Energy density theory formulation and interpretation of cracking behavior for piezoelectric ceramics

J.Z. Zuo a, G.C. Sih b,*

a Department of Engineering Mechanics, Xi'an Jiaotong University, Xi'an 710049, People's Republic of China
b Department of Mechanical Engineering and Mechanics, Lehigh University, Bethlehem, Pennsylvania 18015-3006, USA

Abstract

Any attempt made to separate energy into electrical and mechanical parts may lead to inconsistencies as they do not necessarily decouple. This is illustrated by application of the energy density function in the linear theory of piezoelectricity. By assuming that a critical energy density function prevails at the onset of crack initiation, it is possible to establish the relative size of an inner and outer damage zone around the crack tip; they correspond to the ligaments at failure caused by pure electric field and pure mechanical load. On physical grounds, the relative size of these zones must depend on the relative magnitude of the mechanical and electrical load. Hence, they can vary in size depending on the electromechanical material and damage resistance properties. Numerical results are obtained for the PZT-4, PZT-5H, and P-7 piezoelectric ceramics. These two ligaments for the two damage zones may coincide for appropriate values of the applied electrical field and mechanical load.

Explicit expression of the energy density factor $S$ is derived showing the mixed mode electromechanical coupling effects. The factor $S$ can increase or decrease depending on the direction of the applied electric field with reference to the poling direction. This is in contrast to the result obtained from the energy release rate quantity, which remains unchanged for electric field in the direction of poling or against it. © 2000 Elsevier Science Ltd. All rights reserved.

1. Introduction

Electromechanical coupling effects for ferroelectric crystals have been known for sometime. However, only in recent years much interest has been generated because of their application to electronic devices such as transducers, sensors and actuators. Concern for reliability and durability of these devices necessitates a fundamental understanding of the damage and fracture process of piezoelectric ceramics. This has led to a host of research findings [1–6] concerned with electromechanical interactive phenomena that remain not understood. The widely quoted work [7] on the fracture mechanics of piezoelectric materials assumes crack growth to occur under the static adiabatic condition while others [8,9] propound for consideration of material damage at different scale levels. The implication is that electric and mechanical energy transfer may not be synchronized in time for a given size of region over which the physical parameters are being averaged. For a multiscale process, attention needs to be focused on the space/time...
interaction effects. Additional complexities are sure to rise if dissipative effects are to be included as well [10].

The enhancement and retardation of crack growth in piezoelectric materials [11] have been identified, respectively, with the application of a positively and negatively applied electric field. The former refers to electric flow in the direction of poling while the opposite prevails for the latter. Although the above phenomenon was confirmed in [12] for the PZT-4 material, the quantitative assessment of such a behavior was not successful when using the energy release rate quantity as it was unaffected by the direction of the applied electric field. This is in contrast to the experimental observations. Only the mechanical part of the total energy was thus used to correlate the test data [12]. The argument was that the electrical portion of the energy had no influence on crack energy release. An alternate approach based on a strip polarization saturation model and a ‘local’ energy release rate was proposed in [6]. A straight line relation between the failure stress and electric field was obtained with a negative slope; it differed from that in [12] by a factor of two. Again, the sign of the electrical field played no role [6]. Electrical nonlinearity was claimed as a factor giving rise to these unexplained physical phenomena.

What have not been considered in previous works are the spatial and temporal interactions that may not be explainable by using classical continuum theories. Physical parameters should be defined in accordance with the scale level at which the observations and/or analyses are being made. Nonequilibrium effects become dominant as the space and time scale are reduced [10]. Lacking in particular is a quantitative assessment of the limitation of the linear theory of piezoelectricity and/or application of a more general failure criterion. When applying the energy release rate criterion, it is necessary to specify whether the energy is released with reference to the creation of macroscopic, mesoscopic or microscopic crack surface area. For example, the release of elastic and plastic energy does not occur at the same scale level nor at the same location and time. Such a distinction has eluded the attention of many past investigators. The justification perhaps could be claimed on the grounds that the difference in location and time are smeared over a sufficiently large area and long time as an average. For the uniaxial test of polycrystals (macroscopically homogeneous) under moderate strain rate, the time average could be minutes and the space average could be centimeters. These restrictions may well apply to the fracture behavior of piezoelectric ceramics. It is therefore, prudent to select a failure criterion [14] that could be applied to linear and nonlinear and dissipative and non-dissipative materials for closed and open thermodynamic systems [10].

The energy density criterion [14] makes no a priori assumptions for the direction of crack initiation and applies to mixed mode load in three-dimensions as easily as in two-dimensions. Moreover, the same criterion remains valid for determining the onset of crack initiation, growth (stable) and final termination (unstable).

Material damage in general is governed fundamentally by the proportion of how each element distorts and dilates in the continuum regardless of whether the energy used in the process is electrical or mechanical; their interaction would vary in location and time. Limitations imposed by the continuum mechanics theory of piezoelectricity should be distinguished from those arising from the failure criterion or vice versa. The latter applies to the energy release rate quantity, the application of which has led to conclusions that are not consistent with experiments [11–13].

