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Fracture of Piezoelectric Materials: Energy Density Criterion

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Abstract

In this paper, the concept of energy density factor S for piezoelectric materials is presented. In addition to the mechanical energy the electrical energy is included as well. The direction of crack initiation is assumed to occur when S_{min} reaches a critical value S_{cr} that can be used as an intrinsic materials parameter and is independent of the crack geometry and loading. The result agrees with empirical evidence qualitatively and explain rationally the effect of applied electric field on fracture strength: positive electric fields decrease the apparent fracture toughness of piezoelectric materials while negative electric fields increase it.

1. Introduction

Piezoelectric materials have been found wide technological applications for transducers, sensors and actuators due to their inherent coupled electromechanical behavior. Fracture behaviors of these materials under a combined electric-mechanical loading have drawn increasing attention in both the academic and engineering communities. Some basic crack problems in linear piezoelectric materials have been solved in [1-7]. However, there are some unexplained discrepancies between theory and experiments. A field is defined as positive or negative when it is parallel or anti-parallel. The fracture criterion based on energy release rate indicates that the presence of electric fields always impedes crack propagation. However, all available experimental results imply otherwise. Mode I and mixed mode fracture tests were made [4] for PZT-4 ceramics. It was observed that a positive electric field tends to open the crack and reduce the fracture load while a negative electric field increases it. In vickers indentation experiments, It was observed [8] that cracks tends to be longer in the presence of a positive electric field than cracks in the absence of a electric field. Conversely, shorter cracks were observed when a negative electric field was applied. In order to derive a fracture criterion which corresponds more closely with the empirical observations, proposed in [4] is to use only the mechanical part of the energy release rate in a fracture criterion, arguing that fracture is a mechanical process and should be controlled only by the mechanical part of the energy. It seems rather difficult to defend this argument on physical grounds because all mechanical forces are of electromagnetic origin. There is no fundamental reason to separate a physical process into an electric part and a mechanical part [9]. As an alternative explanation of the discrepancies between theory and experiments, a strip polarization saturation model was proposed [9]. A "local" energy release rate, obtained by evaluating a path independent integral along an infinitesimal contour near the crack tip. This was used as a fracture criterion. This model has not been verified experimentally. In fact, it has been shown that polarization switching would occur near the crack tip under combined electrical and mechanical loads. A 180° domain switching cannot be modeled by polarization saturation.

More than two decades ago, the volume energy density was proposed [10] as a fracture criterion in contrast to the idea of Griffith's energy release rate. This provided an alternative approach to failure prediction for the same stress solution. The

distinctions were emphasized in the series Mechanics of Fracture [11]. The theory requires no calculation on the energy release rate and thus possesses the inherent advantage of being able to treat all mixed mode crack extension problems. Unlike the conventional theory of G and K which measures only the amplitude of the local stress, the fundamental parameter in this theory, the strain energy theory density factor S which is defined as the coefficient of $1/r$ singular behavior of the volume energy density dW/dV, is also direction sensitive. The stationary values of S with reference to the coordinates of the element under consideration are assumed to coincide with the location of crack initiation. The direction of crack initiation is assumed to occur when $S_{\min}$ reaches a critical value S_{cr} that can be used as an intrinsic materials parameter and is independent of the crack geometry and loading. This theory gained momentum and credibility in engineering. A review on the use of the volume energy density can be found in [12,13].

Since the stress intensity factor and energy release rate are not suitable as a fracture criterion for piezoelectric materials, the energy density theory [14] is applied to piezoelectric materials as a fracture criterion. The theoretical result agrees qualitatively with empirical evidence, i.e. positive electric fields aid crack propagation, while negative electric fields impede crack propagation.

2. The Inner Energy Density Concept and Hypotheses

The constitutive relations for linear piezoelectric solid can be written as

$$\begin{aligned} \sigma_{ij} &= c_{ijkl}\gamma_{kl} - e_{lij}E_l \\ D_i &= e_{ikl}\gamma_{kl} + \varepsilon_{il}E_l \end{aligned} \tag{1}$$

where σ_{ij} are the stress tensor, D_i the electric displacement vector, γ_{ij} the strain tensor and E_i the electric field vector. c_{ijkl}, e_{ikl} and ε_{ij} are the elasticity constants, piezoelectricity constants and permittivity constants, respectively. Adopt the convention that upper-case subscripts rang from 1 to 4, while lower-case subscripts rang from 1-3, the constitutive equations can be written as

$$\Phi_{iJ} = \begin{cases} \sigma_{ij} & \text{if } J = 1,2,3 \\ D_i & \text{if } J = 1,2,3 \end{cases} \tag{2}$$

$$E_{iJKl}=\begin{cases} c_{ijkl} & \text{if } J,K=1,2,3 \\ e_{lij} & \text{if } J=1,2,3;K=4 \\ e_{ikl} & \text{if } K=1,2,3;J=4 \\ -\varepsilon_{il} & \text{if } J,K=4 \end{cases}$$

