (15) is developed into

$$\left\{ \begin{bmatrix} G & 0 \\ 0 & G \end{bmatrix} - \frac{1}{a} \begin{bmatrix} \eta Q & 0 \\ 0 & \eta Q \end{bmatrix} \right\} \{C\} = 2\left[\Lambda_0\right]\{b_\infty\} . \tag{19}$$

Taking $M = 1$ as example, the solutions of sliding displacement, electric potential jump along the crack faces, stress and electric displacement intensity factors can be obtained as follows:

$$\delta w = \frac{2a\left(\bar{\Lambda}_{11}\tau_\infty + \bar{\Lambda}_{12}D_\infty\right)}{1-\eta/a}, \tag{20.1}$$

$$\delta \phi = \frac{2a\left(\bar{\Lambda}_{21}\tau_\infty + \bar{\Lambda}_{22}D_\infty\right)}{1-\eta/a}, \tag{20.2}$$

$$K_{\mathrm{III}} = \frac{\sqrt{\pi a}\tau_\infty}{1-\eta/a}, \tag{20.3}$$

$$K_D = \frac{\sqrt{\pi a}D_\infty}{1-\eta/a}. \tag{20.4}$$

Let $\eta = 0$, then we can also obtain the sliding displacement δw_o, electric potential jump along the crack faces $\delta\phi_o$, the stress intensity factor $K_{\mathrm{III}o}$, and electric displacement intensity factor K_{Do} which ignored the surface piezoelectric effect, i.e. the linear elastic fracture mechanics solution. It follows from Eq. (20) that

$$\frac{\delta w}{\delta w_o} = \frac{\delta\phi}{\delta\phi_o} = \frac{K_{\mathrm{III}}}{K_{\mathrm{III}o}} = \frac{K_D}{K_{Do}} = \frac{1}{1-\eta/a}. \tag{21}$$

According to the method of determining the value of the character factor for an anti-plane problem [21], let $\eta = -1$ nm. Obviously, the characteristic length parameter of the piezoelectric material l_c can be expressed as $l_c = -\eta$. As argued by Andreussi and Gurtin [25], it is feasible to apply the continuum surface model for structures at a few nanometers scale. It can be seen from Eq. (21) that the influence of the surface effect is not related to the applied load, but only related to the normalized half crack length a/l_c. The above results are obtained under the crack impermeable assumption. For the crack permeable assumption, the electric potential across the crack is continuous, the solution is more easily obtained, and the corresponding equations can be derived as

$$\left\{ \begin{bmatrix} G & 0 \\ 0 & G \end{bmatrix} - \frac{1}{a} \begin{bmatrix} \eta Q & 0 \\ 0 & \eta Q \end{bmatrix} \right\} \begin{Bmatrix} C_{wm} \\ 0 \end{Bmatrix} = 2\left[\Lambda_0\right] \begin{Bmatrix} \tau_\infty \\ D_\infty - D_0 \end{Bmatrix} \tag{22}$$

where D_0 is the unknown constant that can be calculated as $D_0 = \left(\bar{\Lambda}_{21}\tau_\infty + \bar{\Lambda}_{22}D_\infty\right)/\bar{\Lambda}_{22}$. In the case of $M = 1$, the corresponding normalized solutions are:

$$\frac{\delta w}{\delta w_o} = \frac{K_{\mathrm{III}}}{K_{\mathrm{III}o}} = \frac{K_D}{K_{Do}} = \frac{1}{1-\eta/a}. \tag{23}$$

It can be seen from Eq. (22) that the sliding displacement, the stress and electric displacement intensity factors are the same as those under the crack impermeable condition. Therefore, in this section only the surface effect

