Multiscale behavior of crack initiation and growth in piezoelectric ceramics

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Abstract

The multiscale nature of cracking in ferroelectric ceramics is explored in relation to the crack growth enhancement and retardation behavior when the direction of applied electric field is reversed with reference to that of poling. An a priori knowledge of the prevailing fracture behavior is invoked for the energy dissipated in exchange of the macro- and micro-crack surface. To avoid the formalism of developing a two-scale level model, a single dominant crack is considered where the effect of microcracking could be reflected by stable crack growth prior to macro-crack instability. This is accounted for via a length ratio parameter \( k \). Micro- and macro-crack damage region would necessarily overlap in the simplified approach of applying equilibrium mechanics solutions to different scale ranges that are connected only on the average over space and time. The strain energy density theory is applied to determine the crack growth segments for conditions of positive, negative and zero electric field. The largest and smallest crack segments were found to correspond, respectively, to the positive and negative field. All of the three piezoceramics PZT-4, PZT-5H and P-7 followed such a trend. This removes the present-day controversy arising from the use of the energy release rate concept that yields results independent of the sign of the electric field. Interaction of non-similar crack growth with the direction of electric field is also discussed in relation to Mode II cracking. The crack initiation angle plays a dominant role when the growth segment is sufficiently small. Otherwise, a more complex situation prevails where consideration should also be given to the growth segment length. Failure stresses of Modes I and II cracking are also obtained and they are found to depend not only on the electric field density but also on crack length and the extent of slow crack growth damage. These findings suggest a series of new experiments. © 2000 Elsevier Science Ltd. All rights reserved.

1. Introduction

The demand for use specific materials in the electronics industry has necessitated a more in-depth understanding of how piezoelectric materials are damaged, particularly when physical size is scaled down to the dimensions of the material microstructure. Of concern are the group of ferroelectric ceramics that are vulnerable to cracking at the micro-, meso- and macro-scale levels. A revival of interest in the fracture mechanics of ferroelectric ceramics can be evidenced in [1–4] and the host of references mentioned there in. The exclusive use of the energy release rate concept in these works have led to a diversification of results and conclusions that has became a focal point of controversy.
One of the main issues of discussion were concerned with characterizing the failure of a single dominant crack for poled (or unpoled) lead–zirconate–titanate (PZT) ceramics. To this end, it is worthwhile to first clarify how a multiscale fracture process could be analyzed using fracture mechanics that is not limited to the concept of energy release rate. When energy is dissipated in exchange of free surface and/or intergranular defect growth, it is necessary not only to identify the directional character of the process but also the scale level at which the process is occurring. For a dominant crack in metals that undergo elastoplastic deformation, the creation of macrocrack surface along the main crack (Mode I) path should be distinguished from the creation of microcrack surfaces off to the side of the main crack [5,6] where the plastic enclaves are located. In this sense, elastoplastic fracture is also a multiscale process. A portion of the total energy is first dissipated to distort and reorient the grains while the remaining available energy can be used to drive the main crack. The former and latter are released, respectively, at the micro- (or meso-) and macroscale level. As in the application of the strain energy density criterion [7,8], the local plastic energy is dissipated at time \( t - \delta t \) and is no longer available to drive the main crack at \( t + \delta t \). Only the portion of energy density at \( t + \delta t \) is available to create macrocrack surface. In recent works, investigators of experimental mesomechanics [9,10] have emphasized the importance to include the meso effects of “shear + rotation” for the grains in polycrystals subjected to mechanical loads. It was further elaborated in [11] that the conventional dislocation models could not possibly serve as the foundation for developing continuum mechanics theories of elastoplasticity unless the state of affairs at the meso-scale level are also included.

The energy dissipation mechanisms for ferroelectric ceramics are different from those of metal alloys. Coupled electromechanical actions can alter the crystal microstructure in different ways. One of the main sources of energy dissipation near a crack tip is domain switching that gives rise to nonlinearity in ferroelectric ceramics similar to plasticity for metals. Such a local phenomenon could occur even though the remote field intensity is less than the coercive value. Experiments [12] have shown that the dominant crack model holds well for field intensity near the coercive value, i.e., \( E \approx 0.9 - 1.0E_c \) for PZT-5. When \( E \) is reduced to 0.80 to 0.83\( E_c \), massive cracking at locations away from the main crack tends to occur. The extend to which microcracking cuts down the driving force of the main crack remains to be assessed. Attempts have been made to predict the onset of domain switching by applying a criterion that is intimately associated with the strain energy density function [7,8], i.e., the change of the energy density function [13,14]. The same approach was also applied in [15,16] to investigate the effect of domain switching in the vicinity of a crack tip.

Past experience for elastoplastic fracture mechanics tends to suggest that the energy release rate concept could not be used directly to address multiscale processes unless additional independent assumptions are invoked. What remains unexplained up to this date is the experimental observation [17,18] that crack growth is enhanced for positive \( E \) and retarded for negative \( E \). The results for \( E = 0 \) are used as a base for comparison. Here, \( +E \) and \( -E \) correspond, respectively, to electric field applied in the same and opposite direction of poling. More specifically, the indentation tests in [15,16] used a mechanical load of 500 g to produce cracks in PZT-8 ceramics. A base reference crack length of 32 \( \mu m \) was obtained for \( E = 0 \). The test is then repeated to find crack lengths of 54 and 22 \( \mu m \) for positive and negative \( E \) of \( 4.7 \times 10^3 \) V/m, respectively. Experiments for pre-cracked PZT-4 compact tension specimens subjected to mechanical and electric loading were also made in [4]. The same conclusion was obtained. That is the crack initiation load was found to be greater for negative \( E \) and smaller for positive \( E \). The experimental data, however, did not agree with the energy release rate predictions that gave the same crack length regardless of whether \( E \) is positive or negative [3,4].