2. Basic equations of linear piezoelectricity

The constitutive equations for the stresses $\sigma_{ij}$ and strains $\gamma_{ij}$ as associated with the electric displacements $D_i$ and electric field components $E_i$ can be expressed by

$$
\sigma_{ij} = C_{ijkl} \gamma_{kl} - e_{ijk} E_k, \quad D_i = e_{ikl} \gamma_{kl} + \varepsilon_{ik} E_k
$$

(1)
for the linear case. In Eqs. (1), the elastic, piezoelectric and dielectric constants are denoted, respectively, by $C_{ijkl}, e_{ijk}$ and $e_{ij}$. The inverse of Eqs. (1) can be written as

$$\gamma_{ij} = H_{ijkl} \sigma_{kl} + g_{kl} D_k, \quad E_i = -g_{ikl} \sigma_{kl} + \beta_{kl} D_k.$$  

Here, $H_{ijkl}, g_{ijk}$ and $\beta_{ij}$ stand, respectively, for the compliance piezoelectric and dielectric impermeability constants. In the absence of body forces and free electric volume charge, the equilibrium equations and Gauss’ Law of Electrostatics take the forms

$$\sigma_{ij, j} = 0, \quad D_{ij} = 0.$$  

The kinematic equations are given by

$$\gamma_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}), \quad E_i = -\phi_i.$$  

Note that $u_i$ and $\phi$ are the elastic displacements and electric potential, respectively.

If $L$ denotes a surface free of electric charge or traction, while $x_i$ are points on $L$, then the following boundary conditions can be stated:

$$t_i = 0, \quad D_i n_i = 0 \quad \text{on} \quad x_i \in L.$$  

The boundary value problem can thus be formulated in terms of complex variables in two-dimensions similar to those in [15,16] for problems involving lines of discontinuities.

3. Energy density field

Consider a unit volume of material such that a mechanical load would give rise to an electric field while an electric field could cause mechanical deformation. Such materials belonging to the ferroelectric crystal group are known as piezoelectric ceramics. Regardless of the electromechanical interaction, energy state in the continuum is assumed to behave as a continuous function of time and space. On fundamental grounds, it is not possible to separate the internal energy induced by different external disturbances let it be electrical, mechanical, thermal or otherwise. Without loss in generality, the energy density function at a given location $x_i$ and time $t$ can be written as

$$\left( \frac{dW}{dV} \right)_{x_i,t} = \left( \frac{dW}{dV} \right)_{x_i,t-\Delta t} + \left( \frac{dW}{dV} \right)_{x_i,t+\Delta t}.$$  

To be understood is that $dW/dV$ at $t - \Delta t$ and $t + \Delta t$ would correspond, respectively, to the dissipated and available energy density at $t$ as $\Delta t \to 0$. In the theory of elastoplasticity, the former would be referred to as the plastic energy density and the latter as elastic energy density. Philosophically speaking, Eq. (6) states that the ‘present’ could not be stated without an a priori knowledge of the past and future.

3.1. Implication of specimen testing results

It suffices therefore to express all disturbance such as electrical, mechanical, acoustic, etc. by the movement of molecules. This was accomplished in the isoenergy density theory [10] by application of the nonequilibrium temperature in relation to displacement. The quantity $dW/dV$ at $t - \Delta t$ represents the dissipation energy density which has been measured experimentally [17] for composite materials with a dominant crack. The results were startling as they tend to depend specifically on the specimen test condition, particularly at the load grips. Similar observations concerning the initiation of mesobands have also been made in [18]. This implies that experimental data are very sensitive to specimen testing conditions,
particularly when the specimen dimensions are reduced. Hence, the possible use of small specimen data in application must be scrutinized.

3.2. Limitation of classical approaches

Classical continuum mechanics theories neglect the spatial size effect by letting the rate change of volume with surface to vanish in the limit. This decouples the thermal and mechanical effects. Dissipation can no longer be included as an inherent behavior of the continuum but only as an after thought. Invoking the classical assumptions is equivalent to assuming that the influence of material can be decoupled from the effects of loading and geometry. This permits the independent specification of the constitutive relation. Such a simplifying assumption reduces the isoenergy density theory [10] to the energy density criterion [14]. Despite the simplifications, the classical approach has provided the type of ‘consistency’ in general; application that nonlinear theories could not match. It is in this spirit that linear piezoelectricity will be applied in conjunction with the energy density criterion to better understand whether the discrepancies between theory and experiment are caused by deficiencies in the classical continuum theories, the failure criteria or both.

4. Interaction of electromechanical effects

The literature on piezoelectricity assumes that the energy density function can be regarded as the linear superposition of two parts

\[ \frac{dW}{dV} = \left( \frac{dW}{dV} \right)_M + \left( \frac{dW}{dV} \right)_E. \] (7)

The subscripts M and E refer, respectively, to the mechanical and electrical portion of the energy density function such that they are expressible in the forms

\[ \left( \frac{dW}{dV} \right)_M = \frac{1}{2} \sigma_{ij} \gamma_{ij}, \quad \left( \frac{dW}{dV} \right)_E = \frac{1}{2} D_i E_i \] (8)

and hence

\[ \frac{dW}{dV} = \frac{1}{2} \sigma_{ij} \gamma_{ij} + \frac{1}{2} D_i E_i. \] (9)

At first glance, the neglect of \( (dW/dV)_E \) would appear to have excluded the electrical part of the energy density function. A closer examination shows otherwise.

