Discussion of fracture criterions associated with the crack surface boundary conditions of piezoelectric materials

By Rong Jiao

Department of Aerospace Engineering and Engineering Mechanics

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Abstract: The fracture criterions of piezoelectric materials are different from those of common brittle and ductile materials due to their particular electrical-mechanical responses under the electrical-mechanical loading fields. There have five different fracture criterions for the crack in piezoelectric materials: (1) maximum loop stress; (2) total energy release rate (TERR); (3) mechanical strain energy release rate (MSERR); (4) local and global energy release rate only coming from the electrical yielding; (5) influence of mode-mixity on fracture. Using of these criterions is associated with the selections of the electrical boundary conditions including: (1) impermeable and mechanical traction free cracks surface; (2) permeable and mechanical traction free cracks surface; (3) exact electrical boundary and traction free cracks surface.

In this term paper, two criterions (TERR and MSERR) under various mechanical and electrical loading fields for the impermeable crack surface and the permeable crack surface are discussed and for the impermeable crack, the mechanical strain energy release rate is reasonable while for the permeable crack, the total energy release rate is more reasonable.

Introduction:
In the last two or three decades, the piezoelectric materials have been used increasingly in the smart structures and adaptive technologies such as sensors, transducers and large displacement actuators. The most commonly used piezoelectric ceramics are PZT (PbZrO₃-PbTiO₃) and they are very brittle and very easy to induce fracture in its applications. So it’s important to study fracture behavior for the piezoelectric material and to discuss the reasonable fracture criteria for crack propagation. However, due to the particular electrical-mechanical responses under the electrical-mechanical loading, the fracture behavior of the piezoelectric ceramics is more complicated than those common materials which the Linear Elastic Fracture Mechanics can be used.

In this term paper, two criterions (TERR and MSERR) under various mechanical and electrical loading fields for the impermeable crack surface and the permeable crack surface are discussed and for the impermeable crack, the mechanical strain energy release rate is a reasonable fracture criterion while for the permeable crack, the total energy release rate is more reasonable.

Fundamental fracture mechanics for piezoelectricity:
Governing field equations:

\[ \sigma_{i,j} + f_i = 0 \]  \hspace{1cm} (1)

\[ D_{i,j} = q_b \]  \hspace{1cm} (2)

There, \( \sigma_{i,j} \) is the stress tensor, \( f_i \) is the body force and \( D_{i,j} \) is the electric displacement, \( q_b \) is the body charge.
Boundary conditions:

\[ \sigma_{ij} n_j = T_i \]  \hspace{1cm} (3)
\[ D_i n_i = -q_s \]  \hspace{1cm} (4)

There, \( T_i \) is the traction vector on the boundary, \( q_s \) is the surface change and \( n_i \) is the unit normal outward to the boundary surface.

Constitutive equations,

\[ \sigma_{ij} = C_{ijkl} s_{kl} - e_{ijk} E_k \]  \hspace{1cm} (5)
\[ D_j = e_{ijkl} s_{kl} + \varepsilon_{ijk} E_k \]  \hspace{1cm} (6)

There, \( C_{ijkl} \) are the elastic modules, \( \varepsilon_{ij} \) are the dielectric constants and \( e_{ijk} \) are the piezoelectric constants.

For a generalized plane problem where all qualities in a 3D are not zero but they depends only on two Cartesian coordinates \( x_1 \) and \( x_2 \), Suo et al. (1992) developed Stroh's complex potential theorem with four complex argument and gave a compact expressions form associated with the field equations (3) and the boundary conditions (4) as following:

\[ u = [u_k, \phi]^T = a f(z), \quad z = x_1 + px_2 \]  \hspace{1cm} (7)

There, \( u_k \) is the displacement and \( \phi \) is the electric potential. \( f(z) \) is an arbitrary function of the complex variable \( z \) and the complex constant \( p \) and the vector \( a \) are unknown currently and they can be solved out from the following eigen function:

\[ \begin{bmatrix} Q + p(R + R^T) + p^2 T \end{bmatrix} h = 0 \]  \hspace{1cm} (8)

The requirement of the non-trivial solution of equation (8) gives four pairs of complex conjugate eigen roots \( p_{\alpha} (\alpha = 1,2,3,4) \) with the positive imaginary parts and the corresponding eigen vector \( a_{\alpha} (\alpha = 1,2,3,4) \).

