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**On the Crack Face Boundary Conditions in Electromechanical Fracture
and An Experimental Protocol for Determining Energy Release Rates**

by

Wenyuan Li

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APPROVED, THESIS COMMITTEE:

Chad M. Landis, Associate Professor, Chair
Mechanical Engineering & Materials Science

Ed Akin, Professor
Mechanical Engineering & Materials Science

Michael M. Carroll, Professor
Mechanical Engineering & Materials Science

Satish Nagarajaiah, Professor
Civil and Environmental Engineering

HOUSTON, TEXAS

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ABSTRACT

On the Crack Face Boundary Conditions in Electromechanical Fracture and An Experimental Protocol for Determining Energy Release Rates

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An experimental protocol for measuring the energy release rate in a non-linear reversible electromechanical body is proposed and summarized. The potential results are capable of shedding light on the true physical nature of the conditions prevailing at the crack surface and in the space within the crack. The experimental procedure is simulated numerically for a linear piezoelectric specimen in a four point bending configuration subjected to electrical loading perpendicular to the crack. Two efficient finite element formulations are presented for nonlinear crack face boundary conditions. Methods for the numerical determination of the crack tip energy release rate and the simulation of the experimental method for obtaining the total energy release rate are developed. It is shown that the crack tip energy release rate calculated under energetically consistent boundary conditions is equal to the total energy release, when the exact boundary conditions are used, there is no such agreement.

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1. Introduction

Over the past few decades, a rather large literature has developed for the fracture mechanics of linear piezoelectric material, and a review of recent work can be found in McMeeking[8]. As yet, there has been little success in the attempts to correlate experimental data with the predictions of theoretical and computational models for the initiation of crack growth in piezoelectric materials. Only when *ad hoc* assumptions with little grounding in physics are utilized can models be made to agree with experimental observations. A possible reason for this situation is that the relevance of the experimental data is uncertain. No fundamental experiments for measuring the energy release rate for cracks in piezoelectric materials have been successfully completed. In principle, the method of compliance calibration, as used for isotropic, linear elastic materials [13] is available. We are aware of only one attempt to provide such data for a piezoelectric material [14], but this effort is as yet incomplete. The experimental difficulties standing in the way of the successful completion of such measurements is considerable. To motivate further work on such experiments, we lay out below the principles upon which the energy release rate may be deduced from tests in which the applied load and the electric potential drop across the specimen are measured as functions of the load point displacement and the charge on the specimen electrodes. These data are then manipulated to obtain the potential energy for the specimen at chosen levels of load and electric potential difference, and upon differencing with respect to crack areas, the energy release rate in the piezoelectric specimen at the chosen levels of load and potential difference is obtained. Such an experimental protocol, if it could be completed successfully, would yield unambiguous data for the critical energy release rate for crack

propagation in situations where various combinations of mechanical load and electric field are being applied.

Another reason for the failure to achieve consistency between experimental data and theoretical and computational fracture mechanics simulations for piezoelectric materials is the primitive nature of the models so far utilized. In attempts to remedy this situation, the simulations have been extended to try to bring more realistic features into the fracture mechanics. For example, different models of the electrical boundary conditions on the crack surfaces have been proposed based on differing assumptions about the electrical characteristics of the medium within the crack gap [3,5,6,9,10,11,12]. Within linearized analysis of material behavior, the “exact” crack model [5] represents the most ambitious attempt at physical consistency. In this model, the crack gap is treated as a capacitor and the electric field between the faces is thus dependent on the crack opening displacement and the electric field in the adjacent material. In contrast, the permeable [10] and impermeable [3,11,12] models of the crack are more simplistic. In the former, the crack is assumed to cause no perturbation to the electric field, whereas the electric field cannot penetrate the crack at all in the latter case. All three of these crack models assume that the crack faces are traction free.