4.1. Stress and electric displacement

Eq. (2) may be substituted into Eqs. (8) to eliminate the strains \( \gamma_{ij} \) and electric field components \( E_i \), such that \( dW/dV \) in Eq. (9) can be expressed in a positive definite form

\[ \frac{dW}{dV} = \frac{1}{2} \sigma_{ij} H_{ijkl} \sigma_{kl} + \frac{1}{2} D_i \beta_{ij} D_j \] (10)
such that
\[
\left( \frac{dW}{dV} \right)_M = \frac{1}{2} \sigma_{ij} H_{ijkl} \sigma_{kl} + \frac{1}{2} D_k g_{kj} \sigma_{ij},
\]
(11)
\[
\left( \frac{dW}{dV} \right)_E = -\frac{1}{2} D_i g_{ki} \sigma_{kl} + \frac{1}{2} D_j \beta_{ij} D_j.
\]
(12)
Note that the neglect of \((dW/dV)_E\) in Eq. (12) does not exclude the effect of electrical energy. There remains the interaction term between \(D_i\) and \(\sigma_{ij}\) in Eq. (11).

4.2. Strain and electric field

Similarly, Eqs. (1) may be inserted into Eqs. (8) to eliminate the stresses \(\sigma_{ij}\) and electric displacements \(D_i\) such that \(dW/dV\) in Eq. (9) can be written as
\[
\frac{dW}{dV} = \frac{1}{2} \gamma_{ij} C_{ijkl} \gamma_{kl} + \frac{1}{2} E_i \epsilon_{ij} E_j.
\]
(13)
According to the form in Eq. (7), there renders
\[
\left( \frac{dW}{dV} \right)_M = \frac{1}{2} \gamma_{ij} C_{ijkl} \gamma_{kl} - \frac{1}{2} E_k \epsilon_{kij} \gamma_{ij},
\]
(14)
\[
\left( \frac{dW}{dV} \right)_E = \frac{1}{2} E_k \epsilon_{kij} \gamma_{ij} + \frac{1}{2} E_i \epsilon_{ij} E_j.
\]
(15)
Here again, the neglect of \((dW/dV)_E\) in Eqs. (15) does not imply the complete exclusion of electrical portion of the energy as the quantity \(E_k\) prevails in \((dW/dV)_M\).

4.3. Canonical forms

In view of the aforementioned comments with reference to Eqs. (11) and (12) or Eqs. (14) and (15), Eqs. (10) and (13) in canonical forms offer another possibility for discussing electrical and mechanical energy density function, i.e.
\[
\frac{dW}{dV} = \left( \frac{dW}{dV} \right)_\sigma + \left( \frac{dW}{dV} \right)_D \quad \text{or} \quad \frac{dW}{dV} = \left( \frac{dW}{dV} \right)_\gamma + \left( \frac{dW}{dV} \right)_\epsilon
\]
(16)
such that
\[
\left( \frac{dW}{dV} \right)_\sigma = \frac{1}{2} \sigma_{ij} H_{ijkl} \sigma_{kl} \quad \text{and} \quad \left( \frac{dW}{dV} \right)_D = \frac{1}{2} D_k g_{kj} \sigma_{ij}
\]
(17)
and
\[
\left( \frac{dW}{dV} \right)_\gamma = \frac{1}{2} \gamma_{ij} C_{ijkl} \gamma_{kl} \quad \text{and} \quad \left( \frac{dW}{dV} \right)_\epsilon = \frac{1}{2} E_i \epsilon_{ij} E_j.
\]
(18)
Suppose that \((dW/dV)_D\) in Eq. (17) or \((dW/dV)_\epsilon\) in Eq. (18) were set to zero. By means of Eqs. (1) and (2), it is not difficult to show that
\[
\left( \frac{dW}{dV} \right)_\sigma = \frac{1}{2} \sigma_{ij} \gamma_{ij} - \frac{1}{2} D_k g_{kj} \sigma_{ij}
\]
(19)
and
\[
\left( \frac{dW}{dV} \right)_r = \frac{1}{2} \sigma_{ij} \epsilon_{ij} + \frac{1}{2} E_k \kappa_{kj} \epsilon_{ij}. \tag{20}
\]
Again, the electric effects are not eliminated. They are still contained in \((dW/dV)_\sigma\) and \((dW/dV)_\epsilon\) as shown in Eqs. (19) and (20) although the first of Eqs. (17) and (18) do not reveal the electric effects explicitly.

5. Energy density criterion

As stated earlier, the energy density criterion applies in general to any materials including piezoelectric ceramics [19]. It can be stated in general by the following hypotheses for solids with and without an initial defect such as a crack for at least two relative scale levels such as damages due to elastic and plastic actions.

5.1. Basic hypotheses

For simplicity, the criterion will be stated in terms of \(dW/dV\) for a macrocrack in a piezoelectric material.