The main objective of this work is to reexamine some of the previously unexplained phenomena of cracking in PZT ceramics by application of the energy density criterion [7,8]. The examples are limited to those situations where energy dissipation by cracking is dominated by a single
macrocrack such that the fracture toughness concept [5] can be applied to characterize the resistance of PZT ceramics against fracture. Efforts will be made to quantify the crack growth enhancement and retardation behavior of PZT ceramics based on the crack solution obtained from the linear theory of piezoelectricity. Since the energy density criterion applies equally well to materials with nonlinear behavior that are dissipative or non-dissipative, there are no difficulties to extend the present treatment to include nonlinear behavior of ferroelectric ceramics.

2. Description of crack growth

The scale level at which the crack growth process should be modelled depends on the rates at which energy are being pumped into the system and the mechanisms of energy dissipation. When modelling crack growth, non-uniform crack growth segment should be considered. Arbitrary assumption of crack growth segments can lead to non-unique solutions [19]. The path dependent nature of crack growth cannot be ignored.

2.1. Thresholds

Uniaxial stress–strain curves for metal alloys in tension are identified with thresholds such as yield strength, ultimate strength, ultimate strain, etc. The stress–strain behavior for ferroelectric ceramics is quite different and data are usually obtained in compression because it is difficult to pull ceramics which are susceptible to fracture at the clamps. A typical curve for a soft PZT-51 ceramic is shown in Fig. 1. The direction of poling and compression correspond to the $x_3$-axis along which $\sigma_{33}$ is applied. Note that the curve is concaved instead of convexed for metals and there is no sign of yielding in the mechanical sense. Unloading follows the dotted curve that did not return to the origin, leaving a large remanent axial strain $\gamma_{33}$.

![Stress versus strain in compression for PZT ceramic.](image)

2.2. Initiation, growth and termination

Fracture is a process that necessarily involves crack initiation, growth and rapid propagation. These three stages are in fact one of the same process and should be assessed accordingly in order to avoid inconsistencies. The energy density criterion [7,8] can satisfy the aforementioned requirement and be stated in terms of three hypotheses:

- The location of fracture initiation is assumed to coincide with the maximum of minimum of $(dW/dV)_c$ or $(dW/dV)_{\text{min}}^{\text{max}}$.
- Failure by crack initiation and growth is assumed to occur when $(dW/dV)_c^{\text{max}}$ reaches a critical value $(dW/dV)_c$ being characteristics of the material.
- Stable crack growth increments $r_1$, $r_2$, etc., are assumed to be governed by

$$\left( \frac{dW}{dV} \right)_c = \frac{S_1}{r_1} = \frac{S_2}{r_2} = \cdots = \frac{S_j}{r_j} = \cdots = \frac{S_c}{r_c}.$$  \hspace{1cm} (1)

Unstable fracture is assumed to take place when

$$\left( \frac{dW}{dV} \right)_c = \frac{S_c}{r_c},$$  \hspace{1cm} (2)

where $r_c$ is the critical ligament ahead of a crack.

2.3. Fracture toughness

Eqs. (1) and (2) show that crack growth consists of a sequence of nucleation processes involving the burst of isolated energy pockets over the discrete ligaments $r_1$, $r_2$, etc. For monotonically increasing
Recall that for a linear elastic homogeneous material $S_c$ can be related to the ASTM valid $K_{IC}$ plane strain value as

$$S_c = \frac{(1 + \nu)(1 - 2\nu)K_{IC}^2}{2\pi E_0},$$  

where $\nu$ is the Possion’s value and $E_0$ the Young’s modulus. For instance, an approximate value of $K_{IC} \approx 0.79$ MN/m$^{3/2}$ for PZT-4 can be estimated from the fracture data in [4].

For a linear transversely anisotropic but homogeneous piezoceramic material subjected to mechanical loads only, Eq. (5) takes the form

$$S_c = B_{11} K_{IC}^2.$$  

The expression

$$B_{11} = A_{11} + 2A_{14} \frac{g_{33}}{\beta_{33}} + A_{44} \frac{g_{33}^2}{\beta_{33}^2}$$

has been derived with $A_{11}$, $A_{14}$ and $A_{44}$ being given, respectively, by Eqs. (46), (48) and (50) in [20] while $g_{33}$ and $\beta_{33}$ can be found in [20] as Eqs. (33) and (34), respectively. The parameters $A_{11}$, $A_{14}$, $g_{33}$ etc. in Eq. (7) are related to the elastic constants $C_{11}$, $C_{12}$, ... piezoelectric constants $\varepsilon_{31}$, $\varepsilon_{33}$, ... and dielectric permittivities $\varepsilon_{11}$ and $\varepsilon_{33}$. Their values for several PZT ceramics are given in [20]. Presumably, fracture tests could be carried out to obtain $S_c$ for the dominant crack model.

