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Effect of Electric Field Reversal on Crack Growth Behavior of Poled Piezoelectric Ceramic

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ABSTRACT

A long standing unexplained crack growth behavior of poled PZT ceramics is that crack tends to grow longer under a positively applied electric field and shorter under a negatively applied field as compared to the situation when no electric field is applied. While this behavior was observed experimentally, the prevailing mathematical models have not been able to quantify the results. The attempted explanation speaks of separating the electrical and mechanical parts while realizing that the electromechanical energy field is coupled. The energy in a unit volume of material, once stored, could not distinguish the portion from the electric to the mechanical.

Based on the energy density criterion, an analytical approach is developed to show qualitatively the behavior of crack growth enhancement and retardation when the electric field is reversed. Crack growth segments are computed for the PZT-4 ceramic material to show that indeed a crack tends to grow longer and shorter depending on whether the applied electric is positive or negative. This confirms the experimental observation.

KEYWORDS: Piezoelectric, Crack Growth, Electromechanical

1. INTRODUCTION

Piezoelectric ceramics are prone to cracking because they are inherently brittle, an undesirable character that has limited the use of this class of materials. Much research has been done to understand how electrical and mechanical disturbances could lead to unexpected fracture. Indenters [1,2] have been dropped onto PZT (lead-zirconate-titanate) ceramic specimens to produce longer cracks when the poled direction coincides with that of the electric field. The opposite holds for electric field that is applied against the poled direction. The same phenomenon was observed in PZT-4 for a compact tension specimen with an edge crack [3]. Mathematical models have since been developed to quantify these observations without success. Controversies continue to prevail despite numerous unsuccessful attempts [4-6] of using the energy release rate or path independent integral as the fracture criterion. Only in recent times that the energy density criterion [7,8] was applied and resolved the long standing inconsistencies mentioned earlier [3,6].

In what follows, the energy density criterion shall be used to determine how crack growth would be affected by reversing the direction of applied electric field with reference to the poled direction for a central crack in an infinite body made of PZT-4 material. The crack tip energy density function dW/dV is first computed using the equations of linear piezoelectricity. An energy density factor S near the crack tip can thus be defined; it has the units of energy release rate. The initiation of stable crack growth and rapid crack propagation correspond to dW/dV and S reaching their respective critical values, $(dW/dV)_c$ and S_c. Numerical results are presented to illustrate how the energy density factor is affected by sign change of the applied electric field while the energy release rate criterion has failed to account for such a behavior in the past.

2. THROUGH CRACK MODEL

Depicted in Fig. 1 is a central crack of length 2a in an infinite body. A remote electric field E and uniform mechanical stress σ are applied such that the macrocrack would extend along the x_1-axis while poling is directed in the positive x_3-axis. Plane strain in the x_1x_3-plane is assumed.

Figure 1: Line crack under electrical and mechanical load.

Figure 2: Crack tip decay of volume energy density

2.1 Coupling of electrical and mechanical effects

A complete description of cracking involves the process of initiation, growth and termination. For a solid subjected to both electrical and mechanical disturbances, the energy density function based on the theory of linear piezoelectricity can be computed as

$$\frac{dW}{dV} = \int_o^{\gamma_{ij}} \sigma_{ij} d\gamma_{ij} + \int_o^{D_i} E_i dD_i \quad . \tag{1}$$

In eq. (1), σ_{ij} and γ_{ij} are, respectively, the stress and strain components while E_i and D_i are components of the electric and displacement field. Even though the mechanical and electrical portion of the energy density function would appear to be separated in eq.(1), the equivalents forms of expressing eq. (1) in terms of stresses and electric displacements

$$\frac{dW}{dV} = \frac{1}{2}\sigma_{ij} H_{ijk\ell}\sigma_{k\ell} + \frac{1}{2} D_i \beta_{ij} D_j \tag{2}$$

or in terms of strains and electric fields

$$\frac{dW}{dV} = \frac{1}{2}\gamma_{ij} C_{ijk\ell}\gamma_{k\ell} + \frac{1}{2} E_i \varepsilon_{ij} E_j \tag{3}$$

show that the mechanical and electrical parts of dW/dV are always coupled. They cannot be separated as it was assumed in [3]. In eq. (2), H_{ijkl} and β_{ij} are the elastic and dielectric compliance constants while those in eq. (3) given by C_{ijkl} and ε_{ij} are the elastic and dielectric constants.