**Hypothesis 1:** Crack initiation is assumed to occur in the direction of the maximum of minimum \(dW/dV\) with reference to the space variables, say max. of \((dW/dV)_{\min}\).

**Hypothesis 2:** Crack initiation is assumed to take place when \((dW/dV)_{\min}\) reaches a critical value characteristics of the material, say \((dW/dV)_c\).

**Hypothesis 3:** The onset of rapid crack propagation is assumed to start when the energy density \(S_{\min}\) associated with \((dW/dV)_{\min}\) also reaches a critical value, i.e., \(S_{\min} = S_c\).

5.2. Critical damage zone

When referring to the location where a small crack is likely to nucleate or a pre-existing crack would initiate, it is expedient to introduce a distance \(r\) as illustrated in Fig. 1 such that

![Fig. 1. Local element near damage or failure initiation.](image)

(a) Crack nucleation  
(b) Crack initiation
and \( r \) is required to be non-zero. In the limit as \( r \) approaches the location of defect nucleation Fig. 1(a) or crack initiation Fig. 1(b), \( \frac{dW}{dV} \) becomes unbounded. The decay away from the origin corresponds to the Newtonian potential \( \frac{1}{r} \). The intensity \( S \) has been referred to as the ‘energy density factor’. The problems in Figs. 1(a) and (b) are in fact the same as they both address the threshold for a macro-element to fail. One happens to be ahead of a macrocrack and another near a microdefect the shape and size of which are not considered in the continuum analysis.

It is possible to estimate the relative size of the electrical and mechanical ligament, say \( r_e/r_\sigma \), around the origin of crack nucleation or initiation. In general, both conditions \( r_e < r_\sigma \) in Fig. 2(a) and \( r_e > r_\sigma \) in Fig. 2(b) could prevail depending on the relative magnitude of the applied mechanical load \( \sigma_\infty \) and electrical field \( E_\infty \), i.e., \( E_\infty/\sigma_\infty \). No intention is made to determine the damage zone shape. The parameters \( r_e \) and \( r_\sigma \) are only indicative of the average size.

Suppose that two experiments are performed for a piezoelectric material with a macrocrack. As the electrical field intensity \( E_\infty \) is increased with \( \sigma_\infty = 0 \), \( (dW/dV)_e \) in an element near the crack tip reaches a critical value and the ligament \( r_e \) would fail. Similarly, the same specimen is subjected to mechanical load \( \sigma_\infty \) only while \( E_\infty = 0 \), \( (dW/dV)_\sigma \) in an element at a different distance \( r_\sigma \) would break. Assume that the critical energy density at failure initiation is the same regardless of whether the energy is supplied by an electrical or mechanical source, then it can be deduced from Eq. (21) that

\[
\frac{r_e}{r_\sigma} = \frac{S_e}{S_\sigma} \rightarrow B^* \frac{K_E^2}{K_I^2}
\]

(22)

for cracks that extend in a self-similar manner. In Eq. (22), the parameter \( B^* \) depends on the properties of the piezoelectric material. The quantities \( K_I \) and \( K_E \) are the Mode I stress intensity factors for mechanical and electrical loadings; they depend only on the load type and crack configuration.

6. Central crack specimen

To be specific, the central crack configuration will be considered. Refer to Fig. 3 for the case of a line crack extending from \( x_1 = -a \) to \( x_1 = a \) in the \( x_1x_3 \) plane. The boundaries of the region are sufficiently far away such that they would not interact with the crack. A uniform electric displacement \( D_\infty \) and stress \( \sigma_\infty \) are applied with the respective orientations of \( z_e \) and \( z_\sigma \) as shown in Fig. 3. The piezoelectric material is poled in the positive \( x_3 \) direction.
6.1. Specification of stress and electric displacement

The expressions for the singular in-plane stresses and electric displacements can be found in [3]. They are given by:

\[ \sigma_{11} = \frac{1}{\sqrt{2\pi r}} \text{Re} \left[ \sum_{j=1}^{3} \frac{C_j \mu_j^2}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right], \]

\[ \sigma_{33} = \frac{1}{\sqrt{2\pi r}} \text{Re} \left[ \sum_{j=1}^{3} \frac{C_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right], \tag{23} \]

\[ \sigma_{13} = -\frac{1}{\sqrt{2\pi r}} \text{Re} \left[ \sum_{j=1}^{3} \frac{C_j \mu_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right], \]

and

\[ D_1 = \frac{1}{\sqrt{2\pi r}} \text{Re} \left[ \sum_{j=1}^{3} \frac{C_j \lambda_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right], \]

\[ D_3 = -\frac{1}{\sqrt{2\pi r}} \text{Re} \left[ \sum_{j=1}^{3} \frac{C_j \lambda_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right], \tag{24} \]

where \( \mu_j \) and \( \lambda_j \) are complex parameters which depend only on the mechanical and electric properties of the piezoelectric material. The symbol \( \text{Re} \) denotes the real part of a complex function and the parameter \( C_j \) depends on the loading conditions at infinity as

\[ C_j = A_{j1} K_1 - A_{j2} K_{II} - A_{j3} K_D. \tag{25} \]
The complex parameters \( A_{jk} \ (j,k = 1,2,3) \) are related to the material properties; they are given in Appendix A.1. The stress and electric displacement intensity factorss \( K_1, K_{II} \) and \( K_D \) take the forms

\[
K_1 = \sigma_\infty \sin \alpha \sqrt{\pi \alpha}, \quad K_{II} = \sigma_\infty \cos \alpha \sqrt{\pi \alpha}, \quad K_D = D_\infty \sin \alpha \sqrt{\pi \alpha}.
\]