2.4. Microcracking

When microcracking becomes appreciable, the foregoing approach requires modification in a manner similar to elastoplastic fracture mechanics [21,22]. It becomes necessary to determine the energy density $(dW/dV)^{\text{micro}}$ dissipated at the microscale and energy density $(dW/dV)^{\text{macro}}$ available at the macroscale. That is $dW/dV$ could be decomposed into two parts:

$$\frac{dW}{dV} = \left( \frac{dW}{dV} \right)^{\text{micro}} + \left( \frac{dW}{dV} \right)^{\text{macro}}.$$  

The computational details are outlined in [21,22] for crack growth in an elastic–plastic material. The first term in Eq. (8) was attributed to plastic deformation and the second term is identified with the available energy that could do further damage. The inference made here in Eq. (8) is of a more general character as in [11] where an additional term $(dW/dV)^{\text{meso}}$ could be added. What should be emphasized is that $(dW/dV)^{\text{micro}}$ and $(dW/dV)^{\text{macro}}$ are consumed at different location and time. In general, if the decomposition of $(dW/dV)^{\text{micro}}$ and $(dW/dV)^{\text{macro}}$ in Eq. (8) is sufficiently accurate to represent the total energy density $dW/dV$, then the addition of $(dW/dV)^{\text{meso}}$ would serve only as minor refinement.
2.5. Crack arrest

In situations where the loads transmitted to the crack tip decrease monotonically, then the inequalities in Eqs. (3) and (4) are reversed as
\[ r_1 > r_2 > \cdots > r_j > \cdots > r_a \]
and
\[ S_1 > S_2 > \cdots > S_j > \cdots > S_a. \]
This would result in crack arrest as in the indentation tests [17,18]. In general, the load may fluctuate and the description of crack growth will correspond to a combination of Eqs. (3) and (9) as dictated by the load spectrum.

3. Mode I cracking

Consider a line crack of length 2a centered at the origin along the \( x_1 \)-axis while the material is poled in the \( x_3 \) direction normal to the crack. Both the normal stress \( \sigma \) and electric field \( E \) are uniform; they are oriented normal to the crack as shown in Fig. 3. For in-plane extension and symmetric crack growth \( K_{II} = 0 \), the expression for the energy density factor \( S \) in [20] reduces to

\[
S = B_{11}K_1^2 + 2B_{14}K_1E + B_{44}K_E^2.
\]

Substituting
\[ K_1 = \sigma \sqrt{\pi a} \quad \text{and} \quad K_E = E \sqrt{\pi a} \]
into Eq. (11) yields

\[
S = \sigma^2 \pi a \left[ B_{11} + 2B_{14} \frac{E}{\sigma} + B_{44} \left( \frac{E}{\sigma} \right)^2 \right].
\]

Again, the values of \( B_{11}, B_{14} \) and \( B_{44} \) can be computed from the expressions given in [20].

3.1. Direction of crack growth

The first step in applying the energy density criterion is to determine the angle \( \theta_0 \) of crack initiation. Positive direction of \( \theta \) in Fig. 3 is counterclockwise. For a fixed distance \( r \) from the crack tip, the minimum of \( dW/dV \) is equivalent to the minimum of \( S \) which can be found from the conditions:

\[
\frac{\partial S}{\partial \theta} = \sigma^2 \pi a \left[ \frac{\partial B_{11}}{\partial \theta} + 2 \frac{\partial B_{14}}{\partial \theta} \frac{E}{\sigma} + \frac{\partial B_{44}}{\partial \theta} \left( \frac{E}{\sigma} \right)^2 \right] = 0
\]
and

\[
\frac{\partial^2 S}{\partial \theta^2} = \sigma^2 \pi a \left[ \frac{\partial^2 B_{11}}{\partial \theta^2} + 2 \frac{\partial^2 B_{14}}{\partial \theta^2} \frac{E}{\sigma} + \frac{\partial^2 B_{44}}{\partial \theta^2} \left( \frac{E}{\sigma} \right)^2 \right] > 0.
\]

Denoting \( p = E/\sigma \), it can be shown from Eq. (14) that \( \theta_0 = 0 \) is the root of Eq. (14) for any value of \( p \). Substituting \( \theta_0 = 0 \) into Eq. (15), a curve plotting \( \partial^2 S/\partial \theta^2 \) versus \( p = E/\sigma \) is obtained as illustrated in Fig. 4. It can be shown that the maximum of minimum \( dW/dV \) or \( S \) always occur at \( \theta_0 = 0 \) if the ratio \( p = E/\sigma \) is kept within the inequality:

\[
p_1 < \frac{E}{\sigma} < p_2.
\]

The parameters \( p_1 \) and \( p_2 \) depend only on the material properties of the piezoceramics. Using the elastic constants, piezoelectric constants and
dielectric permittivities of PZT-4, it is found that
\[ \hat{\varepsilon}_1 = 0.23 \text{ m}^2/\text{C} \] and
\[ \hat{\varepsilon}_2 = 0.117 \text{ m}^2/\text{C}. \]
Similar values of \( \hat{\varepsilon}_j \) for PZT-5H and P-7 can also be obtained from the respective physical properties given in [20].

Displayed in Fig. 5 are the angular variations of the normalized strain energy density factor for different values of the field intensity to normal stress ratio \( p \). Excluding the extreme values at the crack boundaries, all curves possess a minimum at \( \theta_0 = 0 \). This indicates that crack would initiate along the axis of load symmetry under Mode I.