There, the matrix \( Q, R \) and \( T \) in equation (8) are related to the material mechanical, dielectric and piezoelectric constants in equation (5) and (6) by:

\[ Q = \begin{bmatrix} C_{ijkl} & e_{i1} \\ e_{ik}^T & -\varepsilon_{11} \end{bmatrix}, \quad R = \begin{bmatrix} C_{ijkl} & e_{21} \\ e_{ik}^T & -\varepsilon_{12} \end{bmatrix}, \quad T = \begin{bmatrix} C_{ijkl} & e_{21} \\ e_{ik}^T & -\varepsilon_{22} \end{bmatrix} \]  \hspace{1cm} (9)

After given a particular expression of \( f(z) \), the stress and the electric displacement
can be gained:

\[
\begin{align*}
\begin{cases}
\sigma_{22}^z = (R + pR^T)af^+(z) \\
D_2^z = (Q + pR)af^-(z)
\end{cases}
\end{align*}
\]  

(10)

Or more compact forms from Suo et al. (1992):

\[
\begin{align*}
\mathbf{u} &= 2 \text{Re}[\mathbf{A}f(z)] \\
[\sigma_{12}] &= 2 \text{Re}[\mathbf{B}f^+(z)] \\
[\sigma_{ii}] &= 2 \text{Re}[\mathbf{L}f^+(z)]
\end{align*}
\]

(11) (12) (13)

With:

\[
\mathbf{u} = [u_1, u_2, u_3, \phi]^T
\]

(14)

\[
[\sigma_{ii}] = [\sigma_{11}, \sigma_{21}, \sigma_{31}, D_1]^T, [\sigma_{12}] = [\sigma_{12}, \sigma_{22}, \sigma_{32}, D_2]^T
\]

(15)

\[
f(z) = [f_1(z_1), f_2(z_2), f_3(z_3), f_4(z_4)]^T
\]

(16)

\[
\mathbf{A} = [\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4], \mathbf{B} = [\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3, \mathbf{b}_4], \text{ with } \mathbf{b} = (\mathbf{R}^T + p\mathbf{T})\mathbf{a}
\]

(17)

\[
\mathbf{L} = [-\mathbf{b}_1\mu_1, -\mathbf{b}_2\mu_2, -\mathbf{b}_3\mu_3, -\mathbf{b}_4\mu_4]
\]

(18)

Next, the solutions under the impermeable and permeable crack boundary conditions

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{crack_surface.png}
\caption{The crack surface under the remote mechanical and electric loading}
\end{figure}

Two surfaces of an impermeable crack are charge-free, or in the other words, the
normal components of dielectric displacement $D_2$ along the crack surface are zero:

$$D_2^+(x) = D_2^-(x) = 0 \quad x \in (-a, a) \quad (19)$$

Just as we did in the Linear Elastic Fracture Mechanics, the mechanical quantities on the crack surfaces for the traction free conditions are:

$$\sigma_{12}^+(x) = \sigma_{12}^-(x) = 0 \, , \quad \sigma_{22}^+(x) = \sigma_{22}^-(x) = 0 \quad x \in (-a, a) \quad (20)$$

By the same dimensional analysis used in LEFM, for the impermeable crack, the square root singularity still exists for both the stress and electric fields near the crack-tip. So, the crack-tip stress intensity factors (SIF) and the electric displacement intensity factor (EDIF) are associated with the remote mechanical and electric loading by:

$$K_I = \sigma_{22}^{\infty} \sqrt{\pi a} \quad (21)$$

$$K_{II} = \sigma_{12}^{\infty} \sqrt{\pi a} \quad (22)$$

$$K_e = D_2^{\infty} \sqrt{\pi a} \quad (23)$$

From the expressions of equations (21-23), it’s evident that for an impermeable crack in an infinite plane piezoelectric material, the SIF’s do not depend on of remote electric loading $D_2^{\infty}$ while EDIF does not depend on the remote mechanical loading $\sigma_{22}^{\infty}$ and $\sigma_{12}^{\infty}$, neither. For the impermeable crack surface, the SIFs was suggested as a fracture criterion which is exactly we use in LEFM. But this is in contrary with the classical Vickers indentation experiments under an applied electric field, in which the fracture toughness dose depends on the electric field, may either decrease or increase, depending upon the direction of the applied electric field. So, SIFs is not a good fracture criterion for the impermeable crack since they do not consider the influence of the electric field on fracture.

Park and Sun (1995) used the complex Fourier transformation to calculate the hoop stress near the crack-tip as function of angle $\theta$ for PZT-4 under the purely mechanical loading, pure electric loading and the combined mechanical-electric loading remote conditions, and the results are shown in Figure 2 and Figure 3.
Figure 2: Distribution of hoop stress at the tip of an impermeable crack under a purely mechanical or a pure loading (Park and Sun, 1995)

Figure 3: Distribution of hoop stress at the tip of an impermeable crack surface under a combined mechanical and electric loading (Park and Sun, 1995)

These two figures show that the angle $\theta$ for the maximum hoop stress is greatly influenced by the remote electric loading and we know that in the case of pure mechanical loading in LEFM, the maximum hoop stress is at $\theta = 0$. But here, this position is affected by the applied electric loading and maybe it’s not at $\theta = 0$.

In LEFM, the $J$-integral is equivalent to the crack-tip energy release rate (ERR) per unit crack extension (also known as the total potential energy release rate, shortly by
TPERR) that includes both mechanical and electric energy. So, consequently, TPERR has been suggested to be used as the fracture criterion for piezoelectric material. $J$-integral can be calculated as follows;

$$J = \oint_C \left[ \sigma_{ij} s_{ij} dx_{2} - n_i \sigma_{ip} \frac{\partial u_p}{\partial x_1} ds \right] - \left( D_i E_i dx_{2} + n_i D_i \frac{\partial \phi}{\partial x_1} ds \right) \quad i, j, p = 1,2 \quad (24)$$

There, $C$ denotes the closed contour surrounding the crack tip and in the paper Suo et al (1992), the $J$-integral was associated with the SIFs by:

$$J = \frac{1}{4}(K_{II}, K_I, K_e)H^* \begin{pmatrix} K_{II} \\ K_I \\ K_e \end{pmatrix} \quad (25)$$

There $H^*$ is a $3 \times 3$ matrix and is related to the piezoelectric material constants as:

$$H^* = 2 \text{Re}(iA^*B^{-1}) \quad (26)$$

$$A^* = \begin{bmatrix} p_1 & p_2 & p_3 \\ q_1 & q_1 & q_1 \\ r_1 & r_1 & r_1 \end{bmatrix} \quad (27)$$

$$B^* = \begin{bmatrix} -\mu_1 & -\mu_2 & -\mu_3 \\ 1 & 1 & 1 \\ -\lambda_1 & -\lambda_1 & -\lambda_1 \end{bmatrix} \quad (28)$$

In the paper of Park and Sun (1995), for the model-I crack normal to the poling direction and the applied electric field in PZT-4, the expression of TPERR was:

$$G_I = \frac{\pi a}{2} \left[ 1.48 \times 10^{-11} (\sigma_{22}^e)^2 + 5.34 \times 10^{-2} \sigma_{22}^e D_{22}^e - 8.56 \times 10^{7} (D_{22}^e)^2 \right] \quad (29)$$

In this expression, besides the mechanical part, the TPERR also includes the electric part and the coupling term of mechanical and electric loading. But the problem is the last term square $D_{22}^e$ is negative, and consequently, for different $\sigma_{22}^e$ and $D_{22}^e$, the value of TPERR may be zero or even negative. So, for a fixed mechanical loading, use of the TPERR as the fracture criterion will always block crack propagation under an applied electric loading, whatever the direction of the applied electric loading is. Moreover, if there has no mechanical loading, a purely eclectic loading never drives the crack since the last term in equation (29) is always negative. These deductions obviously do not coincide with all available experimental observations and common sense. So, for the impermeable crack, the total energy release rate TPERR can not be used as the fracture criterion.