Substituting Eqs. (23) and (24) into Eq. (10) and solving for \( S \) with the aid of Eq. (21), there results

\[
S = A_{11}K_1^2 + A_{22}K_{II}^2 + A_{44}K_D^2 + 2A_{12}K_1K_{II} + 2A_{14}K_1K_D + 2A_{24}K_{II}K_D,
\]

where the coefficients \( A_{11}, A_{22}, A_{44}, A_{12}, A_{14} \) and \( A_{24} \) can be found in Appendix A.2. They depend only on the materials constants and angle \( \theta \) measured from the crack plane. The main difference between Eq. (27) and other fracture criteria for piezoelectric materials is that Eq. (27) includes the additional terms \( A_{12}, A_{14} \) and \( A_{24} \) that reflect interactions between the electrical and mechanical loading.

Unlike the empirical failure criteria expressed in quadratic form where the coefficients are determined by curve fitting, the functions \( A_{ij} \) in Eq. (27) depend on the angle \( \theta \) and material properties; they are obtained by application of Hypothesis (2) and reflect the proportion of the distortional and dilatational effects.

### 6.2. Specification of stress and electric field

When an electric field \( E_\infty \) is applied instead of \( D_\infty \), Eqs. (1) and (2) may be used to obtain the relation

\[
E_\infty \sin \alpha = -g_{33} \sigma_\infty \sin \alpha + \beta_{33} D_\infty \sin \alpha.
\]

Thus, the electric displacement intensity factor \( K_D \) can be rewritten as

\[
K_D = \frac{1}{\beta_{33}} (E_\infty \sin \alpha + g_{33} \sigma_\infty \sin \alpha) \sqrt{\pi \alpha}.
\]

Substituting Eq. (29) into Eq. (27), it is found that

\[
S = B_{11}K_1^2 + B_{22}K_{II}^2 + B_{44}K_D^2 + 2B_{12}K_1K_{II} + 2B_{14}K_1K_D + 2B_{24}K_{II}K_D,
\]

where

\[
K_E = E_\infty \sin \alpha \sqrt{\pi \alpha}.
\]

The coefficients \( B_{ij} \) are related to \( A_{ij} \) as:

\[
B_{11} = A_{11} + 2A_{14} \frac{g_{33}}{\beta_{33}^2} + A_{44} \frac{g_{33}^2}{\beta_{33}^2}, \quad B_{22} = A_{22}, \quad B_{44} = \frac{A_{44}}{\beta_{33}^2},
\]

\[
B_{12} = A_{12} + A_{24} \frac{g_{33}}{\beta_{33}^2}, \quad B_{14} = \frac{A_{14}}{\beta_{33}^2} + A_{44} \frac{g_{33}}{\beta_{33}^2}, \quad B_{24} = \frac{A_{24}}{\beta_{33}^2},
\]

In view of the dependencies of \( A_{ij} \) on the angle \( \theta \), \( B_{ij} \) would also be a function of \( \theta \) via Eqs. (32). Note that \( g_{33} \) and \( \beta_{33} \) are related to the basic constants for the piezoelectric material as

\[
g_{33} = \frac{1}{\det(B)} \left[ 2C_{13} e_{31} (C_{11} - C_{12}) - (C_{11}^2 - C_{12}^2) e_{33} \right],
\]

\[
\beta_{33} = \frac{1}{\det(B)} \left[ 2C_{11}^2 (C_{11} - C_{12}) - (C_{11}^2 - C_{12}^2) C_{33} \right]
\]
with
\[
\det(B) = \begin{vmatrix}
C_{11} & C_{12} & C_{13} & e_{31} \\
C_{12} & C_{11} & C_{13} & e_{31} \\
C_{13} & C_{13} & C_{33} & e_{33} \\
e_{31} & e_{31} & e_{33} & -e_{33}
\end{vmatrix}.
\] (35)

6.3. Inner and outer region of damage

To be more specific, three different piezoelectric ceramics are selected: they are PZT-4, PZT-5H and P-7 with the properties given in Tables 1–3 inclusive.

