Energy Release Rate for a Crack or a Cavity in a Piezoelectric Material

T.Y. Zhang

Department of Mechanical Engineering, The Hong Kong University of Science and Technology,
Clear Water Bay, Kowloon, Hong Kong

Keywords: Fracture, Piezoelectric Materials, Energy Release Rate, Elliptical Cavity

ABSTRACT

The present paper studies thermodynamic functions and energy release rate for an elliptical cylinder cavity or an opened crack inside an infinite piezoelectric medium under combined mechanical-electrical loadings. The energy release rate for the cavity propagation is formulated under the condition that the ratio of the minor semi-axis to the major semi-axis of the ellipse remains unchanged. For an insulating crack, the applied electric field contributes nothing to the energy release rate when the undeformed crack profile is used, while the electric field resists crack propagation when the deformed crack profile is used. For a conducting slit crack, the energy release rate is independent of the applied electric field perpendicular to the crack, and is enhanced by the applied electric field parallel to the crack.

1. INTRODUCTION

Piezoelectric materials are widely used as active elements of sensors and actuators in the electronics industry due to their pronounced piezoelectric, dielectric and pyroelectric properties. Fracture behaviors of these materials under combined electric-mechanical loadings have drawn increasing attentions in both academic and engineering communities [1-16]. However, there is still confusion regarding the effect of electric field on the fracture behavior and criterion. In cases where a crack is treated as a mathematical slit without any thickness and has a finite dielectric constant, the energy release rate for crack propagation evaluated from linear fracture mechanics is positive definite and independent of applied electric fields when the electric field inside the crack is considered [6, 14]. On the other hand, the energy release rate is not positive definite and the electric loading would always impede crack propagation if the electric field inside the crack is ignored [8, 11]. Park and Sun [16] argued that the fracture process is mechanical in nature and, therefore, only the mechanical energy release rate should be used as a fracture criterion, which linearly depends on the applied electric field. Recently Gao, Zhang and Tong [15] proposed an electric strip saturation model and hence derived the local and global energy release rates. Under small-scale yielding conditions, the global energy release rate is equal to that of a linear piezoelectric crack without electrical yielding. The local energy release rate gives linear predictions similar to the results of the mechanical energy release rate [16].

When the crack is treated as a mathematical slit crack, the electric field inside cannot be calculated and, consequently, the energy release rate cannot be perfectly evaluated. In a previous study, we developed a self-consistent method to calculate the crack opening profile in a piezoelectric material under combined mechanical and electric loadings [17]. The energy release rate for crack propagation should be evaluated using the opened crack profile (after deformation), because the crack opens first and then propagates. The present work reports the details of derivation of the energy release rate for a cavity in a piezoelectric material.

2. ANALYSIS

Parton and Kudryavtsev [18] summarized the thermodynamic functions for piezoelectric materials. The internal energy, electric enthalpy and full Gibbs energy are briefly described here. The internal energy per unit volume, u , is expressed in a differential form as

$$du = \sigma_{ij} d\epsilon_{ij} + E_i dD_i + T ds, \quad (1)$$

where s is the entropy per unit volume; T is the absolute temperature; $\mathbf{E}$ and $\mathbf{D}$ are respectively the electric field strength and electric displacement vectors; and σ_{ij} , and ϵ_{ij} are respectively the components of stress and strain tensors. Define the free energy per unit volume, f , as

$$f = u - Ts, \quad \text{for which} \quad df = \sigma_{ij} d\epsilon_{ij} + E_i dD_i - s dT. \quad (2)$$

The electric enthalpy per unit volume, h , is defined as

$$h = u - E_i D_i - Ts, \quad \text{for which} \quad dh = \sigma_{ij} d\epsilon_{ij} - D_i dE_i - s dT. \quad (3)$$

Introduce the mechanical enthalpy per unit volume, w , as

$$w = u - \sigma_{ij} \epsilon_{ij} - Ts, \quad \text{for which} \quad dw = -\epsilon_{ij} d\sigma_{ij} + E_i dD_i - s dT. \quad (4)$$

The full Gibbs function per unit volume, g , is defined as

$$g = u - \sigma_{ij} \epsilon_{ij} - E_i D_i - Ts, \quad \text{for which} \quad dg = -\epsilon_{ij} d\sigma_{ij} - D_i dE_i - s dT. \quad (5)$$