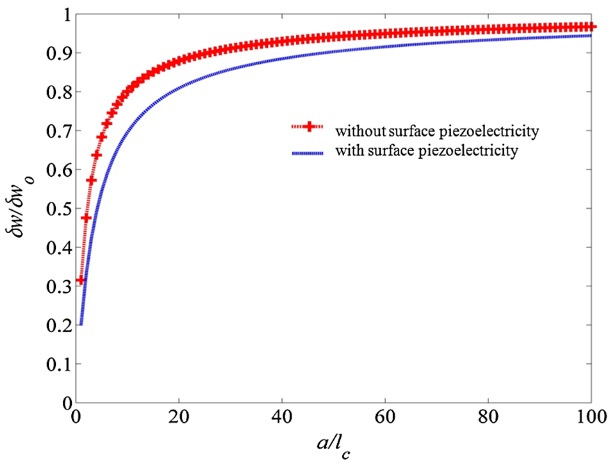

Fig. 2 Normalized sliding displacement as a function of normalized half crack length

under the impermeable crack condition is given. Next, with increasing M, the solutions are very close to the exact solutions. Then, with the consideration of surface piezoelectricity, the normalized results as functions of the normalized half crack length are given. To compare the results with and without the surface piezoelectricity, the normalized solutions which only incorporate the influence of the surface elasticity are also given, i.e. terms related to e_{15}^{s} and $\in_{11}^{s}$ in Eq. (19) are ignored. To obtain the corresponding results one can see the similar work where only the residual surface stress is included [26]. Similar to this work, Ref. [22] also found that the electric displacement intensity factor is related to the electric boundary condition. These two results are all normalized by the linear elastic fracture mechanics solutions.

How the surface piezoelectricity affects the sliding displacement is plotted in Fig. 2. It can be seen that surface piezoelectricity decreases the value of the sliding displacement which is the same as that of surface elasticity. However, these two effects have different degree; obviously the influence incorporated by surface piezoelectricity has far more effect on the sliding displacement. For example, when $a/l_c = 80$, the normalized sliding displacement $\delta w/\delta w_o = 0.94$, i.e., with consideration of surface piezoelectricity, the value of the sliding displacement is 6 % less than that of linear elastic fracture mechanics theory, while ignoring the surface piezoelectricity the normalized sliding displacement is $\delta w/\delta w_o = 0.98$, i.e., if only surface elasticity is considered, the value of the sliding displacement is 2 % less than that of linear elastic fracture mechanics theory; when $a/l_c = 20$, with the consideration of surface piezoelectricity, $\delta w/\delta w_o = 0.81$, i.e. in this case the value of sliding displacement is 19 % less than that of linear elastic fracture mechanics theory; while ignoring the surface piezoelectricity the obtained solution is $\delta w/\delta w_o = 0.89$, i.e. the value of sliding displacement is 11 % less than that of linear elastic fracture mechanics theory.

Figure 3 depicts the normalized electric potential jump along the crack faces as a function of normalized the half crack length with and without consideration of surface piezoelectricity. It is found that all the curves in this figure approach 1. Similar to sliding displacement, the value of the electric potential jump along the crack faces is decreased with the influence of surface elasticity and surface piezoelectricity, especially for the latter. In other words the two effects have the same tendency, but with different degree of variations.

Incorporating the surface piezoelectricity, the variation of the normalized stress intensity factor $K_{\mathrm{III}}/K_{\mathrm{III}o}$ with the normalized half crack length is displayed in Fig. 4. It can be seen that similar to $\delta w/\delta w_o$ and $\delta\phi/\delta\phi_o$, the normalized stress intensity factor approaches 1 with the increase in a/l_c. It means that when the size of the piezoelectric material shrinks to nanoscale, the surface elasticity and surface piezoelectricity cannot be ignoring. Furthermore, ignoring the surface piezoelectricity will overestimate the stress intensity factor.

Finally, Fig. 5 gives the relation between the normalized electric displacement intensity factor and the half crack length. It is found that the normalized solution K_D/K_{Do} is equal to 1, i.e. ignoring the surface piezoelectricity, the solution of K_D is the same as that of linear elastic fracture mechanics theory. Under such circumstances if only the surface elasticity is considered, the electric displacement is independent of the surface effect. However, when the surface piezoelectricity is included, the influence of surface piezoelectricity on the electric displacement intensity factor is remarkable. Apparently, under the two different electric boundaries, the surface effect on the electric displacement is different when the surface piezoelectricity is ignored. With the consideration of surface piezoelectricity, the surface effect does not rely on the electric boundary conditions.