Consider the two-dimensional case of a crack in a combined mechanical and electrical field and focus attention on a coordinate system (x_1, x_2, x_3) shown in Fig. 1 with the x_1-axis normal to the crack, the x_3-axis perpendicular to the crack plane and the x_2–axis tangent to the crack border. From the solution obtained in [4], the near tip stresses and the electric displacement are expressed in polar coordinates (r, θ) originated at the right crack tip (see Fig. 1) as

$$\begin{aligned} \mathbf{t}_3 &= \left[\sigma_{31} \quad \sigma_{32} \quad \sigma_{33} \quad D_3\right]^T = \frac{\sqrt{\pi a}}{\sqrt{2\pi r}} \mathrm{Re}\{\mathbf{B}\,\mathrm{diag}[1/\sqrt{\cos\theta + \mathrm{p}_K \sin\theta}]\mathbf{B}^{-1}\mathbf{T}\} + O(1) \\ \mathbf{t}_1 &= \left[\sigma_{11} \quad \sigma_{12} \quad \sigma_{13} \quad D_1\right]^T = \frac{\sqrt{\pi a}}{\sqrt{2\pi r}} \mathrm{Re}\{\mathbf{B}\,\mathrm{diag}[\mathrm{p}_K/\sqrt{\cos\theta + \mathrm{p}_K \sin\theta}]\mathbf{B}^{-1}\mathbf{T}\} + O(1) \end{aligned} \tag{3}$$

where $\mathbf{T} = \left[\sigma_{13}^{\infty} \quad \sigma_{23}^{\infty} \quad \sigma_{33}^{\infty} \quad D_3^{\infty}\right]^T$ represents remote mechanical and electrical loadings, a is a half crack length, p_K $(K = 1, 2, 3, 4)$ are eigenvalues of a characteristic equation, and **B** are coefficient matrix, diag[ ] denotes a diagonal matrix, Re{ } denotes the real part of the complex function in the bracket. It is noted that the higher order terms in r have been neglected.

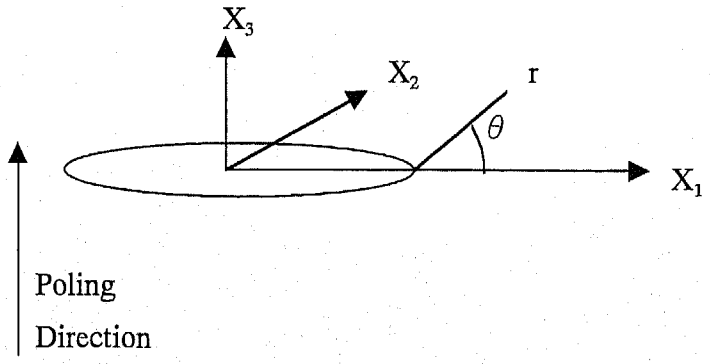

Fig. 1 Crack tip in a piezoelectric material

Using the conventionally defined stress and electric displacement intensity factor, stress and displacement at the crack plane, $\theta = 0$, are given as

$$\sigma_{23} = \frac{K_{III}}{\sqrt{2\pi r}} \quad \sigma_{13} = \frac{K_{II}}{\sqrt{2\pi r}} \quad \sigma_{33} = \frac{K_I}{\sqrt{2\pi r}} \quad D_3 = \frac{K_D}{\sqrt{2\pi r}} \tag{4}$$

where

$$K_I = \sigma_{33}^{\infty}\sqrt{\pi a} \quad K_{II} = \sigma_{13}^{\infty}\sqrt{\pi a} \quad K_{III} = \sigma_{23}^{\infty}\sqrt{\pi a} \quad K_D = D_3^{\infty}\sqrt{\pi a} \tag{5}$$

Equation (4) shows that stresses and electric displacement are uncoupled in this plane, that means the electric loading alone can not produce mechanical stress in the crack plane ahead of the crack tip and vice versa. If the stress intensity factor is used as a fracture criterion, the effect of the electric field can not be accounted for. Hence, stress intensity factor is not suitable as a fracture criterion for piezoelectric materials.