### 3.2. Failure stress: normal extension

Let \( \sigma_f \) represent the critical stress that sets off cracking when an electric field \( E \) is applied while \( K_{IC} = \sigma_c \sqrt{\pi a} \) corresponds to the onset of rapid fracture with no electric field applied. Since
\[
\left( \frac{dW}{dV} \right)_c = \frac{S_c}{r} \rightarrow \frac{S_c}{r_c}
\]
in general, Eqs. (6) and (13) may be substituted into Eq. (17) for \( \sigma = \sigma_f \), the following quadratic relation
\[
\sigma_f^2 + 2 \frac{B_{14}}{B_{11}} \sigma_f E + \frac{B_{44}}{B_{11}} E^2 = \frac{K_{IC}^2}{\pi a}
\]
is obtained. This gives a relation between \( \sigma_f \) and \( E \):
\[
\sigma_f = \frac{-B_{14}}{B_{11}} E \pm \sqrt{\frac{K_{IC}^2}{\pi a} + \left( \frac{B_{14}}{B_{11}} - \frac{B_{44}}{B_{11}} \right) E^2}.
\]
A necessary condition is that \( \lambda = (r/r_c) \ll 1 \) with \( r_c \) being the terminal ligament that triggers off global instability. Failure is understood to include stable cracking in this work.

Once the fracture toughness value \( K_{IC} \) is measured for a given piezoceramic material, the mechanical failure stress \( \sigma_f \) can be predicted for a given half crack length \( a \) and electric field intensity \( E \). Numerical calculations have been made for the case of a line crack in a large body under plane strain condition, Fig. 3. Calculations have been made for the PZT-4 material with \( K_{IC} \approx 0.79 \text{ MN/m}^{3/2} \). They are displayed graphically in Figs. 6(a), (b) and (c) for \( \lambda = 0.01, 0.1 \) and 1.0, respectively. For each \( \lambda \), a family of \( \sigma_f \) vs. \( E \) curves is obtained to show how crack length affects failure stress. For values of \( E \) that are about one order of magnitude lower than the coercive value \( (\sim 10^5 \text{ V/m}) \), the variations of \( \sigma_f \) with \( E \) are nearly linear. Fig. 6(a) shows that \( \sigma_f \) decreases with increasing half crack length from 0.5 to 9.0 mm for \( \lambda = 0.01 \). Failure by cracking is confined to the crack tip region. The local region of failure increases dramatically when the failure stress is approximately tripled. Such an effect is shown by the
length on failure stress. Results based on the energy release rate criterion [3,4] were not able to exhibit the effect of crack length on the variations of $\sigma_f$ with $E$. Alternatively, Eq. (19) can be rearranged into the form

$$\sigma_f = \frac{K_{IC}}{\sqrt{\pi a}} \sqrt{\frac{\lambda}{1 + 2(B_{14}/B_{11})p + (B_{44}/B_{11})p^2}}$$

(20)
to reflect the variations of $\sigma_f$ with $p = E/\sigma$, i.e., the relative magnitude of electric field to normal stress. For the same values of $\lambda = 0.01$, 0.1 and 1.0, Figs. 8(a), (b) and (c) give the numerical results. The curves are no longer straight lines for different crack sizes. Deviations from linearity tend to imply that the effects of geometry for mechanical stress and electric field are not the same.

3.3. Crack growth enhancement and retardation

As mentioned earlier with reference to the works in [4,17,18] that crack growth enhancement and retardation behavior could not be assessed using the energy release rate approach. The strain energy density criterion [20,23–25] has been used in recent times to explain the fracture behavior of piezoceramics. Variations of the energy density factor $S$ with the electric field intensity $E$ [20,25] were found to behave differently from those obtained by the total energy release rate $G$. It increases and decreases as $E$ is increased monotonically from the negative to the positive range with a peak near $E = 0$. This implies that crack tends to arrest as $E$ is decreased in the negative direction and increased in the positive direction. Such a conclusion cannot be correct on physical grounds. In contrast to $G$, $S$ was found to increase monotonically with $E$. Making use of Eq. (13), the normalized energy density factor $S/\sigma^2a$ can be computed for different piezoceramics as a function of $E/\sigma$. The values of $B_{11}$, $B_{14}$ and $B_{44}$ for PZT-4, PZT-5H and P-7 in Eq. (13) for Mode I crack growth are given in Table 1. They are used to obtain the normalized energy density factor $(S/\sigma^2a) \times 10^{-12}$ for different $E/\sigma$. Table 2 gives the numerical values that are shown graphically in Fig. 9. All the curves increase monotonically with $E/\sigma$. Moreover, it can be seen from Eq. (13) that
the term \(2B_{14}(E/\sigma)\) would affect the magnitude of \(S\) depending on whether \(E\) is positive, negative or zero. According to the third hypothesis of the stress energy density theory stated by Eq. (1), this would affect the crack growth behavior as the sign of the electric field intensity is altered with reference to poling.