At a constant temperature, Eqs. (2), (3), (4) and (5) reduce respectively to

$$df = \sigma_{ij} d\epsilon_{ij} + E_i dD_i, \quad (6)$$

$$dh = \sigma_{ij} d\epsilon_{ij} - D_i dE_i, \quad (7)$$

$$dw = -\epsilon_{ij} d\sigma_{ij} + E_i dD_i, \quad (8)$$

$$dg = -\epsilon_{ij} d\sigma_{ij} - D_i dE_i, \quad (9)$$

There are two independent variables, one mechanical and the other electrical, determining the four thermodynamic functions at a constant temperature. The independent mechanical variable can be the strains or the stresses, while the independent electric variable can be the electric field strengths or the electric displacements. If the strains and electric field strengths are considered as independent variables, the stresses and electric displacements are given by

$$\sigma_{ij} = c_{ijkl}^E \epsilon_{kl} - e_{kij} E_k, \quad D_i = e_{ikl} \epsilon_{kl} + \kappa_{ik}^E E_k, \quad (10)$$

where $c_{kl ij}^E$ are the isothermal elastic constants, e_{mij} are the piezoelectric constants, and κ_{ik}^E are the isothermal dielectric constants at constant strains. If another two variables are treated as independent variables, the corresponding constitutive equations can be obtained by re-arranging Eq. (10).

From Eqs. (6-9), we have the following statements of the total virtual work for the entire domain, Π , for an isothermal process

$$\int_{\Gamma} (t_i \delta u_i - \phi n_i \delta D_i) d\Gamma - \int_{\Pi} \delta f d\Pi = 0, \quad (11)$$

$$\int_{\Gamma} (t_i \delta u_i + D_i \delta \phi n_i) d\Gamma - \int_{\Pi} \delta h d\Pi = 0, \quad (12)$$

$$\int_{\Gamma} (-u_i \delta t_i - \phi n_i \delta D_i) d\Gamma - \int_{\Pi} \delta w d\Pi = 0, \quad (13)$$

$$\int_{\Gamma} (-u_i \delta t_i + D_i \delta \phi n_i) d\Gamma - \int_{\Pi} \delta g d\Pi = 0, \quad (14)$$

where u_i is a component of the displacement vector, ϕ is the electric potential, $\mathbf{t}$ is the traction along the boundary, $\mathbf{n}$ is the unit vector normal to the boundary, and Γ denotes the boundary of the entire domain which may include a crack or a cavity. Eq. (14) was derived before by Zhang [19]. The first term in each of Eqs. (11-14) represents the thermodynamic work done by the surrounding and the second term represents the corresponding thermodynamic function in the domain. From the thermodynamics point of view, the total virtual work may be regarded as the isothermal energy conservation for each thermodynamic function. Introduce four isothermal potential energies as

$$P_F = \int_{\Gamma} (t_i u_i - D_i \phi n_i) d\Gamma - \int_{\Pi} f d\Pi, \quad (15)$$

where the prescribed properties on the boundary are stresses and electric potential;

$$P_H = \int_{\Gamma} (t_i u_i + D_i \phi n_i) d\Gamma - \int_{\Pi} h d\Pi, \quad (16)$$

where the prescribed properties on the boundary are stresses and electric displacements;

$$P_W = \int_{\Gamma} (-u_i t_i - D_i \phi n_i) d\Gamma - \int_{\Pi} w d\Pi, \quad (17)$$

where the prescribed properties on the boundary are displacements and electric potential;

$$P_G = \int_{\Gamma} (-u_i t_i + D_i \phi n_i) d\Gamma - \int_{\Pi} g d\Pi, \quad (18)$$

where the prescribed properties on the boundary are displacements and electric displacements. Thus, Eqs. (11-14) can be re-written as

$$\delta P_F = \int_{\Gamma} (t_i \delta u_i - \phi n_i \delta D_i) d\Gamma - \int_{\Pi} \delta f d\Pi = 0, \quad (19)$$

$$\delta P_H = \int_{\Gamma} (t_i \delta u_i + D_i \delta \phi n_i) d\Gamma - \int_{\Pi} \delta h d\Pi = 0, \quad (20)$$

$$\delta P_W = \int_{\Gamma} (-u_i \delta t_i - \phi n_i \delta D_i) d\Gamma - \int_{\Pi} \delta w d\Pi = 0, \quad (21)$$

$$\delta P_G = \int_{\Gamma} (-u_i \delta t_i + D_i \delta \phi n_i) d\Gamma - \int_{\Pi} \delta g d\Pi = 0. \quad (22)$$