So, Park and Sun (1995) used a new fracture criterion based on mechanical strain energy release rate (MSERR) since they believed that the fracture is a mechanical process and it’s more reasonable to only use the mechanical strain energy released during crack propagation. The MSERR is the crack closure integral for the mechanical...
part, which can be defined as follows:

\[
G_I^M = \lim_{\delta \to 0} \frac{1}{2\delta} \int_0^\delta \sigma_{22}(x) \Delta u_2(\delta - x) \, dx \quad \text{(Mode I)}
\]  

(29)

\[
G_{II}^M = \lim_{\delta \to 0} \frac{1}{2\delta} \int_0^\delta \sigma_{12}(x) \Delta u_1(\delta - x) \, dx \quad \text{(Mode II)}
\]  

(30)

Also, Park and Sun (1995) proposed the expression of \( MSERR \) for an impermeable crack normal to the poling direction of PZT-4:

\[
G^M = \frac{\pi D}{2} \left[ 1.48 \times 10^{-11} (\sigma_{xx}^{\infty})^2 + 2.67 \times 10^{-2} \sigma_{22}^{\infty} D_{22}^{\infty} \right]
\]  

(31)

Now from this expression, we found that the negative term disappears and the \( MSERR \) has the linear relationship to the remote electric loading under non-zero mechanical loading. Park and Sun found that a positive electric field decreases the critical stress at which the fracture occurs and hence accelerates crack growth while a negative electric field increases the fracture stress hence blocks crack growth. This conclusion matches the experiments they did very well, which is shown in the figure 4 and figure 5.

![Center Crack](image)

*Figure 4: Fracture load as a function of electric field for a center crack in PZT-4 (Park and Sun, 1995)*
By the comparison of the experiments and the prediction of $G^M$, it is concluded that the $MSERR$ is a better fracture criterion than the $TPERR$ when the crack surface are charge-free. Park and Sun (1995) suggested that the charge-free crack surface can be obtained by putting a crack specimen in the silicone oil.

**Permeable crack model:**

In the impermeable crack model, the normal electric displacement and the corresponding electric potential are assumed zero. But actually, the magnitude of the normal electric displacement on crack surfaces does not vanish and they should be continuous through the two surfaces of the crack:

\[ D_2^+(x_i) = D_2^-(x_i) \]  \hspace{1cm} (32)

\[ \phi_2^+(x_i) = \phi_2^-(x_i) \]  \hspace{1cm} (33)

For the permeable crack model, it’s significant to find the distributed normal electric displacement $D_2^0(x_i)$ which is the difference between the two surfaces of the crack.

It is found that under the uniform far-field loading, $D_2^0(x_i)$ is constant. So, equation (33) is reduced to:

\[ E_2^+(x_i) = E_2^-(x_i) \]  \hspace{1cm} (34)

Xu and Rajapakse (2001) found that the normal electric displacement on crack surfaces is related to the uniform far-field loadings by:
\[ D_2^0 = \frac{\text{Im} \sum_{k=1}^{3} \kappa_k \left( -A_{k1} \sigma_{22}^\infty + A_{k2} \sigma_{12}^\infty \right)}{\text{Im} \sum_{k=1}^{1} \kappa_k A_{k3}} + D_2^\infty \]  

(35)

There, the constants \( \kappa_k \) and \( A_{ki} \) are related to equation (27). From equation (35), we found that as the complex coefficient in the complex potentials are not dependent to the remote electric displacement \( D_2^\infty \) itself, but the electric quantity \( D_2^0 - D_2^\infty \). Also, Xu and Rajapakse (2001) proposed the following expression for the field intensity factors:

\[ K_I = \sigma_{22}^\infty \sqrt{\pi a} \]  

(36)

\[ K_{II} = \sigma_{12}^\infty \sqrt{\pi a} \]  

(37)

\[ K_e = (D_2^\infty - D_2^0) \sqrt{\pi a} \]  

(38)

Here, for a conducting crack, the remote electric loading \( D_2^\infty \) has no influence on the complex potential solutions and this implies that for a conducting crack, the remote mechanical loading plays a much more significant role than the remote electric loading and consequently, the traditional mechanical SIFs may be used as a fracture criterion for conduction cracks.