The permeable and impermeable models have obvious deficiencies in regard to representing the interaction of the electric field and the crack. Furthermore, there are no experimental data that confirm the utility of these models as the basis of fracture mechanics for piezoelectric materials. On the other hand, the exact model would seem to

provide a more realistic approach to modeling the electrical behavior of cracks, albeit at the expense of nonlinear features that are introduced into the analysis. However, a discrepancy was found between the total and the crack tip energy release rates by McMeeking [9], when he investigated these for a Griffith crack having the exact crack face boundary conditions in a piezoelectric material. The crack tip energy release rate is that calculated as the flux of mechanical and electrical work to an extending crack tip, whereas the total energy release rate is the rate at which the potential energy of the systems falls as the crack extends. These two concepts should yield the same value as in a conservative system, such as those represented by a brittle piezoelectric material with a crack. Recently, this discrepancy was repaired by Landis [6] through implementation of energetically consistent boundary condition, where the electrically “exact” boundary condition is augmented by tractions on flaw faces tending to close the crack. When such boundary conditions are imposed in the problems solved by Landis [6], the total and crack tip energy release rates are identical.

An additional phenomenon that is thought to occur within the crack in a piezoelectric material is electrical discharge. Since the dielectric constant of technologically important piezoelectric materials is typically very high (of the order 10^3), the electric field within the crack can be very high even if the potential difference across the specimen is modest. In many cases, the predicted electric field within the crack is much higher than the known breakdown strength of air. As a consequence, it must be assumed that electrical discharge takes place in the crack, and this effect should be accounted for in simulations of cracks in piezoelectric specimens subject to electric loading.

With such ideas in hand, it is desirable to obtain results in which the energy release rate is simulated analytically or computationally for piezoelectric specimens containing cracks, where the component is subject to applied load and an electric field. Although some analytical solutions for cracks in loaded piezoelectric components are available, their scope is limited and numerical methods are necessary to solve problems with complicated or finite geometries. Given the difficulty of carrying out experiments on piezoelectric materials with cracks, the need for computational results, *e.g.* from the finite element method, is particularly great for verifying fracture mechanics models by comparing theoretical and the experimental results. Among the different finite element methods available for linear piezoelectric materials and structures [2], the most popular one is the standard scalar potential formulation proposed by Allik and Hughes [1]. On the other hand, Ghandi and Hagood [4] developed a hybrid finite element formulation that includes electric displacement degrees of freedom within the element over and above the standard one. In addition, Landis [7] developed an alternative formulation, deriving the electric displacement from the components of a vector potential utilized as a nodal degree of freedom. The comparison of the standard scalar potential formulations and the vector potential method can be found in [7]. The vector potential method is particularly advantageous when an electrical discharge model is used within the crack gap, and so it will be used for the computations in this paper.

For the results below, a linear, piezoelectric beam in bending is analyzed, where an electric field is applied transverse to the flaw. A non-linear, electrical discharge model is

used within the crack and the energy release rate is computed when the beam is under various combinations of applied load and electric field. In some cases, the energetically consistent boundary conditions are utilized, causing a tensile stress to be present effectively within the crack. In other situations, this tension is omitted. Three different methods of calculating the energy release rate are presented. One method is based on the computation of compliance calibrations and is akin to the method we propose for measuring the energy release rate experimentally. Another technique presented is the use of a domain integral method, analogous to utilization of a path integral. This approach is used to obtain both crack tip and total energy release rates, with and without the energetically consistent crack surface boundary conditions. These results are compared to the ‘experimental’ value of the energy release rate to verify that when energetically consistent crack surface boundary conditions are used, the resulting crack tip energy release rate is indeed equal to the total energy release rate.

2. An experimental protocol for determining the energy release rate in cracked electromechanical bodies

Consider a crack of area A in a body with nonlinear but reversible electromechanically coupled constitutive response. The body is contained in another nonlinear dielectric medium, whose properties include the possibility of electric breakdown, *e.g.* air, vacuum, or an electrically inert liquid. The arguments presented here can also be rigorously applied to irreversible behavior as long as no non-proportional loading has occurred at any point in the body. For the sake of simplicity in the presentation we assume that the

mechanical loading is characterized by a point load P and a displacement of the load point Δ . Similarly, the electrical loading is characterized by an electric potential drop of magnitude V between two electrodes and the total charge of magnitude Q that resides on those electrodes. The energy that is stored in the system U , including both the cracked body and its surroundings, is given by

$$U = \int_0^\Delta P(\Delta', Q') d\Delta' + \int_0^Q V(\Delta', Q') dQ' \quad (2.1)$$

Here Δ_0 and Q_0 are the initial or reference load point displacement and electrode charge.