For Mode I crack extension, \( z_\sigma = 0 \) and \( K_{II} = 0 \) Eq. (30) contains only the \( K_I \) terms. Using Eq. (21), it can be shown that
\[
\left( \frac{dW}{dV} \right)_1 = \frac{B_{11}K_I^2}{r_\sigma}, \quad K_I = \sigma_\infty \sqrt{\pi a}
\] (36)
for \( E_\infty = 0 \) and
\[
\left( \frac{dW}{dV} \right)_E = \frac{B_{44}K_E^2}{r_E}, \quad K_E = E_\infty \sqrt{\pi a}
\] (37)

Table 1
Elastic constants \((\times 10^{10} \text{Nm}^2)\)
<table>
<thead>
<tr>
<th>Materials</th>
<th>(C_{11})</th>
<th>(C_{12})</th>
<th>(C_{13})</th>
<th>(C_{44})</th>
<th>(C_{44})</th>
</tr>
</thead>
<tbody>
<tr>
<td>PZT-4</td>
<td>13.9</td>
<td>7.78</td>
<td>7.43</td>
<td>11.3</td>
<td>2.56</td>
</tr>
<tr>
<td>PZT-5H</td>
<td>12.6</td>
<td>5.5</td>
<td>5.3</td>
<td>11.7</td>
<td>3.53</td>
</tr>
<tr>
<td>P-7</td>
<td>13.0</td>
<td>8.35</td>
<td>8.25</td>
<td>11.9</td>
<td>2.46</td>
</tr>
</tbody>
</table>

Table 2
Piezoelectric constants \((\text{C/m}^2)\)
<table>
<thead>
<tr>
<th>Materials</th>
<th>(e_{31})</th>
<th>(e_{33})</th>
<th>(e_{15})</th>
</tr>
</thead>
<tbody>
<tr>
<td>PZT-4</td>
<td>-6.98</td>
<td>13.84</td>
<td>13.44</td>
</tr>
<tr>
<td>PZT-5H</td>
<td>-6.5</td>
<td>23.3</td>
<td>17.0</td>
</tr>
<tr>
<td>P-7</td>
<td>-10.34</td>
<td>14.66</td>
<td>13.55</td>
</tr>
</tbody>
</table>

Table 3
Dielectric permittivities \((\times 10^9 \text{C/Vm}^2)\)
<table>
<thead>
<tr>
<th>Materials</th>
<th>(\varepsilon_{11})</th>
<th>(\varepsilon_{33})</th>
</tr>
</thead>
<tbody>
<tr>
<td>PZT-4</td>
<td>6.00</td>
<td>5.47</td>
</tr>
<tr>
<td>PZT-5H</td>
<td>15.1</td>
<td>13.0</td>
</tr>
<tr>
<td>P-7</td>
<td>9.65</td>
<td>8.31</td>
</tr>
</tbody>
</table>
for $\sigma_\infty = 0$. Following the reason how Eq. (22) was derived, the parameter $B^*$ in Eq. (22) can be identified as

$$B^* = \frac{B_{44}}{B_{11}}$$

(38)

by application of Eqs. (36) and (37). It follows that

$$\frac{r_e}{r_\sigma} = \frac{B_{44}}{B_{11}} \left( \frac{E_\infty}{\sigma_\infty} \right)^2.$$  

(39)

Shown in Table 4 are the values of $r_e/r_\sigma$ for different values of $E_\infty/\sigma_\infty$. For $\theta = \theta^\circ$, $B_{44}/B_{11}$ in Eqs. (32) is found to be 519.33 for PZT-4. Note that $r_e$ can be greater or smaller than $r_\sigma$ depending on whether the effect of applied electric field $E_\infty$ is greater or smaller than the applied mechanical load $\sigma_\infty$ or $E_\infty/\sigma_\infty$, as it should. The work in [6] considered only the case for $r_e > r_\sigma$. For $r_e = r_\sigma$, $E_\infty/\sigma_\infty = 0.0439$. This corresponds to the situation when the critical ligament size for pure electric loading is the same as that for pure mechanical loading. In general, $r_e$ and $r_\sigma$ would compete. This is illustrated in Figs. 2(a) and (b). Values of $r_e/r_\sigma$ for PZT-5H and P-7 are also given in Table 4. They correspond, respectively, to $B_{44}/B_{11} = 1264.96$ and 801.84. The trends are similar. Since $r_e$ and $r_\sigma$ would not be equal in general, the foregoing results suggest the strong possibility of an inner and outer zone of damage around the crack tip, one being more intensified than the other. The size of these two zones would be sensitive to inhomogeneities of the local material microstructure.

### 7. Crack growth affected by reversal of electric field with respect to poling

As mentioned earlier with reference to the work in [13], the application of an electric field in the direction of poling assisted crack growth while the opposite occurred when the direction of electric field is reversed. No criterion up to now could explain this phenomena although many unsuccessful attempts have been made in the past. The strain energy density criterion offers a possible explanation based on the promise that the energy stored in a continuum per unit volume can be uniquely characterized by the amplitude and frequency of the excitation regardless of the form of external disturbance. For the sake of illustration, consider the case for $\alpha_\sigma = \alpha_e = 90^\circ$, hence, Eq. (30) reduces to

$$S = B_{11}K_1^2 + 2B_{14}K_4K_E + B_{44}K_E^2.$$  

(40)

Since $K_1$ and $K_E$ are known from Eq. (26), the expression for $S$ in Eq. (40) reduces to