2.2 Energy density criterion

At the continuum scale level, the sharp crack tip is assumed to lie within a macroscopic size core region with radius r_o, Fig. 2. Mathematically speaking, the energy density function becomes unbounded as the crack tip is approached or as $r \to 0$ since

$$\frac{dW}{dV} = \frac{S}{r} \tag{4}$$

The relationship of eq. (4) is shown in Fig. 2 where S represents the area of the dW/dV versus r plot for a given level of dW/dV.

The form of eq. (4) does not limit the criterion of energy density to linear elasticity even though the inverse square root of r stress singularity would correspond to 1/r for dW/dV. Note from Fig. 2 that r adopts a much more general interpretation since it is simply the linear distance measured from the crack tip. The following hypotheses applied to dW/dV are in general valid for any nonlinear constitutive relations, large deformation theories with or without dissipation. When applied to a local region ahead of the crack tip, they can be stated as [9]:

- Hypothesis I: Location of crack initiation is assumed to coincide with the maximum of the minimum dW/dV or $(dW/dV)_{min}^{max}$.
- Hypothesis II: The onset of stable crack growth is assumed to occur when $(dW/dV)_{min}^{max}$ reaches a critical value $(dW/dV)_c$.
- Hypothesis III: Stable crack growth segments r_1, r_2, etc., are assumed to be governed by

$$\left(\frac{dW}{dV}\right)_c = \frac{S_1}{r_1} = \frac{S_2}{r_2} = \cdots = \frac{S_j}{r_j} = \cdots = \frac{S_c}{r_c} \tag{5}$$

The onset of rapid fracture is assumed to take place when

$$\left(\frac{dW}{dV}\right)_c = \frac{S_c}{r_c} \tag{6}$$

The ways with which S_c are related to K_{1c} for Mode I crack extension depends on the constitutive relations and the kinetics of cracks under consideration. For a crack under static load applied to an isotropic, homogeneous and elastic body, it has been shown in [9] that

$$S_c = \frac{(1+\nu)(1-2\nu)K_{1c}^2}{2\pi E_o} \tag{7}$$

in which ν is the Poisson's ratio and E_o the Young's modulus. For the PZT material considered in this work, the equivalent of eq. (7) takes the form

$$S_c = A_{11} + 2A_{14}\frac{g_{33}}{\beta_{33}} + A_{44}\frac{g_{33}^2}{\beta_{33}^2} \tag{8}$$

Here, A_{11} , A_{14} , A_{44} , g_{33} and β_{33} are complicated functions related to the elastic, piezoelectric and dielectric constants of the ferroelectric ceramics. The specific expressions can be found in [8]. Another set of B_{ij} connected with specifying electric field E can be defined instead of A_{ij} related specifying the electric displacements D.

2.3 Mode I crack extension

Referring to Fig. 1, both the applied stress σ and the electric field E are such that the crack would extend straight ahead along the x_1-axis where S possesses a relative minimum with reference to the angle θ in Fig.

1 such that Hypothesis I is satisfied. Under the above considerations, the work in [7,8] gives the expression of S for the present problem:

$$S = B_{11}K_1^2 + 2B_{14}K_1K_E + B_{44}K_E^2 \tag{9}$$

in which

$$K_1 = \sigma\sqrt{\pi a} \qquad \text{and} \qquad K_E = E\sqrt{\pi a} \tag{10}$$

where both σ and E are constants. The quantities B_{11} , B_{14} and B_{44} for PZT-4 can be found in [7,8]. Substituting eqs. (10) into eq. (9), it can be shown that

$$S = K_1^2\left[B_{11} + 2B_{14}p + B_{44}p^2\right] \tag{11}$$

Defined in eq. (11) is a load parameter p = E/σ. It is now more pertinent to examine whether a crack would grow longer or shorter when the direction of the applied electric field is reversed by using the solution for no applied electric field as the base of reference.

3. **ENHANCEMENT AND RETARDATION OF CRACK GROWTH**

The phenomenon of crack growth enhancement and retardation due to applied electric field reversal has been known for sometime by experiments [1-3]. Attempts made in [3,6] to explain the observation have all failed because the energy release rate result could not distinguish a positive electric field from that of a negative one. Hence, the arguments presented for these unsuccessful attempts are also suspect.