It follows from Equation (2.1) and the path independence of these integrals implied by reversibility that the force P and the voltage V can be obtained from the stored energy as

$$P = \frac{\partial U}{\partial \Delta} \quad \text{and} \quad V = \frac{\partial U}{\partial Q} \quad (2.2)$$

Then, accounting for the work done by the electrical and mechanical loads, the total potential energy of the system Π is

$$\Pi = U - P\Delta - VQ \quad (2.3)$$

Figure 1. A schematic of a cracked body with mechanical loading by a force P and load point displacement Δ , and electrical loading by a voltage drop V and electrode charge Q .

Note that the second term on the right hand side of Equation (2.3) is not necessary under fixed displacement conditions, and the last term is not necessary under fixed charge conditions. Also note that the independent variables for the potential energy of the system are the load point displacement Δ , the charge on the electrodes Q , and the crack area A . Given a specific state of these variables we would like to determine the reduction in potential energy for an incremental increase in the crack area. Depending on the type of loading, such an increment in the crack area can also produce changes in the load point displacement and the electrode charge. Therefore, the change in potential energy for such a crack advance, in the direction of the crack, can be written as

$$d\Pi = \frac{\partial \Pi}{\partial \Delta} d\Delta + \frac{\partial \Pi}{\partial Q} dQ + \frac{\partial \Pi}{\partial A} dA + O(d\Delta^2, dQ^2, dA^2) \quad (2.4)$$

Given that the equilibrium conditions

$$\frac{\partial \Pi}{\partial \Delta} = 0 \text{ and } \frac{\partial \Pi}{\partial Q} = 0 \quad (2.5)$$

then to first order the change in the potential energy for an incremental change in the crack area is simply

$$d\Pi = \frac{\partial \Pi}{\partial A} dA \quad (2.6)$$

Note that this result is independent of the type of loading, be it fixed load and charge, or fixed displacement and voltage, or any other electromechanical combination. The reduction in the potential energy per increase in the crack area is defined as the energy release rate, i.e.

$$\mathcal{G} = -\frac{\partial \Pi}{\partial A} \quad (2.7)$$

Again, the energy release rate $\mathcal{G}$ represents the decrease in the potential energy of the system associated with an incremental increase in the crack area A . For a reversible system, $\mathcal{G}$ can be interpreted as the energy flux to the crack front, which drives the creation of new crack surface. In other words $\mathcal{G} \delta A$ represents energy that is lost to the crack tip if the crack grows by the area δA . Hence, from this interpretation it should be clear that $\mathcal{G}$ as defined by Equation (2.7) is also the crack tip energy release rate.

Equations (2.1)-(2.7) can be used for an experimental determination of the energy release rate for a cracked electromechanical body and its surroundings. This is accomplished by comparing the electromechanical response of two samples that differ only in their crack area, see Figure 1. For a two dimensional specimen, which characterizes most experimentally significant geometries, the change in crack area dA is, of course, directly related to the change in crack length. The two different cracked bodies are loaded to the same electromechanical “level”. The electromechanical load level can be characterized by any combination of load/displacement and voltage/charge, where, by Equation (2.6), any differences in the approximated energy release rate for different load combinations will be of order dA^2 . For each specimen the load versus displacement and voltage versus charge response must be measured and Equation (2.1) can be used to compute the stored energy in the cracked body and its surroundings. Equation (2.3) can then be used to compute the potential energy and the following difference equation can be implemented to approximate the energy release rate

$$\mathcal{G}_{A+dA/2} = \frac{\Pi(A) - \Pi(A + dA)}{dA} \quad (2.8)$$

This procedure is illustrated schematically in Figure 2. Let us assume that the load-displacement and voltage-charge plot for the specimen illustrated in Figure 1 are given in Figure 2. The upper P - Δ curve and lower V - Q curve correspond to the crack area A , and the other two curves correspond to the crack area $A+dA$. The dashed lines correspond to constant load and constant charge approximations for the energy release rate. Then, the

approximation for the energy release rate at a crack length of $A+dA/2$ is simply the area 1 minus area 2 divided by dA .

Figure 2. A schematic of the load-deflection and voltage-charge curves for samples with different crack areas A and $A+dA$. The mechanical load is applied first holding the charge fixed at zero, then the electrical load is applied holding the load fixed. The approximation to the energy release rate for this loading scenario is then $\mathcal{G}_{A+dA/2} \approx (\text{Area 1} - \text{Area 2}) / dA$.