<table>
<thead>
<tr>
<th>$E_\infty/\sigma_\infty$ ($\text{m}^2/\text{C}$)</th>
<th>$r_e/r_\sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>PZT-4</td>
</tr>
<tr>
<td>0.07</td>
<td>2.545</td>
</tr>
<tr>
<td>0.06</td>
<td>1.870</td>
</tr>
<tr>
<td>0.05</td>
<td>1.298</td>
</tr>
<tr>
<td>0.04</td>
<td>0.831</td>
</tr>
<tr>
<td>0.03</td>
<td>0.467</td>
</tr>
<tr>
<td>0.02</td>
<td>0.208</td>
</tr>
<tr>
<td>0.015</td>
<td>0.117</td>
</tr>
<tr>
<td>0.010</td>
<td>0.0519</td>
</tr>
</tbody>
</table>
According to Eq. (41), $S$ can be interpreted as the energy dissipated as the crack advances by an amount $r$ shown in Fig. 4. In this sense, $S$ could also be regarded as a crack driving force. It suffices to show that $S$ for positive $E_\infty$ is greater than $S$ for $E_\infty = 0$ while $S$ for negative $E_\infty$ is smaller than $S$ for $E_\infty = 0$. This will be shown in a separate communication for stable crack growth in piezoelectric ceramics.

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

Fig. 4. Crack driving force $S$.

8. Concluding remarks

Linear piezoelectricity can be used to explain certain inconsistencies not in the theory but in the ways of how the theoretical results are used in conjunction with energy release rate criterion or path independent integral. Limitations inherent in the equilibrium theories limited to closed thermodynamic systems cannot be corrected by advocating nonlinearity.

The separation of electrical and mechanical energy could be problematic because $E_i$ is implicitly contained in $\sigma_{ij}$ and $D_{ij}$ in $\gamma_{ij}$ as indicated by Eqs. (1) and (2), respectively. Depending on how the electric energy and mechanical energy are defined, the neglect of one or the other may not imply that the electrical and mechanical effects are uncoupled. Assumptions that may seem appealing at first glance could lead to inconsistent results. This has been shown by the examples depicted in this work. What is meant by mechanical and electrical energy becomes ambiguous if the two effects are indeed coupled.

On physical grounds, energy induced by electric source would yield nonuniform distribution in space and time and differ from that produced by mechanical disturbance. The different response in terms of particle displacements, however would be interwoven such that they are no longer separable. The equilibrium theories of continuum mechanics smear any inhomogeneous effects by taking averages. Hence, they
could not explain multiscale processes except in a piece meal fashion. This work in connection with those published earlier tends to suggest that

- Test data for material and strength properties tend to become more specimen specific when specimens are reduced in size.
- Unless scaling in size and time is better understood for piezoelectric ceramics, it would be difficult to establish rules for design.
- While the energy density factor $S$ does account for the sign change of the applied electric field, this effect should be quantified more precisely by experiments.
- Crack initiation and propagation under static and cyclic mixed mode conditions could be analyzed theoretically and experimentally for piezoelectric ceramics.

To reiterate, consistency and generality are important considerations for the selection of a damage or failure criterion, particularly for multiscale processes [20,21].

Appendix A. Coefficients in the energy density factor

A.1. Expressions for $A_{jk}$

The coefficients $A_{jk}$ $(j, k = 1, 2, 3)$ in Eq. (25) are given in the matrix

$$
[A_{jk}] = \frac{1}{\Delta} \begin{bmatrix}
\mu_2\lambda_3 - \mu_3\lambda_2 & \lambda_2 - \lambda_3 & \mu_3 - \mu_2 \\
\mu_3\lambda_1 - \mu_1\lambda_3 & \lambda_3 - \lambda_1 & \mu_1 - \mu_3 \\
\mu_1\lambda_2 - \mu_2\lambda_1 & \lambda_1 - \lambda_2 & \mu_2 - \mu_1
\end{bmatrix},
$$

(A.1)

where

$$
\Delta = (\lambda_2 - \lambda_3)\mu_1 + (\lambda_3 - \lambda_1)\mu_2 + (\lambda_1 - \lambda_2)\mu_3,
$$

(A.2)

$$
\lambda_j = \frac{(b_{31} + b_{15})\mu_j^2 + b_{33}}{\delta_{11}\mu_j^2 + \delta_{33}} \quad (j = 1, 2, 3),
$$

(A.3)

$$
b_{31} = g_{31} - \frac{H_{12}}{H_{11}}g_{31}, \quad b_{33} = g_{33} - \frac{H_{13}}{H_{11}}g_{31}, \quad b_{15} = g_{15},
$$

(A.4)

The parameters $\mu_j$ $(j = 1, 2, 3)$ in Eq. (A.3) are the roots of characteristic equation of piezoelectric materials, which only depend on the mechanical and electric material constants, as shown in Tables 1–3. The material constants $H_{ij}, g_{ij}$ are the components of coefficient matrices in Eq. (2).