If the generalized force, P , the generalized displacement, Δ , the generalized voltage, V , and the generalized charge, Q , are used, then the changes in the total free energy, F , the total electric enthalpy, H , the total mechanical enthalpy, W , and the total full Gibbs energy, G , for the entire sample are given by

$$dF = Pd\Delta + VdQ, \quad (23)$$

$$dH = Pd\Delta - QdV, \quad (24)$$

$$dW = -\Delta dP + VdQ, \quad (25)$$

$$dG = -\Delta dP - QdV. \quad (26)$$

Now, consider a piezoelectric material containing a pre-crack. Adding the energy change associated with the crack extension into each of Eqs. (23-26) leads to

$$dF = Pd\Delta + VdQ - JdA, \quad (27)$$

$$dH = Pd\Delta - QdV - JdA, \quad (28)$$

$$dW = -\Delta dP + VdQ - JdA, \quad (29)$$

$$dG = -\Delta dP - QdV - JdA, \quad (30)$$

where A is the crack area; and J is the energy release rate for crack propagation and defined as

$$J = -\left(\frac{\partial F}{\partial A}\right)_{\Delta, Q} = -\left(\frac{\partial H}{\partial A}\right)_{\Delta, V} = -\left(\frac{\partial W}{\partial A}\right)_{P, Q} = -\left(\frac{\partial G}{\partial A}\right)_{P, V}. \quad (31)$$

Alternatively, the energy release rate can be evaluated by following Rice's treatment [20] of elastic fracture mechanics and is given by

$$J = \frac{\partial P_F}{\partial A} = \frac{\partial P_H}{\partial A} = \frac{\partial P_W}{\partial A} = \frac{\partial P_G}{\partial A}. \quad (32)$$

Using the methodology described above and the potential associated with the electric enthalpy, we derive the energy release rate for an elliptical cavity under the condition that the ratio of the minor semi-axis to the major semi-axis, $\alpha = b/a$ is maintained. When the elliptical cavity reduces to a slit crack, the energy release rate will automatically respond to slit crack propagation. Since only two-dimensional problems are treated here, all properties are calculated per thickness. Thus, the energy release rate is given by

$$2J = \frac{\partial P_H}{\partial a} = \int_{\Gamma} (t_i \frac{\partial u_i}{\partial a} + D_i \frac{\partial \phi n_i}{\partial a}) d\Gamma - \frac{\partial}{\partial a} \int_{\Pi} h d\Pi. \quad (33)$$

A factor of two is added here due to two crack tips in this system. Using the solutions for a cavity in a piezoelectric material under combined mechanical-electrical loadings [21] and after tedious algebraic calculation we finally have

$$\begin{aligned} J = & \frac{\pi a}{4} \left[(\Sigma_1^\infty)^T (\mathbf{B} + \bar{\mathbf{B}}) \Sigma_2^\infty - (1 + \alpha) (\Sigma_2^\infty)^T (\mathbf{B}\bar{\mathbf{d}} + \bar{\mathbf{B}}\mathbf{d}) + \alpha^2 (\Sigma_1^\infty)^T (\mathbf{B} + \bar{\mathbf{B}}) \Sigma_1^\infty \right. \\ & - i\alpha (1 + \alpha) (\Sigma_1^\infty)^T (\mathbf{B}\bar{\mathbf{d}} - \bar{\mathbf{B}}\mathbf{d}) - \left[i(1 + \alpha)(\bar{\mathbf{d}} - \mathbf{d}) - 2\alpha \Sigma_2^\infty \right]^T (\mathbf{A}\mathbf{a}_1 + \bar{\mathbf{A}}\bar{\mathbf{a}}_1) \\ & \left. - \alpha \left[(1 + \alpha)(\bar{\mathbf{d}} + \mathbf{d}) - 2\Sigma_2^\infty \right]^T [\mathbf{A} < p_\alpha > \mathbf{a}_1 + \bar{\mathbf{A}} < \bar{p}_\alpha > \bar{\mathbf{a}}_1] \right], \end{aligned} \quad (34)$$

where Σ_2^a is a 4-dimensional vector for applied loadings, $<>$ denotes a diagonal matrix, p_i ($i=1, 2, 3, 4$) are the eigen-roots with positive imaginary parts determined by the material properties and crack orientation, $\mathbf{a}_1$ is a 4-dimensional vector depending on the remote loadings, $\mathbf{B}$ and $\mathbf{A}$ are 4x4 matrixes depending on the material properties and crack orientation, $\mathbf{d} = (0, 0, 0, d)^T$, and d is a parameter relating the electric field inside the cavity or crack (see [21] for details). Eq. (34) shows that the energy release rate for an elliptical cavity growth depends on both mechanical and electric loads, as well as on the ratio of $\alpha = b/a$ and the value of the dielectric constant κ^c inside the cavity.