The protocol just described can be implemented experimentally or computationally. The barriers to experimental implementation are formidable, but will not be discussed here. In the following Sections we will implement the procedure just described computationally on a linear piezoelectric four-point bend specimen. The purpose of these studies will be to investigate the accuracy of the proposed procedure, and to characterize numerically the effects of several different types of boundary conditions used to model

the electrical conditions on the crack surface. In what follows, we will designate as the “experimental procedure” the numerical implementation of the protocol for obtaining the energy release rate that we have just described.

In the following Section we will numerically implement the experimental procedure described here on an idealized linear piezoelectric four-point bend specimen. The purpose of these studies will be to investigate the accuracy of the proposed procedure and to analyze the effects of several different types of boundary conditions used to model piezoelectric fracture.

3. Fundamentals of linear piezoelectricity

Prior to presenting the specific geometry that we intend to investigate, some theoretical preliminaries associated with the fracture mechanics of linear piezoelectric bodies will be discussed. For a linear piezoelectric solid material, the equations governing a small deformation, small electric field, electrically quasi-static, isothermal boundary value problem for this solid will be reviewed in this section. Assume the volume of material is V and the boundary surface is S , the mechanical equilibrium equations are given by

$$\sigma_{ji,j} + b_i = 0 \quad \text{and} \quad \sigma_{ij} = \sigma_{ji} \quad \text{in } V \quad (3.1)$$

$$\sigma_{ji} n_j = t_i \quad \text{on } S \quad (3.2)$$

Here σ_{ij} represents the symmetric Cauchy stress tensor, b_i represents the body of force per unit volume, n_i represents the unit vector normal to the surface pointing from the volume, and t_i represents the surface traction. In this section, summation is implied over repeated indices, and $_{,i}$ is the partial differentiation with respect to the x_i direction.

The infinitesimal strain tensor ϵ_{ij} is linked to mechanical displacement components u_i as

$$\epsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}) \quad (3.3)$$

The electric displacement governed by Guass's law is written as

$$D_{i,i} = q \quad \text{in } V \quad (3.4)$$

$$D_i n_i = -\omega \quad \text{on } S \quad (3.5)$$

Under quasi-static conditions, electric field can be written as the gradient of the potential

$$E_i = -\phi_{,i} \quad (3.6)$$

Here D_i is the electric displacement, q is the free charge per unit volume, ω is the free charge per unit area, E_i is the electric field, and ϕ is the scalar electric potential.

For conservative materials, an electrical enthalpy density h can be de defined as

$$h = \hat{u} - E_i D_i \quad (3.7)$$

Here $\hat{u}$ is the internal energy density. The electrical enthalpy is introduced because it is used with the electromechanical form of the J-integral and used as a method for calculating the energy release rate.

Finally, the linear piezoelectric constitutive law relating the four electromechanical field quantities can be given in four different combinations. Two of these forms relevant to this work are given as,

$$\sigma_{ij} = c_{ijkl}^E \epsilon_{kl} - e_{kij} E_k, \quad D_i = e_{ikl} \epsilon_{kl} + \kappa_{ij}^E E_j \quad (3.8)$$

or

$$\sigma_{ij} = c_{ijkl}^D \epsilon_{kl} - h_{kij} D_k, \quad E_i = -h_{ikl} \epsilon_{kl} + \beta_{ij}^E D_j \quad (3.9)$$

Here c_{ijkl}^E and c_{ijkl}^D are fourth rank tensors of elasticity, e_{kij} and h_{kij} are third rank tensors of piezoelectricity, and κ_{ij}^E and β_{ij}^E are second rank dielectric tensors.

Equations (3.1)-(3.6) can also be stated in the following two weak forms as

$$\int_V \sigma_{ij} \delta \epsilon_{ij} - D_i \delta E_i dV = \int_V b_i \delta u_i - q \delta \phi dV + \int_S t_i \delta u_i - \omega \delta \phi dS \quad (3.10)$$

or

$$\int_V \sigma_{ij} \delta \epsilon_{ij} + E_i \delta D_i dV = \int_V b_i \delta u_i + \phi \delta q dV + \int_S t_i \delta u_i + \phi \delta \omega dS \quad (3.11)$$

Equation (3.10) is the foundation for a scalar potential finite element formulation that implements the electric potential ϕ as nodal degrees of freedom. For such a formulation the variational quantities $\delta \epsilon_{ij}$ and δE_i must satisfy Equations (3.3) and (3.6), and then the constitutive equations (3.8) are applied. For boundary value problems with body charge $q = 0$, the variational quantities δD_i and $\delta \omega$ must satisfy $\delta D_i = \epsilon_{ijk} \delta \psi_{j,k}$ and $\delta \omega = -\epsilon_{ijk} n_i \delta \psi_{j,k}$, where ϵ_{ijk} is the permutation tensor. For the vector potential formulation the constitutive form of Equation (3.9) is required. Then, Equation (3.11) leads to the vector potential finite element formulation, which uses the vector potential components ψ_i as nodal degrees of freedom.