A.2. Energy density factor coefficients

Once $A_{jk}$ are known from Eqs. (40) to (A.2), the energy density factor coefficients $A_{ij}$ in Eq. (27) can be determined from the following expression:

$$
A_{11} = \frac{a_{11}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j1}\mu_j^2}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right)^2 + \frac{a_{33}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j1}}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right)^2
$$

$$
+ \frac{a_{13}}{2\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j1}\mu_j^2}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right) \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j1}}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right)
$$
\begin{align}
A_{44} &= \frac{a_{11}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j1} \mu_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right)^2 + \frac{a_{33}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j1} \mu_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right)^2 \\
+ \frac{a_{13}}{2\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j3} \mu_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right)^2 + \frac{\delta_{11}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j1} \lambda_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right)^2 \\
&\quad + \frac{\delta_{33}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j3} \lambda_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right)^2,
\end{align}

A_{12} = -\frac{a_{11}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j1} \mu_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right) \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j2} \mu_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right) \\
- \frac{a_{33}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j3} \mu_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right) \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j2} \mu_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right) \\
- \frac{a_{13}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j1} \mu_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right) \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j2} \mu_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right) \\
- \frac{a_{13}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j3} \mu_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right) \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j2} \mu_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right) \\
- \frac{a_{13}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j3} \mu_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right) \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j1} \mu_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right) \tag{A.5}
\end{align}
\[
A_{14} = -\frac{a_{11}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{1j} \mu_{j}}{\sqrt{\cos \theta + \mu_{j} \sin \theta}} \right) \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j3} \mu_{j}}{\sqrt{\cos \theta + \mu_{j} \sin \theta}} \right)
\]
\[
\quad - \frac{a_{33}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j2} \mu_{j}}{\sqrt{\cos \theta + \mu_{j} \sin \theta}} \right) \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j3} \mu_{j}}{\sqrt{\cos \theta + \mu_{j} \sin \theta}} \right)
\]
\[
\quad - \frac{a_{13}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j3} \mu_{j}}{\sqrt{\cos \theta + \mu_{j} \sin \theta}} \right) \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j2} \mu_{j}}{\sqrt{\cos \theta + \mu_{j} \sin \theta}} \right)
\]
\[
\quad - \frac{a_{13}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j3} \mu_{j}}{\sqrt{\cos \theta + \mu_{j} \sin \theta}} \right) \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j2} \mu_{j}}{\sqrt{\cos \theta + \mu_{j} \sin \theta}} \right)
\]
\[
\quad - \frac{a_{44}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j2} \mu_{j}}{\sqrt{\cos \theta + \mu_{j} \sin \theta}} \right) \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j3} \mu_{j}}{\sqrt{\cos \theta + \mu_{j} \sin \theta}} \right)
\]
\[
\quad - \frac{\delta_{13}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j2} \mu_{j}}{\sqrt{\cos \theta + \mu_{j} \sin \theta}} \right) \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j3} \mu_{j}}{\sqrt{\cos \theta + \mu_{j} \sin \theta}} \right) \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j2} \mu_{j}}{\sqrt{\cos \theta + \mu_{j} \sin \theta}} \right),
\]
\[\text{(A.8)}\]

\[
A_{24} = \frac{a_{11}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j2} \mu_{j}}{\sqrt{\cos \theta + \mu_{j} \sin \theta}} \right) \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j3} \mu_{j}}{\sqrt{\cos \theta + \mu_{j} \sin \theta}} \right)
\]
\[
\quad + \frac{a_{33}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j2} \mu_{j}}{\sqrt{\cos \theta + \mu_{j} \sin \theta}} \right) \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j3} \mu_{j}}{\sqrt{\cos \theta + \mu_{j} \sin \theta}} \right)
\]
\[
\quad + \frac{a_{13}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j2} \mu_{j}}{\sqrt{\cos \theta + \mu_{j} \sin \theta}} \right) \left( \text{Re} \sum_{j=1}^{3} \frac{A_{j3} \mu_{j}}{\sqrt{\cos \theta + \mu_{j} \sin \theta}} \right)
\]
\[\text{(A.9)}\]
\[ + \frac{a_{11}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{1j} \mu_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right) \left( \text{Re} \sum_{j=1}^{3} \frac{A_{1j}}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right) + \frac{a_{44}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{1j} \mu_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right) \left( \text{Re} \sum_{j=1}^{3} \frac{A_{1j} \mu_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right) + \frac{\delta_{11}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{1j} \lambda_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right) \left( \text{Re} \sum_{j=1}^{3} \frac{A_{1j} \lambda_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right) + \frac{\delta_{33}}{4\pi} \left( \text{Re} \sum_{j=1}^{3} \frac{A_{1j} \lambda_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right) \left( \text{Re} \sum_{j=1}^{3} \frac{A_{1j} \lambda_j}{\sqrt{\cos \theta + \mu_j \sin \theta}} \right). \tag{A.10} \]

Note that
\[ a_{11} = H_{11} - \frac{H_{12}^2}{H_{11}}, \quad a_{33} = H_{33} - \frac{H_{13}^2}{H_{11} H_{113}} = H_{13} - \frac{H_{12} H_{13}}{H_{11}}, \quad a_{44} = H_{44}, \quad \delta_{11} = \beta_{11}, \quad \delta_{33} = \beta_{33} + \frac{S_{31}^2}{S_{11}}. \tag{A.11} \]

The material constants \( H_{ij}, \beta_{ij} \) are the components of coefficient matrices in Eq. (2).

References