Fig. 2. Electric field and energy release rate as a function of applied mechanical loading for a vacuumed elliptical cavity.

applied electric field. Either a positive or a negative applied electric field decreases the energy release rate. When the cavity is reduced to a slit crack, the electric field inside the crack is around 1,000 times as high as the applied electric field and the energy release rate becomes independent of the applied electric loading.

Fig. 3. Electric field and energy release rate as a function of applied electrical loading for a vacuumed elliptical cavity.

definite with the change of applied mechanical loading as shown in Fig. 5, which also differs from that for a vacuumed elliptical cavity as shown in Fig. 2 in which J could be negative when the mechanical

high as the applied electric field and increases its absolute magnitude with increase of the applied stress. The energy release rate increases as the absolute value of the applied stress increases. It could hold for an elliptical cavity that the energy release rate increases with increasing absolute value of a compressive-applied stress as long as the upper and lower faces do not contact each other. When the upper and lower faces of the cavity contact, which could happen when a slit crack is under compress, the traction-free condition along the cavity faces does not hold any more, and then the energy release rate loses its meaning. Under a constant applied stress, Fig. 3 shows the electric field inside the cavity and the energy release rate as a function of the applied electric field. The electric field inside the cavity is about five times as high as the

In Figs. 2 and 3, the medium inside the cavity is considered a vacuum that has the smallest dielectric constant. To demonstrate the influence of the cavity medium, we now consider another extremity, i.e., an infinitely large dielectric constant for the cavity that represents a conducting cavity. Fig. 4 shows the energy release rate J as a function of the applied electric loading. In this case, the energy release rate J is positive definite with the change of applied electric loading, which is totally different from that for a vacuumed elliptical cavity as shown in Fig. 3. In particular, the electric field parallel to the major semi-axis does contribute very much to the energy release rate. The phenomenon is mainly due to the electrostriction effect which has been discussed by McMeeking [22]. The energy release rate J is also positive

When the cavity reduces to a slit crack (i.e., $\alpha = b/a = 0$) and the dielectric constant of the crack medium κ^c has a finite value (for example, $\kappa^c = 8.85 \times 10^{-12}$ F/m for a vacuum crack), d is real and the energy release rate for the crack propagation is reduced to

$$J = \frac{\pi a}{4} [(\Sigma_2^\infty)^T (\mathbf{B} + \bar{\mathbf{B}})(\Sigma_2^\infty - \mathbf{d})]. \quad (35)$$

If the crack is an electrically conductive crack with κ^c being infinite, the energy release rate is

$$J = \frac{\pi a}{4} [(\Sigma_2^\infty)^T (\mathbf{B} + \bar{\mathbf{B}})\Sigma_2^\infty - (\Sigma_2^\infty)^T (\mathbf{B}\bar{\mathbf{d}} + \bar{\mathbf{B}}\mathbf{d}) - i(\bar{\mathbf{d}} - \mathbf{d})^T (\mathbf{A}\mathbf{a}_1 + \bar{\mathbf{A}}\bar{\mathbf{a}}_1)]. \quad (36)$$

If the parameter $d=0$, however, the energy release rate for the crack propagation is

$$J = \frac{\pi a}{4} (\Sigma_2^\infty)^T (\mathbf{B} + \bar{\mathbf{B}})\Sigma_2^\infty. \quad (37)$$

Eq. (37) is the conventional result [11] from the electric boundary condition that the electric displacement component perpendicular to the crack faces is zero along the crack faces.