4. Boundary conditions

When solving a linear piezoelectric boundary value problem it is of course necessary to specify both mechanical and electrical boundary conditions on all surfaces. Here we will first discuss the conditions which are commonly used to model non-crack face surfaces and then we will move on to the more interesting crack face boundary conditions. For non-crack face surfaces, within linear piezoelectric theory, no distinction is made between the deformed or undeformed configuration of the body, and hence complications associated with tractions due to Maxwell stresses do not arise. The mechanical boundary conditions on such surfaces effectively reduce to known applied tractions or known

applied displacements. On surfaces with attached electrodes the electrical boundary condition is that the electric potential is fixed and constant over any part of the surface connected to the same electrode. On surfaces without electrodes the electrical boundary conditions are not as clear. Since the air/fluid surrounding any specimen has dielectric properties, energy and electrical fields can be transmitted across the specimen boundaries. To account for this physical behavior a solution for the electric field in all of the surrounding space is required. Such solutions can be obtained using boundary elements or a Dirichlet to Neumann map on the surface of the geometry. However, such complete solutions are rarely carried out. Standard practice recognizes that the dielectric constants of most piezoelectric materials of technological interest are 100-1000 times larger than that of free space, and hence it is usually assumed that it is valid to take the limit that the dielectric constant of the surrounding medium is zero. This approximation at non-electroded boundaries forces the normal component of the electric displacement to vanish at the boundary. Hence, the usual electrical boundary conditions are that either the potential ϕ is specified, or the surface charge density ω is taken to be zero.

Several different modeling approaches for the boundary conditions on crack faces have appeared in the literature, [3,5,6,9,10,11,12]. These boundary conditions and the rationale behind them will be presented and discussed in the following sub-sections.

4.1 *Permeable boundary conditions*

The permeable boundary conditions were first proposed by Parton[10]. This model for the crack recognizes that within the assumptions of linear piezoelectricity there is no distinction between the deformed and undeformed configurations of the material. In the undeformed configuration the crack faces are closed, and in such a situation the electrical fields will distribute themselves as if the crack did not exist. The mathematical statements that describe these electrical conditions are that electric potential and the normal component of the electric displacement are continuous across the crack, i.e.

$$D_n^+ = D_n^- ; \quad \phi^+ = \phi^- \quad (4.1)$$

Here the superscripts + and - denote the top and bottom crack faces. It should be obvious that the physical arguments used to justify the permeable boundary conditions are weak because upon loading the crack will open and the medium that fills the crack gap will be able to support an electrical potential drop across the opening.

4.2 *Impermeable boundary conditions*

The impermeable boundary condition model, proposed by Deeg [3], was introduced to address the fact that fracture generally occurs when cracks are open. The same argument used to justify the charge free boundary conditions on non-crack face surfaces is used to motivate the impermeable crack face boundary conditions. Due to the fact that the permittivity of the medium within the crack gap is usually much lower than that of the solid body, it is assumed that the permittivity of the crack gap can be approximated as

zero. This assumption then implies that the normal components of electric displacement on both crack faces are zero, i.e.

$$D_n^+ = D_n^- = 0 \quad (4.2)$$

The obvious physical question that arises for the impermeable boundary conditions is how does the assumption of a zero permittivity crack gap affect solutions?