For a piezoelectric material, the energy stored in a volume element $dV=dxdydz$ under a general three-dimensional system is

$$dW = [\frac{1}{2}\sigma_{ij}\gamma_{ij} + \frac{1}{2}E_i D_i]dV \tag{6}$$

which is positive definite. And the electric enthalpy is defined by

$$d\psi = [\frac{1}{2}\sigma_{ij}\gamma_{ij} - \frac{1}{2}E_i D_i]dV = \frac{1}{2}\Phi_{IK}E_{KlJ}^{-1}\Phi_{iJ}dV \tag{7}$$

So, the inner energy density can be written as

$$\frac{dW}{dV} = \frac{1}{2}\Phi_{IK}E_{KlJ}^{-1}\Phi_{iJ} - D_l E_{4lJ}^{-1}\Phi_{iJ} \tag{8}$$

Inserting the stresses and the electric displacements in equation (3) into the inner energy density function (8) to yield an expression involving $1/r$ the coefficient of which is the energy density factor for generalized two-dimensional problem

$$S = r\frac{dW}{dV} = \mathbf{K}^T\mathbf{M}\mathbf{K} \tag{9}$$

where $\mathbf{K} = [K_{II} \quad K_{III} \quad K_I \quad K_D]^T$, the elements of positive definite matrix $\mathbf{M}$ are complicated function of the piezoelectric material constants and depend on the angle θ through p_K. Define $S = S_M + S_E$ such that

$$S_M = \frac{r}{2}(\sigma_{ij}\gamma_{ij}) = \frac{r}{2}[\Phi_{IK}E_{KlJ}^{-1}\Phi_{iJ} - D_l E_{4lJ}^{-1}\Phi_{iJ}] \tag{10}$$

is the factor corresponding to mechanical part of energy and

$$S_E = \frac{r}{2}(D_l E_i) = -\frac{r}{2}D_l E_{4lJ}^{-1}\Phi_{iJ} \tag{11}$$

is the factor corresponding to electric part of energy.

As in [14], two fundamental hypotheses of crack extension in piezoelectric material can be stated:

Hypothesis (1): **For piezoelectric materials, crack initiation will start in a radial direction along which the inner energy density is a minimum.**

Hypothesis (2): **The critical intensity S_{cr} of this inner energy field governs the onset of crack propagation.**

The physical grounds and explanation of these hypotheses are the same as that for the strain energy density theory for structural materials in [14]. Note that for crack propagation to take place in the x_1x_3-plane the direction of relative minimum inner energy density must be found. In two-dimensional problems, the direction of crack propagation can be determined by a single variable θ and hence hypothesis (1) can be satisfied by the application of the calculus of variations. A necessary condition for the inner energy density S to have a stationary value is that

$$\frac{\partial S}{\partial \theta} = 0 \quad \text{at } \theta = \theta_0 \tag{12}$$

The value of θ_0 which makes S a minimum determines the angle of the plane along which the crack spreads and can be found by further requiring that

$$\frac{\partial^2 S}{\partial \theta^2} > 0 \quad \text{at } \theta = \theta_0 \tag{13}$$

which is a position of unstable equilibrium. Equation (12) and (13) are the necessary and sufficient conditions for S to be a minimum at $\theta = \theta_0$.

It is noted that the above criterion is based on the local density of the inner energy field in the crack tip region and requires no special assumption on the direction in which the energy released by the separating crack surfaces is computed as in the Griffith theory.

For comparison, we also write down the energy release rate G

$$G = \int_\Gamma \left[\psi n_1 - \sigma_{ij} n_j u_{,1} - D_i n_i \varphi_{,1} \right] d\Gamma \tag{14}$$

where u and φ are displacements and electric potential, respectively; Γ is an integration contour around the crack tip, **n** is the unite normal vector to the contour. The integral given by equation (14) is also path-independent. The energy release rate can also be derived using the Irwin closure integral as

$$G = \lim_{\delta \to 0} \frac{1}{2\delta} \int_0^\delta \left[\sigma_{i3}(x_1) \Delta u_i(\delta - x_1) + D_3(x_1) \Delta \varphi(\delta - x_1) \right] dx_1 \tag{15}$$

where δ is assumed crack extension.