More specifically, let the superscripts \(-, 0, +\) denote, respectively, the situations for negative, zero and positive \(E\). The corresponding crack growth segments are denoted by \(r_{1}, r_{2}, \ldots, r_{1}^{0}, r_{2}^{0}, \ldots\), and \(r_{1}^{+}, r_{2}^{+}, \ldots\), while the strain energy density factors are given by \(S_{1}^{-}, S_{2}^{-}, \ldots, S_{1}^{0}, S_{2}^{0}, \ldots\), and \(S_{1}^{+}, S_{2}^{+}, \ldots\). Application of Eq. (1) yields

\[
\left(\frac{dW}{dV}\right)_{c} = \frac{S_{1}^{-}}{r_{1}^{+}} = \frac{S_{2}^{-}}{r_{2}^{+}} = \cdots = \frac{S_{1}^{0}}{r_{1}^{0}} = \frac{S_{2}^{0}}{r_{2}^{0}} = \cdots = \frac{S_{1}^{+}}{r_{1}^{+}} = \frac{S_{2}^{+}}{r_{2}^{+}} = \cdots = \text{const.} \tag{21}
\]

It follows that for the \(j\)th segment of crack growth there prevails the relationship

\[
\frac{S_{j}^{-}}{S_{j}^{0}} = \frac{r_{j}^{-}}{r_{j}^{0}}, \quad j = 1, 2, \ldots \tag{22}
\]

or

\[
\frac{S_{j}^{+}}{S_{j}^{0}} = \frac{r_{j}^{+}}{r_{j}^{0}}, \quad \frac{S_{j}^{-}}{S_{j}^{0}} = \frac{r_{j}^{-}}{r_{j}^{0}}, \quad j = 1, 2, \ldots \tag{23}
\]

Fig. 7. Mode I slope of failure stress versus electric field for: (a) \(\lambda = 0.01\), (b) \(\lambda = 0.1\) and (c) \(\lambda = 1.0\).
For $E = 0, \pm 0.005, \pm 0.01$ and $\pm 0.015$ Vm/N, the results in Table 2 show that

\[ S_j^- < S_j^0 \quad \text{and} \quad S_j^+ > S_j^0. \]  

(24)

Eqs. (23) and (24) can be further applied to show that

\[ r_j^- < r_j^0 \quad \text{and} \quad r_j^+ > r_j^0. \]  

(25)

Table 3 summarizes the normalized crack growth results for the $j$th segment $r_j^+$ where $r_j^0$ corresponds to $E = 0$.

The results of Eqs. (25) are summarized schematically in Figs. 10(a)–(c). Using the crack growth segment $r_j^0$ as a base line of comparison, crack growth is enhanced ($r_j^+ > r_j^0$) when $E$ is in the direction of poling and is retarded ($r_j^- < r_j^0$) when $E$ is opposite to the direction of poling. Results for the three piezocermics in Table 3 are plotted in Fig. 11. Note that all curves are above and below the line $r_j/r_j^0 = 1$ for positive and negative $E$, respectively. These results agree with the
experimental observations in [4,17,18]. It is a first-order effect obtained from the solution of linear piezoelectricity although consideration of nonlinear effects may lead to further refinements. The energy release rate approach appears to be limited to the $K_{IC}$ type of failure where the energy has to be released instantly. Stable and unstable cracking could not be accounted for the same process in tandem.

4. Mode II cracking

Suppose that the normal stress $\sigma$ in Fig. 3 is removed with other conditions being the same. The only difference is that an in-plane shear $\tau$ is now applied, as illustrated in Fig. 12. This gives rise to

$$K_1 = 0, \quad K_{II} = \tau \sqrt{\pi a} \quad \text{and} \quad K_E = E \sqrt{\pi a}. \quad (26)$$

Note that $K_E$ remains unchanged in Eq. (12). The general expression of $S$ for mixed mode crack extension in [20] simplifies to

$$S = B_{22}K_{II}^2 + 2B_{24}K_{II}K_E + B_{44}K_E^2 \quad (27)$$

Eqs. (26) may be inserted into Eq. (27) to render

$$S = \tau^2 \pi a \left[ B_{22} + 2B_{24} \frac{E}{\tau} + B_{44} \left( \frac{E}{\tau} \right)^2 \right]. \quad (28)$$

4.1. Non-similar crack growth

Following a procedure similar to that for Mode I, the crack initiation angle $\theta_0$ can be obtained by solving

$$\frac{\partial S}{\partial \theta} = \tau^2 \pi a \left[ \frac{\partial B_{22}}{\partial \theta} + 2 \frac{\partial B_{24}}{\partial \theta} \frac{E}{\tau} + \frac{\partial B_{44}}{\partial \theta} \left( \frac{E}{\tau} \right)^2 \right] = 0 \quad (29)$$

<table>
<thead>
<tr>
<th>Material</th>
<th>$(E/\sigma) \times 10^{-3}$ (Vm/N)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$-15$</td>
</tr>
<tr>
<td>PZT-4</td>
<td>0.760</td>
</tr>
<tr>
<td>PZT-5H</td>
<td>0.782</td>
</tr>
<tr>
<td>P-7</td>
<td>0.679</td>
</tr>
</tbody>
</table>

Table 3

Mode I normalized $j$th crack growth segments $r_j^+ / r_j^-$ for positive and negative electric field and different piezoelectric ceramics

![Image of a table showing normalized energy density factor versus electric field to normal stress ratio for PZT ceramics.](image-url)
The angles \( \theta_0 \) that make \( S \) minimum for different ratios of \( q = E/\tau \) are found numerically and they are plotted graphically in Fig. 13 for PZT-4, PZT-5H and P-7 piezocermics. For \( E = 0 \), the fracture initiation angle is \( \theta_0 = -78.29^\circ \). When \( E \) is increased in the positive direction, \( -\theta_0 \) tends to decrease to a minimum and then increase again. For negative \( E \), \( -\theta_0 \) increase rapidly at first and then remains nearly constant. The trend is similar for the three piezocermics chosen in this study.