4.3 “Exact” or semi-permeable boundary conditions

In order to address the facts that cracks are actually open and that electrical fields can permeate the crack gap, Hao and Shen [5] introduced electrical boundary conditions that treat the crack faces as an aggregate of parallel plate capacitors. In the literature these boundary conditions have been referred to as “exact”, semi-permeable, or Hao and Shen boundary conditions. These conditions assume that the crack gap behaves like a linear dielectric material with permittivity κ_0 and that the electric field and electric displacement within the crack gap are normal to the crack surfaces. Mathematically these conditions are stated as

$$D_n^+ = D_n^- = D_c \quad (4.3)$$

$$D_c = \kappa_0 E_c = -\kappa_0 \frac{\phi^+ - \phi^-}{u_n^+ - u_n^-} = -\kappa_0 \frac{\Delta\phi}{\Delta u_n} \quad (4.4)$$

Here D_c is the normal component of electric displacement supported by the crack gap, E_c is the electric field in the crack gap, $\Delta\phi$ is the potential drop across the crack gap, Δu_n is the crack opening displacement, the subscript n represents the component normal to the crack faces, and κ_0 is the linear dielectric permittivity of the gap, which is usually identified with the permittivity of free space 8.854×10^{-12} C/Vm.

In addition to the stated electrical conditions, each of the crack face boundary conditions in sub-sections 4.1-4.3 also assume that the crack faces is mechanically traction free. Numerous works have focused on the “exact” electrical boundary condition along with traction free mechanical boundary conditions. These boundary conditions appear to be physically sound and justifiable. However, McMeeking [9] has pointed out that there is the discrepancy between the total energy release rate and the crack tip energy release rate for a Griffith crack configuration with this combination of electrical and mechanical boundary conditions. The fundamental reason for this discrepancy is that, when charged, capacitor plates are drawn towards one another such that there is a force between them. Hence, if the crack gap can store energy, then the crack faces are in general not traction free.

4.4 *Energetically consistent boundary conditions*

In order to repair the inconsistency identified by McMeeking[9], Landis[6] proposed energetically consistent boundary conditions, with an electrical component very similar to the “exact” boundary conditions plus an additional closing traction on crack faces. The basic idea of the model is to assign an energy, specifically an electrical enthalpy h_c ,

to the crack gap, and then the variation of this enthalpy with respect to the crack opening displacement is a traction and the variation with respect to the potential drop is a charge.

The energetically consistent crack face boundary conditions for a crack gap are given as

$$\omega^+ = -D_i n_i^+ = D_c = -\frac{dh_c}{dE_c} \quad \text{on } S_c^+ \quad (4.5)$$

$$\omega^- = -D_i n_i^- = -D_c = \frac{dh_c}{dE_c} \quad \text{on } S_c^- \quad (4.6)$$

$$t_i^+ = \sigma_{ji} n_j^+ = \sigma_c n_i^+ = (h_c + E_c D_c) n_i^+ \quad \text{on } S_c^+ \quad (4.7)$$

$$t_i^- = \sigma_{ji} n_j^- = \sigma_c n_i^- = (h_c + E_c D_c) n_i^- \quad \text{on } S_c^- \quad (4.8)$$

where

$$E_c = -\frac{\phi^+ - \phi^-}{u_n^+ - u_n^-} = -\frac{\Delta\phi}{\Delta u_n} \quad (4.9)$$

Here, S_c^+ and S_c^- are the top and bottom crack surfaces; ω^+ and ω^- are the surface charge density applied to these crack surfaces, t_i^+ and t_i^- are the surface tractions applied to the crack surfaces, n_i^+ and n_i^- are the unit normal along the top and bottom crack faces pointing away from the solid material, h_c is the electrical enthalpy density of the crack

gap, which depends only on E_c such that $h_c = h_c(E_c)$, and σ_c is the effective stress within the crack gap such that $\sigma_c = h_c + E_c D_c$.

In general the electrical enthalpy can be non-linear and is intended to model the electrical response of the crack gap. A specific form for the energetically consistent boundary that can be used to model the linear response of the gap at low electric field levels and the non-linear response that occurs during electrical discharge will be presented next. If the dielectric constant of the medium within the crack gap is much lower than that of the material body, then high electric fields are generated within the crack gap. Ultimately high electric fields within the crack gap can lead to electrical breakdown usually in the form of a corona discharge. Following Landis [6], a simple idealized phenomenological model is proposed with a critical electrical discharge level E_d , such that the crack gap behaves in a linear dielectric manner when electric field within crack gap is below this critical value. Beyond the critical point, the crack gap cannot support electric field larger than E_d and charge will flow between the crack surfaces such that the electric field remains at this bounding value. Mathematically the model is stated as