3. Numerical Example

In order to demonstrate the suitability of the energy density theory for the piezoelectric failure problem, consider a cracked piezoelectric material PZT-4. For transversely isotropic piezoelectrics, the coupled constitutive relations can be written in contracted notation in terms of a single 9×9 symmetric matrix

$$\begin{Bmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{33}\\ \sigma_{23}\\ \sigma_{31}\\ \sigma_{12}\\ D_1\\ D_2\\ D_3\end{Bmatrix}=\begin{bmatrix}c_{11} & c_{12} & c_{13} & 0 & 0 & 0 & 0 & 0 & e_{31}\\ & c_{11} & c_{13} & 0 & 0 & 0 & 0 & 0 & e_{31}\\ & & c_{33} & 0 & 0 & 0 & 0 & 0 & e_{33}\\ & & & c_{44} & 0 & 0 & 0 & e_{15} & 0\\ & & & & c_{44} & 0 & e_{15} & 0 & 0\\ & & & & & c_{66} & 0 & 0 & 0\\ & & & & & & -\varepsilon_{11} & 0 & 0\\ & & & & & & & -\varepsilon_{11} & 0\\ & & & & & & & & -\varepsilon_{33}\end{bmatrix}\begin{Bmatrix}\gamma_{11}\\ \gamma_{22}\\ \gamma_{33}\\ 2\gamma_{23}\\ 2\gamma_{31}\\ 2\gamma_{12}\\ -E_1\\ -E_2\\ -E_3\end{Bmatrix} \tag{16}$$

With the material poling axis aligned in the positive x_3 direction, the constants for PZT-4 are as follows:

$$\begin{aligned} c_{11} &= 13.9\times 10^{10}\ N/m^2 & e_{33} &= 13.8C/m^2\\ c_{33} &= 11.3\times 10^{10}\ N/m^2 & e_{31} &= -6.98C/m^2\\ c_{12} &= 7.78\times 10^{10}\ N/m^2 & e_{15} &= 13.4C/m^2\\ c_{13} &= 7.43\times 10^{10}\ N/m^2 & \varepsilon_{11} &= 6.00\times 10^{-9}C/Vm\\ c_{44} &= 2.56\times 10^{10}\ N/m^2 & \varepsilon_{33} &= 5.47\times 10^{-9}C/Vm \end{aligned} \tag{17}$$

$$c_{66}=\frac{1}{2}(c_{11}-c_{12})=3.06\times 10^{10}\ N/m^2$$

After solving the Stroh eigenvalue problem for the plane perpendicular to the crystal x_2-axis, there results

$$\begin{aligned} p_1 &= 1.19041i & p_2 &= -0.27309+1.08717i\\ p_3 &= 0.27309+1.08717i & p_4 &= 1.09343i \end{aligned} \tag{18}$$

and

$$\mathbf{B}=\begin{bmatrix}-0.1370i & 0.1755-0.2400i & -0.1755-0.2400i & 0\\ 0 & 0 & 0 & 0.2404i\\ 0.1151 & 0.2457+0.0996i & 0.2457-0.0996i & 0\\ 0.8265 & 0.6049 & 0.6049 & 0\end{bmatrix} \tag{19}$$

The vector **T** is calculated by inverting equation (16) with plane strain boundary conditions. For a crack along the crystal x_1-axis, with uniaxial loading $(\sigma_{33}^{\infty}, E_3^{\infty})$ perpendicular to the crack plane, the load vector takes the form

$$\mathbf{T} = \left[0 \quad 0 \quad \sigma_{33}^{\infty} \quad 10^{-9}\left(10.0E_3^{\infty} + 0.24\sigma_{33}^{\infty}\right)\right]^T \tag{20}$$

Substituting these expressions into equation (14) and (9) yields

$$G = 10^{-9}a\left[0.036\left(\sigma_{33}^{\infty}\right)^2 + 0.037\sigma_{33}^{\infty}E_3^{\infty} - 13.8\left(E_3^{\infty}\right)^2\right] \tag{21}$$

The expressions for S, S_E and S_M are very complicated, so are omitted here. After obtaining the expression of S, differentiating it with respect to θ and setting the result equal to zero, the values of θ_0 corresponding to S_{min} are found. It is found that $\theta_0 = 0$ over the rang shown in Fig. 2.