Determination of \( B_{ij} \) in Eq. (28) that correspond to minimum \( S \) is more involved for Mode II cracking because there prevails a different set of \( B_{ij} \) for each \( \theta_0 \) as \( E = s \) is altered. Values of \( E/\tau \) are first assigned to Eqs. (29) and (30) which can be solved for \( \theta_0 \) since \( B_{ij} \) are functions of \( \theta_0 \). Once \( \theta_0 \) is known, those \( B_{ij} \) associated with maximum of minimum \( S \) can thus be found. As an example, Table 4 gives the \( B_{ij} \) values for \( \theta_0 = 50^\circ \). A set of \( B_{ij} \) is determined for each of the three piezocermics as given in Table 4. Note that the values of \( B_{44} \) in Table 4 are not the same as those in Table 1 even though the same notation has been used. The functions \( B_{ij} \) are understood to depend on the direction of crack initiation.

Because \( \theta_0 \) is non-zero even for the first segment of crack growth, a bent crack configuration would result giving rise to a mixed mode crack extension situation such that \( S \) would involved both \( K_I \) and \( K_{II} \).
Eq. (1) remains valid for non-self similar crack growth, which would no longer occur along a straight line. Crack initiation angles \( \theta_1, \theta_2, \ldots \), need to be determined for each segments \( r_1, r_2, \ldots \), and they are evaluated by the repeat application of the energy density theory for locating \( S \) minimum. This procedure has been used not only for solving two-dimensional mixed mode crack problems but also for three-dimensional crack problems of elasticity [26,27] and elastoplasticity [6].

4.2. Failure stress: in-plane shear

To determine the in-plane shear stress \( \tau_f \) that would fail the first segment \( r_1 \), it is necessary to consider the extend of stable growth leading to global instability, i.e., \( r \to r_c \) as shown in Eq. (17). The condition of global instability can be defined by

\[
S = B_{11}K_1^2 + B_{22}K_{II}^2 + B_{44}K_E^2 + 2B_{12}K_1K_{II} + 2B_{14}K_1K_E + 2B_{24}K_{II}K_E.
\]

\[ (31) \]

Eq. (1) remains valid for non-self similar crack growth, which would no longer occur along a straight line. Crack initiation angles \( \theta_1, \theta_2, \ldots \), need to be determined for each segments \( r_1, r_2, \ldots \), and they are evaluated by the repeat application of the energy density theory for locating \( S \) minimum. This procedure has been used not only for solving two-dimensional mixed mode crack problems but also for three-dimensional crack problems of elasticity [26,27] and elastoplasticity [6].

\[
S_c = B_{22}K_{II}^2,
\]

\[ (32) \]

where \( B_{22} \) is evaluated in the direction of crack initiation \( \theta_0 = -78.297^\circ \) for pure Mode II mechanical load \( \tau \). Since \( S_c \) is assumed to be characteristics of the material, Eq. (32) may be equated to Eq. (6):

\[
\text{Fig. 13. Mode II failure stress versus electric field for: (a) positive field, (b) no field and (c) negative field.}
\]
\[ K_{\text{HIC}} = \sqrt{\frac{B_{11}(0^\circ)}{B_{22}(-78.297^\circ)}} K_{\text{IC}}. \] (33)

Hence, there is no need to perform separate experiments for finding \( K_{\text{HIC}} \) after Eq. (33) has been validated. The expression for \( B_{11} \) is given by Eq. (7) while \( B_{22} = A_{22} \) corresponds to Eq. (47) in [20]. Both Eqs. (32) and (28) may now be substituted into Eq. (17) to give

\[ \tau_{f}^2 + 2 \frac{B_{24}}{B_{22}} \tau_{f} E + \frac{B_{44}}{B_{22}} E^2 = \frac{\lambda}{B_{22} \pi a} \frac{B_{11}(0^\circ) K_{\text{IC}}^2}{B_{22} \pi a} \] (34)

which can be solved for \( \tau_{f} \)

\[ \tau_{f} = \frac{B_{24}}{B_{22}} E \]

\[ + \sqrt{\frac{\lambda}{B_{22} \pi a} \frac{B_{11}(0^\circ) K_{\text{IC}}^2}{B_{22} \pi a} + \left( \frac{B_{24}^2}{B_{22}^2} - \frac{B_{44}}{B_{22}} \right) E^2}. \] (35)

Recall that \( \lambda = r/r_c \) and is required to be less than unity.

Plotted in Figs. 13(a), (b) and (c) are values of \( \tau_{f} \) in Eq. (35) as a function of \( E \) for \( \lambda = 0.01, 0.10 \) and 1.0, respectively, and half crack length that varies from \( a = 1 \) to 9 mm. The trend of the curves are similar to those in Figs. 6(a)–(c) for Mode I crack extension. Deviations of curves in Figs. 13(a)–(c) from straight lines become more pronounced as the crack length is increased. In order to trigger global instability with little or no stable crack growth, Fig. 13(c) for \( \lambda = 1 \) shows that \( \tau_{f} \) has to increase approximately one order of magnitude.

As in the case of Mode I cracking, Eq. (35) may be rearranged or \( \tau_{f} \) may be solved directly from Eq. (34) to give

\[ \tau_{f} = \sqrt{B_{22}(-78.297^\circ)} \frac{K_{\text{HIC}}}{\sqrt{\pi a}} \sqrt{\frac{\lambda}{B_{22} + 2 B_{24} q + B_{44} q^2}}. \] (36)

A family of curves showing the variations of \( \tau_{f} \) with \( q \) can be obtained for \( \lambda = 0.01, 0.10 \) and 1.0. They are shown in Figs. 14(a)–(c) and tend to deviate from straight lines more significantly than those in Figs. 13(a)–(c) when \( \tau_{f} \) is varied against \( E \) alone.