$$h_c = -\frac{1}{2}\kappa_0 E_c^2, \quad D_c = \kappa_0 E_c, \quad \sigma_c = \frac{1}{2}\kappa_0 E_c^2 \quad \text{if } |D_c| \leq \kappa_0 E_d \quad (4.10)$$

$$\begin{aligned} h_c &= -\frac{1}{2}\kappa_0 E_d^2, \quad D_c = \text{sgn}(\omega_d)\kappa_0 E_d + \omega_d, \\ E_c &= \text{sgn}(\omega_d)E_d, \quad \sigma_c = E_d|\omega_d| + \frac{1}{2}\kappa_0 E_d^2 \quad \text{if } |D_c| \geq \kappa_0 E_d \end{aligned} \quad (4.11)$$

Here, ω_d represents the amount of charge per unit area transferred between the crack faces. A plot of the electrical response for this simple model is shown in Figure 2.

5. Finite element formulations

Several authors have investigated the effects of different crack face boundary conditions using the idealized geometry of a center crack in an infinite two-dimensional linear piezoelectric medium. Even with the non-linearities associated with the “exact” and energetically consistent boundary conditions this model requires only the solution of a quadratic or cubic algebraic equation. For geometries relevant for experimental measurements, analytic solutions of this type are not attainable and numerical methods are required for the model solutions. Here we will present two useful finite element formulations along with model reduction techniques that allow for relatively rapid solutions of the non-linear boundary conditions.

5.1 *Scalar potential formulation*

The scalar finite element formulation for the analysis of linear piezoelectric boundary value problems was first proposed by Allik and Hughes[2]. In the standard scalar potential formulation, the displacements and the electric potential are interpolated from the nodal quantities with a set of shape/interpolation functions which can be represented in matrix form as $[N^u]$ and $[N^\phi]$. The strains and electric fields are also interpolated from the nodal displacements and electric potentials with $[B^u]$ and $[B^\phi]$ matrices. Note

that the components of the $[B]$ matrices are simply spatial derivatives of the components of the $[N]$ matrices.

With these interpolations, the finite element equations can be derived from (3.10) as

$$\begin{aligned} [K^{uu}]\{u^n\} + [K^{u\phi}]\{\phi^n\} &= \int_V [N^u]^T \{b\} dV + \int_S [N^u]^T \{t\} dS \\ [K^{\phi u}]\{u^n\} + [K^{\phi\phi}]\{\phi^n\} &= - \int_V [N^\phi]^T q dV - \int_S [N^\phi]^T \omega dS \end{aligned} \quad (5.1)$$

where

$$\begin{aligned} [K^{uu}] &= \int_V [B^u]^T [c^E] [B^u] dV, \quad [K^{u\phi}] = \int_V [B^u]^T [e] [B^\phi] dV \\ [K^{\phi u}] &= \int_V [B^\phi]^T [e]^T [B^u] dV, \quad [K^{\phi\phi}] = - \int_V [B^\phi]^T [\kappa^E] [B^\phi] dV \end{aligned} \quad (5.2)$$

Equations (5.1) represent the standard scalar potential finite element formulation for piezoelectric materials.

5.2 Vector potential formulation

The vector potential formulation was developed by Landis [7], and its primary advantage is the ability to easily account for electrical non-linearities associated with domain switching and the discharge model of Equations (4.10) and (4.11). The vector potential formulation is most easily applied to problems where the body charge density is zero, such that the electric displacement can be given as

$$D_i = \epsilon_{ijk} \psi_{j,k} \quad (5.3)$$

where ϵ_{ijk} is the permutation tensor.

As for the standard scalar potential formulation, interpolations for the fundamental field quantities are required. For the vector potential formulation the displacements and the vector potential components ψ_i are interpolated from the nodal quantities with a set of shape/interpolation functions which can be represented in matrix form as $[N^u]$ and $[N^\psi]$. The strains and electric displacements are then interpolated from the nodal displacements and vector potential with $[B^u]$ and $[B^\psi]$ matrices.