3.1 Crack growth segments

Consider the situation in Fig. 1 where the crack is subjected to σ and E. The superscripts +, o and – will refer to, respectively, as the positive, zero and negative E field. The corresponding crack growth segments are r_1^+, r_2^+, …, r_1^o, r_2^o, …, and r_1^-, r_2^-, …, while the energy density factors are given by S_1^+, S_2^+, …, S_1^o, S_2^o, …, and S_1^-, S_2^-. Application of Hypothesis III governed by eq. (5) renders

$$\left(\frac{dW}{dV}\right)_c = \frac{S_1^+}{r_1^+} = \frac{S_2^+}{r_2^+} = \cdots = \frac{S_1^o}{r_1^o} = \frac{S_2^o}{r_2^o} = \cdots = \frac{S_1^-}{r_1^-} = \frac{S_2^-}{r_2^-} = \cdots = \text{const}. \tag{12}$$

For the jth segment of crack growth, eq. (12) gives

$$\frac{S_j^+}{r_j^+} = \frac{S_j^o}{r_j^o} = \frac{S_j^-}{r_j^-}, \qquad j = 1,2,\cdots \tag{13}$$

What needs to be shown is that

$$S_j^+ > S_j^o \ \text{ and } \ S_j^- < S_j^o \quad \text{for} \quad j = 1,2,\cdots \tag{14}$$

and

$$r_j^+ > r_j^o \ \text{and} \ r_j^- < r_j^o \quad \text{for} \quad j = 1,2,\cdots \tag{15}$$

Refer to Fig. 3 for an illustration of eq. (15). Recall that positive and negative electric field refer, respectively, to E being in the same and opposite direction of poling.

3.2 Interaction of mechanical and electrical field

The interaction of mechanical and electrical field on crack growth can be exhibited by a plot of energy density factor and/or crack growth as a function of the parameter p or the ratio E/σ. Using the elastic, piezoelectric and dielectric constants of PZT-4, numerical values of S in eq. (11) can be computed for $p \times 10^{-3}$ = -15, -10, -5, 0, 5, 10 and 15 Vm/N. Plotted in Fig. 4 are the normalized values of S as a function of p. The curve increases monotonically.

Figure 3: Enhancement and retardation of crack growth

Figure 4: Energy density and crack growth segment variations with positive and negative electric field strength

Once S can be computed numerically for situations where E changes sign, eq. (13) can be applied to show whether the inequalities in eqs. (15) would hold or not. The other curve in Fig. 4 corresponds to crack growth segments $r_j^{\pm}$ normalized to r_j^o. The point with coordinates $r_j^{\pm}$ = 1.0 and p = 0 corresponds to the crack growth segment r_j^o with E = 0. Summarized in Table 1 are the numerical values of r_j^+ and r_j^- normalized with reference to r_j^o. When E is positive r_j^+/r_j^o is always greater than one.

TABLE 1

Normalized crack growth segments r_j^+/r_j^o and r_j^-/r_j^o for PZT-4 and different $E/\sigma \times 10^{-3}$ values (Vm/N)

-15	-10	-5	0	5	10	15
0.765	0.814	0.894	1	1.132	1.290	1.474

Moreover, r_j^-/r_j^o is always less than one when E is negative. This implies that a crack would grow longer for a positive electric field. Shorter crack growth applies to a negative electric field. For comparing the relative magnitudes of r_j^+, r_j^o and r_j^-, the results in Table 1 are sufficient to validate the experimental findings in [1-3]. There were no need to de-couple the electrical and mechanical effects nor was there the need to include nonlinear effects.

4. CONCLUSIONS

When material microstructure plays a role in failure analyses, the possibility of multiscale cracking should be considered even though it was not needed for illustrating the influence of electric field reversal on crack growth. For a quantitative assessment of the failure stress, however, microcracking would need to be modeled since the compliance of the specimen would be altered. The initiation and growth of the macrocrack would also be affected accordingly. Such a situation has been discussed in [8] where the interaction of micro- and macro-cracking was accounted for by introducing an additional length parameter.

Lacking at present is a knowledge of the initial states of the material microstructure, the behavior of which would depend sensitively on the stress/strain or energy density arising, say from the process of crystal nucleation and formation for metals. If the internal stresses trapped in the grains are of the same orders of magnitude as those induced by the applied loads, then the neglect of the influence of the initial states would leave any predictions in doubt. Such situations are no longer uncommon as the length scale of device components are being reduced to microns in size. Another seemingly innocent pitfall is the use of physical data extracted from test specimens that are orders of magnitude larger than the device under consideration. It appears that data correlation at the nano-, micro-, meso- and macro-scale requires extensive attention. Until the problem of scaling is better understood, the reliable use of ferroelectric ceramics in electronic devices leaves much to be desired.

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