### 4.3. Direction reversal of electric field

Eq. (28) suggests that a similar phenomenon of crack growth enhancement and retardation would prevail in Mode II when the electric field direction is reversed. It also appears that the deviation of crack path from the \( \tau_{1} \)-axis for \( +E \) and \( -E \) would be smaller and greater than that for \( E = 0 \). More precisely, the crack initiation angles are anticipated to satisfy the following conditions:

\[ |\theta_0| < |\theta_0| < |\theta_0|. \] (37)

This implies that the crack would curve less for positive \( E \) and curve more negative \( E \) when compared with \( \theta_0 \) for \( E = 0 \). This is shown schematically in Fig. 15. A less bent crack should extend longer than a more bent one. Even though no experimental observations have been reported for Mode II cracking in the open literature, the behavior in Fig. 15 appears to be intuitively plausible and supported by the analytical results obtained from the energy density theory provided that effect is angle controlled for the situation where the first crack growth segment is sufficiently small. As the crack initiation angle rotates, the crack growth segment size would increase and the starting angle becomes less influential. A more rigorous analysis would be required before making any conclusions.

Refer to Eq. (1) and apply it to the first segment of crack growth \( r_1 \) under Mode II

\[ \left( \frac{dW}{dV} \right)_c = \frac{S_0^+}{r_1} = \frac{S_0}{r_1^0} = \frac{S_0}{r_1^+} = \ldots \] (38)

The superscript notation has the same meaning as before. Eq. (38) would lead to the same results as those in Eqs. (23)–(25) for Mode I with \( j = 1 \) except that \( S_0^- \) and \( S_0^+ \) must now be understood to depend on different crack initiation angles. Since the crack growth enhancement and retardation behavior may not be entirely controlled by the initiation angle, the following possible conditions should be considered.
Condition I: If $|\theta_0^+| < |\theta_0^-|$, then $r_1^+ > r_1^0$ for positive $q$.
Condition II: If $|\theta_0^+| > |\theta_0^-|$, then $r_1^- < r_1^0$ for negative $q$.
Condition III: If $|\theta_0^+| > |\theta_0^-|$, $r_1^+ > r_1^0$ may still hold for positive $q$.
Condition IV: If $|\theta_0^+| < |\theta_0^-|$, $r_1^- < r_1^0$ may still hold for negative $q$. 

Fig. 14. Mode II failure stress versus electric field to shear stress ratio for: (a) positive field, (b) no field and (c) negative field.

Fig. 15. Mode II crack growth initiation behavior due to electric field reversal.

Fig. 16. Mode II normalized energy density factor versus electric field to shear stress ratio for PZT ceramics.
Because the crack initiation direction changes with $E = \tau$, there might be a situation where $|\theta_0|$ is greater than $|\theta_0|$ and $r_1^\pm$ may still be greater than $r_0^\pm$ (Condition III). The situation $|\theta_0| < |\theta_0|$ and $r_1^\pm < r_0^\pm$ (Condition III) is also a possibility. Shown in Fig. 16 are variations of the normalized energy density function $S = s^2p_{\alpha\alpha}10^{-3}$ with $E = \tau$. Keep in mind that a different $S$ being dependent on $\theta_0$ would have to be determined for each different value of $E = \tau$. The conditions in Eq. (24) for $j = 1$ are thus satisfied for PZT-4, PZT-5H and P-7. Numerical values of the curves in Fig. 16 can be found in Table 5.

Based on the results in Fig. 16, the normalized Mode II growth increment $r_1^\pm/r_0^\pm$ can be calculated and plotted in Fig. 17 as a function of $E/\tau$. As in Mode I, all curves intersect at $q = 0$ and $r_1^\pm = r_0^\pm$. The numerical data in Table 6 exhibit the crack growth enhancement and retardation behavior. Except for PZT-5H and P-7, when negative $E/\tau$ values equal to $-0.015$, $r_1^\pm$ becomes larger than $r_0^\pm$. Further clarified in Fig. 18 are the conditions posed in Eq. (39). Region I refers to the crack angle controlled zone where the crack segment $r_1^\pm$ is sufficiently small; it includes both $+E$ and $-E$. Region II exists only for $+E$ and the growth segment $r_1^\pm$ must be sufficiently large.

Table 7 shows the values of $E/\tau$ and $\theta_0$ at which Condition I switches to Condition III. The transition point marked as $T$ in Fig. 18 shows for each material that the crack would bend.
shown in Fig. 17. In addition to $K_E$, both $K_I$ and $K_{II}$ would be present. Each term of $S$ in Eq. (31) would then affect the direction of crack initiation and the failure stress. Applying the same procedure that was used for analyzing Mode I and II cracking, the conditions for determining $S$ minimum, i.e., $\partial S/\partial \theta = 0$ and $\partial^2 S/\partial \theta^2 > 0$ can be applied to obtain the angles of crack initiation $\theta_0$. Without going into details, the results for PZT-4 are plotted in Fig. 18 for different values of $m = E/\sigma$. The mid-point of Fig. 18 at $\theta_0 = 0^\circ$ and $\beta = 0^\circ$ refers to Mode I crack extension where all curves intersect. The curves with negative and positive $m$ correspond, respectively, to positive and negative crack initiation angles. Comparing with the curve for $m = 0$, the crack initiation directions are altered more and more several as $m$ is increased (see Figs. 19 and 20).