3. RESULTS AND DISCUSSION

Consider a mathematical slit crack in an infinite piezoelectric material under combined mechanical and electrical loadings, as shown in Fig. 1, where the crack is perpendicular to the poling direction and applied loadings are applied also in the poling direction. The present work uses the PZT-4 ceramics as a model material. The material constants are given below:

Elastic constants (10^{10} N/m²):

$$c_{11} = 13.9, \quad c_{12} = 7.78, \quad c_{13} = 7.43,$$

$$c_{33} = 11.3, \quad c_{44} = 2.56;$$

Piezoelectric constants (C/m^2):

$$e_{31} = -6.98, \quad e_{33} = 13.84,$$

$$e_{15} = 13.44;$$

Dielectric constants (10^{-9} F/m):

$$\kappa_{11} = 6.00, \quad \kappa_{33} = 5.47;$$

$$\kappa_c = 8.85 \times 10^{-3};$$

where N and C denote, respectively, Newton and Coulomb. The dielectric constant of vacuum, κ_c , is also listed here for convenience. Fig. 2 shows the variations of the electric field inside the cavity and the energy release rate with the applied stress under a constant applied electric field when the cavity medium is considered as a vacuum. The electric field inside the cavity is about five times as

Fig. 1. A slit crack in an infinite piezoelectric medium under combined mechanical and electrical loadings.

Fig. 2. Electric field and energy release rate as a function of applied mechanical loading for a vacuumed elliptical cavity.

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Fig. 4. Energy release rate as a function of applied electrical loading for an electrically conductive elliptical cavity.

Fig. 5. Energy release rate as a function of applied mechanical loading for an electrically conductive elliptical cavity.

Fig. 6. Comparison of the self-consistent calculation with the conventional one for energy release rate.

Fig. 7. Applied mechanical loading as a function of applied electrical loading for a given energy release rate.

loading is low and the electric loading is high. An electrically-positive-defined energy release rate means that the electric loading would enhance the crack propagation rather than impede it.

Since the geometry of a crack affects its propagation and a slit crack opens before propagation, the deformed crack profile should be used in the calculation of the energy release rate. A self-consistent analysis has been developed to count the effects [17, 21]. When the magnitude of crack opening is small, the energy release rate is almost symmetric-about $E_2=0$ for a vacuumed crack, while the energy release rate is roughly a constant for an electrically conducting crack. If the applied electric loading is much larger, the energy release rate would be expected to be asymmetric for a vacuumed crack and inconstant for a conducting crack. Fig. 6 compares the energy release rate obtained from the self-consistent calculation with those from conventional calculations. It is clear that the resistance of the applied electric loading to propagation of a vacuumed crack is overestimated if the electric field inside the crack is ignored, as shown in Fig. 6. For a given piezoelectric material, the fracture toughness should be a constant. When the energy release rate is larger than the fracture toughness the crack will propagate. As illustrated in Fig. 6, the electric field E_2^∞ may be against the mechanical loadings to propagate the crack. In other words, the critical mechanical loading may be enhanced by an applied electric field. In Fig. 7, the energy release rate is fixed at the same value as that under pure mechanical loading, $\sigma_{22}^\infty=20$ MPa. As expected, the applied mechanical loading maintains if the electric field inside the crack is taken into account and the undeformed crack profile is used. For the other two cases, either a positive or a negative applied electric field along the x_2 axis requests a higher mechanical loading to facilitate the crack propagation. Again, the conventional calculation (ignoring the electric field inside the crack and using the undeformed crack profile) leads to a higher level of mechanical loading than that obtained from the self-consistent calculation.

4. CONCLUDING REMARKS

This paper presents the thermodynamic functions and the energy release rate for a crack or a cavity in a piezoelectric material. The energy release rate for the propagation of an elliptical cavity with a constant ratio of the minor semi-axis to the major semi-axis is a function of the combined mechanical-electrical loadings, the ellipse geometry and the dielectric constant of the cavity medium. For an insulating crack, the energy release rate is independent of the applied electric field either perpendicular or parallel to the crack when the electric field inside the crack is taken into account. For a conducting crack, even though the electric field perpendicular to the crack does not contribute to the energy release rate, the applied electric field parallel to the crack drives the crack to propagate. Makino and Kamiya [23] investigated experimentally the effects of applied electric field on the modulus of rupture (fracture strength). Their results show that either a positive or a negative electric field reduces the modulus of rupture. We have comprehensively studied the effects of applied electric field on the modulus of rupture and observed the similar phenomenon [24]. The original insulating crack may breakdown electrically and cause a fundamental change in its behavior. The detailed results will be reported separately.

ACKNOWLEDGMENTS---The author thanks Professor Pin Tong and Professor Huajian Gao from Stanford University for useful discussions and Dr. Caifu Qian for plotting the figures. Financial support from the Hong Kong Research Grants Council under RGC grant HKUST573/94E is gratefully acknowledged.

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