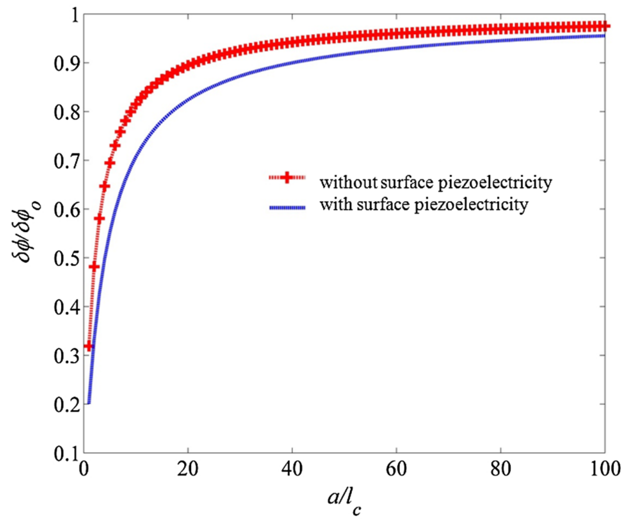

Fig. 3 Normalized electric potential jump across the crack center as a function of normalized half crack length

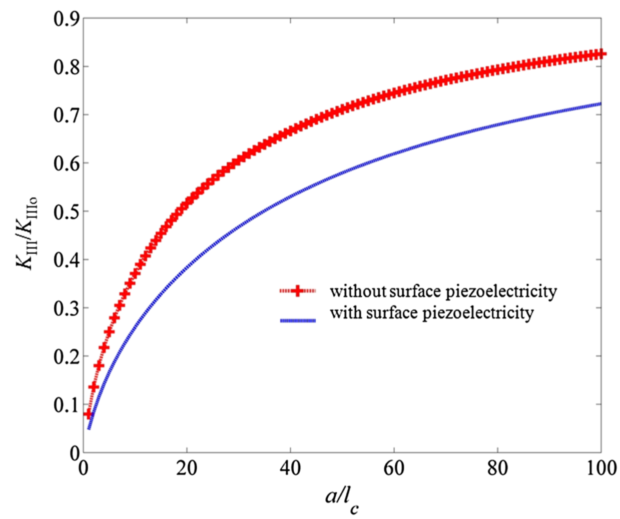

Fig. 4 Normalized crack tip stress intensity factor as a function of normalized half crack length

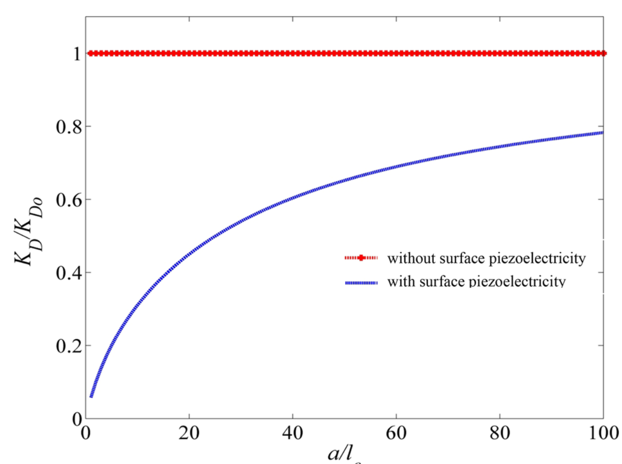

Fig. 5 Normalized crack tip electric intensity factor as a function of normalized half crack length

5 Conclusion

Applying the Fourier integral and the singular integral equation technique, the problem of an infinite piezoelectric material with a nanoscale anti-plane crack is studied. The coupling surface elasticity model is introduced to express the electro-elastic coupling fields. The solutions to the sliding displacement, electric potential jump along the crack faces, stress and electric displacement intensity factors are obtained. The surface piezoelectricity effect is found to be remarkable on the crack deformation and crack near-tip stress field. It is also found that when the influence of surface piezoelectricity is included, the electric displacement intensity factor is independent of the electric boundary conditions on the crack faces. If only the surface elasticity is incorporated, the electric displacement intensity factor is dependent of electric boundary conditions on the crack faces. Finally, influences of surface elasticity and surface piezoelectricity on the solutions of the problem are consistent under the two electric boundary condition assumptions. The obtained theoretical results are helpful for studying the size-dependent fracture phenomena of nanomaterial containing nanoscale cracks and the design nanodevices in NEMS.

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