Failure stress for mixed mode crack initiation can be derived to show that crack growth enhancement and retardation behavior also prevails by reversing the direction of the applied electric field. A detailed discussion would be beyond the objectives of this work.

### Table 7

<table>
<thead>
<tr>
<th>Material</th>
<th>$E/\tau$ (Vm/N)</th>
<th>$\theta_0$ (deg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PZT-4</td>
<td>0.386</td>
<td>−78.30</td>
</tr>
<tr>
<td>PZT-5H</td>
<td>0.506</td>
<td>−77.49</td>
</tr>
<tr>
<td>P-7</td>
<td>5.808</td>
<td>−79.96</td>
</tr>
</tbody>
</table>

**6. Concluding remarks**

Interaction of the electric and mechanical effects for ferroelectric ceramics has been a topic of continuing interest since there still remains many unresolved problems and unexplained physical phenomena. Attempts to develop a theory to describe the fracture mechanics of piezoceramics are confronted with the difficulties of quantifying energy dissipated by changes in the crystal structures (domain switching), alteration in the microstructure (intergranular separation, grain distortion and rotation, etc.) and creation of micro- and
In elastoplastic fracture problems, a two-level model involving strain energy density function could be applied within each scale range. The connection between each scale range depends on a priori assumptions motivated by experimental observations [28] or inspired by the analysts [11]:

\[ \frac{dW}{dV} = \left( \frac{dW}{dV} \right)_{\text{nano}} + \left( \frac{dW}{dV} \right)_{\text{micro}} + \left( \frac{dW}{dV} \right)_{\text{meso}} + \left( \frac{dW}{dV} \right)_{\text{macro}} . \] (40)

In elastoplastic fracture problems, a two-level model involving \((dW/dV)_{\text{micro}}\) and \((dW/dV)_{\text{macro}}\) as shown by Eq. (8) has been used [6,21,22]. A three-level model might be preferred to include \((dW/dV)_{\text{meso}}\) where the effects of so referred to "shear + rotation" [28] could be included. The weak points of such an approach lies in an a priori knowledge of the gap size between the scale ranges. The major advantage is that equilibrium mechanics could be applied within each scale range. The connection between each scale range could be made on the average in time and space without considering the details of how the energy is transferred across surfaces and interphases. Strictly speaking, a multiscale process is highly inhomogeneous and non-equilibrium in character. That is the states traversed by a system cannot be described in terms of physical parameters representing the system as a whole. Ideally speaking, no gaps should prevail between each successive scale range such that the connection would be smooth. This requires a precise consideration of the exchange of surface and volume energy via the rate change of volume with surface \(dV/\Delta A\) [29], a quantity that is assumed to vanish in the limit for equilibrium theories. Keep in mind that boundary conditions for equilibrium theories are preassumed and not determined [30] as required in a truly non-equilibrium theory.

While recognizing that failure by cracking is a multiscale process, a first-order solution for the crack growth enhancement and retardation behavior can be obtained by using only a single level \((dV/\Delta A)_{\text{macro}}\) model with the stipulation that the energy dissipation is not a spontaneous process; it must necessarily consist a stable stage prior to the onset of global instability. The energy release rate approach contains no length parameter to distinguish slow cracking from rapid fracture. It accommodates only instant release of all energy. This is the main reason why it has been traditionally limited to "brittle fracture" à la Griffith. Those attempts made to use energy release rate for describing fracture preceded by slow growth have not been successful. They include the fracture of elastoplastic and piezoelectric materials.

Encouraged by the results in this work, it would appear that the strain energy density function

\[ \frac{dW}{dV} = \int_0^{r_0} \sigma_{ij} \, d\gamma_{ij} + \int_0^{D_i} E_i \, dD_i , \] (41)

could be further used with the criterion for failure [7,8] to resolve additional problems:

- A two-scale level model may be developed to analyze the effect of microcracking on a dominant macrocrack when the intensity of the applied electric field is not so close to the coercive field \(E_c\), say for \(E\) in the range of 0.6–0.8\(E_c\).
- An energy rate driven criterion for domain switching appears to be more plausible than those based on electric field driven, stress driven or the combination. This is reminiscent of microstructure changes in phase transformation of metals [31] where accurate predictions have been made by the strain energy density theory. Similarly, domain switching involves changes of the crystal structure.
- Near the crack tip, energy dissipations other than domain- switching could prevail, particularly for high intensity electric field. The interactive effects of domain switching and microcracking have not received attention.
- Analytical and experimental results for mixed mode cracking could provide information to
control failure by selecting the appropriate directional and fracture resistance properties of the piezoceramics.

Little would be gained to associate damage or microstructure change thresholds with load related parameters such as applied stress or strain for they would not serve a useful purpose in application. The challenge is to find a threshold parameter that could linearize the nonlinear data such that component size and loading rate effects could be resolved by extrapolation to minimize the number of tests. The ultimate objective would be to relate small specimen data to those for large specimens and high loading rate data to those for lower loading rates. Such objectives have been achieved in [6,21,22] for the elastoplastic fracture of metal alloy specimens. Scaling of failure behavior for piezoceramics could alleviate the cumbersome task of testing miniature size specimens that are difficult to handle.

References

[12] Private communication with D.N. Fang, Fracture Mechanics Laboratory, Department of Engineering Mechanics, Tsinghua University, Beijing, China, April 2000.