Xu and Rajapakse (2001) proposed the formula for the total potential energy release rate (TPERR) for a conducting crack including its mechanical and electric parts as following:

\[ G = G^M + G^E = \lim_{\delta a \to 0} \frac{1}{2 \delta a} \int_0^{\delta a} \left( \sigma_{12}(x,0) u_i (\delta a - x, \pm \pi) + D_2(9x,0) \phi (\delta a - x, \pm \pi) \right) dx \]  

(39)

\[ G^M = \frac{m_1}{2} \text{Im} \sum_{k=1}^{3} \left\{ -q_k A_{k1} (\sigma_{22}^\infty)^2 + p_k A_{k2} (\sigma_{12}^\infty)^2 + (q_k A_{k2} - p_k A_{k1}) \sigma_{12}^\infty \sigma_{22}^\infty + \right\} \]  

\[ \left\{ (p_k A_{k3} \sigma_{22}^\infty + q_k A_{k3} \sigma_{12}^\infty) (D_2^\infty - D_2^0) \right\} \]  

(40)

\[ G^E = \frac{m_1}{2} \text{Im} \sum_{k=1}^{3} \left\{ -s_k A_{k1} (\sigma_{22}^\infty)^2 + s_k A_{k2} (\sigma_{12}^\infty)^2 \right\} (D_2^\infty - D_2^0) + s_k A_{k3} (D_2^\infty - D_2^0) \]  

(41)

Using this formulas, Liu and Chen (2002) analyzed the energy for both permeable and impermeable cracks in the piezoelectric materials and the numerical results of \( G^M \), \( G^E \) and \( G \) are plotted in figure 6~8, respectively.
Figure 6: Mechanical part of TPERR against the crack oriented angle (Liu and Chen, 2002)

Figure 7: Electric part of TPERR against the crack oriented angle (Liu and Chen, 2002)
The mechanical part $G^M$ in the $TPERR$ against the crack orientation angle $\alpha$ is always positive for the permeable crack. It’s interesting that under the pure mechanical loading ($E_2 = 0$), the values $G^M$ of for the permeable crack are always bigger than those for the impermeable crack, which means that the permeable crack surface condition enhances the crack propagation compared with the impermeable characteristic. Under the mechanical-electrical loading, the values of $G^M$ is almost constant for the permeable crack irrespective of the applied electric loading and this implies that $G^M$ is independent of the electric loading under the situation of permeable crack boundary conditions. While for the impermeable crack, the mechanical strain release rate $G^M$ is influenced by the applied electric loading: compared with the value of $G^M$ under the pure mechanical loading, the positive electric loading increase $G^M$ while the negative decreases $G^M$.

In the figure 7, the value of $G^E$ is always zero for the permeable crack, which implies that is no electric energy release rate for the permeable crack boundary condition. This can explain that why $TPERR$ criterion could be used as a fracture criterion for the permeable crack, since the electric part $G^E$ vanishes and mechanical part $G^M$ is overwhelming irrespective of the positive or negative electric loading. However, for
the impermeable crack, the applied electric loading influences on $G^E$ and due to the effect of the electric part of $G^E$ in $TPERR$, $TPERR$ criterion can not be used for the impermeable crack. In this situation, by Park and Sun (1995), the mechanical strain energy release rate ($MSERR$) is a good choice.

**Conclusion:**
Several fracture criterions for the piezoelectric materials under impermeable and permeable boundary conditions are discussed here. For the impermeable crack, Park and Sun (1995) concluded that rather than the total energy release rate ($TPERR$), the mechanical strain energy release rate ($MSERR$) can be used as the fracture criterion; while for the permeable crack, $TPERR$ is useful since the electric part $G^E$ is negligible.

**Reference:**