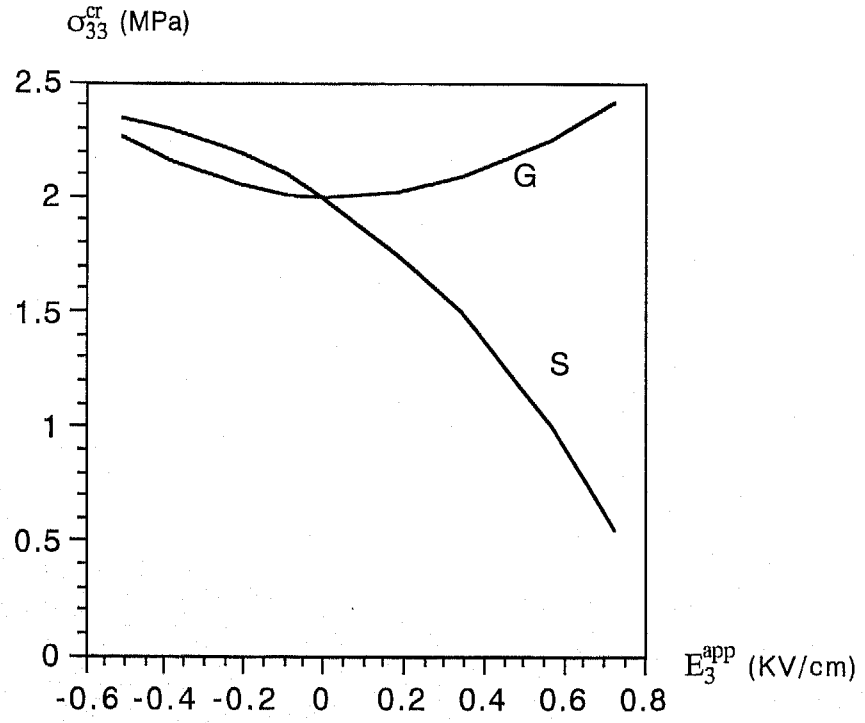

Fig. 2 Fracture load *vs* applied field according to inner density theory and energy release rate

Once a fracture load is measured with no voltage applied, the formulas can be used to predict the change in critical stress as a function of electric field. Fig. 2 shows the field-dependence of fracture load for a crack with half-length $a=1cm$ which extends at a stress of $2MPa$ when no field is applied (the estimate of baseline fracture strength was guided by [4] experiments conducted on PZT-4). In these loading conditions, the

distribution of S is analogous to that of mechanical energy S_M, the plane $\theta_0 = 0$ corresponds to the direction of minimum energy density, a position of unstable equilibrium. For comparison, the fracture toughness according to the energy release rate are also include in Fig. 2.

The local minimum of energy density predicts that the crack extend along the crack plane over the rang shown in Fig. 2 and the positive electrical fields aid crack propagation while negative electric fields impede crack propagation. Such a trend agrees qualitatively with empirical evidence. In contrast, the energy release rate shows no dependence on the sign of the applied electric field, contradicting the experimental observations. For structural materials, the Griffith energy release rate theory is the special case of S-theory when $\theta_0 = 0$. But, for piezoelectric materials, this relation fails.

When the applied electric field is greater than about 0.725kV/cm for PZT-4, (moreover when only the electric field is applied) the distribution of S is analogous to that of electric energy S_E, the position of unstable equilibrium *i.e.* the direction of minimum energy density will locate between $\pi/2$ and π, which may indicate that the failure mode of piezoelectric materials will be dielectric breakdown in these loading conditions. It is an interesting question whether this criterion can describe the crack initiation and breakdown near crack tip in a unified fashion: when the energy density factor S reaches the critical value, the crack initiation will start if the distribution of S is analogous to that of mechanical energy S_M; the crack will breakdown if the distribution of S is analogous to that of electric energy S_E. However, this needs experiment to verify, the further research is being undertaken by the authors.

In other hand, due to its ferroelectricity, PZT-4 will endure nonlinear polarization near the crack tip as the applied electric field is higher (the coercive field of PZT-4 is $1KV/cm$). Thus, the linear solution will overestimate the electric energy, which means the linear solution may underestimate the fracture toughness σ_{33}^{cr} in the case when the applied electric field is higher.

4. Conclusion

In this paper, the concept of energy density factor S for piezoelectric materials has been presented. The stationary values of the energy density factor can predict the direction of crack growth under electric and mechanical combined mixed mode conditions. As In

[14], the critical value S_{cr} is independent of the crack geometry and loading and hence it can be used as a material parameter for measuring the resistance against fracture. The theory result in qualitative agree with empirical evidence. From the present study, it can be concluded that the inner energy density theory is a good fracture criterion for piezoelectric materials; and positive electric fields decrease the apparent fracture toughness of piezoelectric materials while negative electric fields increase it.

In other hand, this theory shows the potential that it can describe the crack initiation and dielectric breakdown near crack tip in a unified fashion. The energy density theory can be immediately applied for resolving many practical electromechanical coupling problems. The superiority of the energy density theory over the energy release rate theory is apparent.

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