With these interpolations, Equation (3.11) yields the vector potential finite element formulation

$$\begin{aligned} [K^{uu}]\{u^n\} + [K^{u\psi}]\{\psi^n\} &= \int_V [N^u]^T \{b\} dV + \int_S [N^u]^T \{t\} dS \\ [K^{\psi u}]\{u^n\} + [K^{\psi\psi}]\{\psi^n\} &= - \int_S [B^\psi]^T \phi \{n\} dS \end{aligned} \quad (5.4)$$

where

$$\begin{aligned} [K^{uu}] &= \int_V [B^u]^T [c^D] [B^u] dV, \quad [K^{u\psi}] = - \int_V [B^u]^T [h] [B^\psi] dV \\ [K^{\psi u}] &= - \int_V [B^\psi]^T [h]^T [B^u] dV, \quad [K^{\psi\psi}] = \int_V [B^\psi]^T [\beta^e] [B^\psi] dV \end{aligned} \quad (5.5)$$

Note that $[K''']$ differs from the analogous form in the scalar potential formulation. Equation (5.4) represents the vector potential finite element formulation for piezoelectric solids.

For the idealized non-linear phenomenological model outlined in Equations (4.10) and (4.11), only this vector potential finite element formulation can be implemented. The standard scalar potential formulation cannot converge when the electric field remains constant during changes in the electric displacement.

5.3 *Nodal stiffness matrix condensation to the crack faces*

When the crack face boundary conditions are linear, e.g. for the permeable and impermeable boundary conditions, then for each geometry only two load cases need to be solved, one mechanical and one electrical, and the solution to any other loading situation can be obtained from linear superposition. However, the “exact” and energetically consistent boundary conditions introduce non-linearity into the solution, and for a given geometry a full solution is required for each loading scenario. Since the bulk material is described by linear piezoelectricity it is very costly and unnecessary to include the nodal degrees of freedom from this region in every non-linear solution step. Hence, in order to reduce the model size and computation time, a condensation technique can be used such that only the nodal degrees of freedom associated with the opening displacement and electric potential or vector potential on the crack faces are included in the non-linear solution procedure. The condensation method is described next.

Both the standard scalar potential and the vector potential finite element formulations can be written as

$$[K]\{u\} = \{F\} \quad (5.6)$$

Here $[K]$ represents the global nodal stiffness matrix, $\{u\}$ represents the generalized displacement vector including both electrical and mechanical degrees of freedom, and $\{F\}$ is the generalized force applied to the body. Next we decompose the global stiffness matrix $[K]$, the displacement vector $\{u\}$, and the applied force vector $\{F\}$ in the following manner,

$$[K] = \begin{bmatrix} [K^{nc}] & [C] \\ [C^T] & [K^c] \end{bmatrix}, \quad \{u\} = \begin{Bmatrix} u^{nc} \\ u^c \end{Bmatrix}, \quad \{F\} = \begin{Bmatrix} F^{nc} \\ F^c \end{Bmatrix} \quad (5.7)$$

Here the superscript nc represents the degrees of freedom that are not on the crack faces, and superscript c represents the degrees of freedom that are on the crack faces. Note that in either the scalar or vector potential formulations the stiffness matrix is symmetric.

Equation (5.6) becomes

$$\begin{bmatrix} [K^{nc}] & [C] \\ [C^T] & [K^c] \end{bmatrix} \begin{Bmatrix} u^{nc} \\ u^c \end{Bmatrix} = \begin{Bmatrix} F^{nc} \\ F^c \end{Bmatrix} \quad (5.8)$$

After matrix manipulation, the non-crack face degrees of freedom can be given in terms of the crack face degrees of freedom as

$$\{u^{nc}\} = [K^{nc}]^{-1} \{F^{nc}\} - [K^{nc}]^{-1} [C] \{u^c\} \quad (5.9)$$

Note that the only non-linearity in the problem arises from the crack face boundary conditions, which are represented by the vector $\{F^c\}$. Hence, the inversion of the matrix $[K^{nc}]$ and its operation on $[C]$ need to be performed only once and can then be stored.

Using (5.9), Equation (5.8) can now be written as

$$\underbrace{([K^c] - [C]^T [K^{nc}]^{-1} [C])}_{[K^{crack}]} \{u^c\} = \underbrace{\{F^c\} - [C]^T [K^{nc}]^{-1} \{F^{nc}\}}_{[F^{crack}]} \quad (5.10)$$

Here, $[K^{crack}]$ is the condensed stiffness matrix. Again, note that non-linearity enters the problem through $\{F^c\}$. A Newton-Raphson method will be implemented to solve the problem, and this technique will introduce additional terms into the condensed Jacobian matrix. Hence, it is not useful to invert the condensed stiffness yet, but it is useful to store this matrix after one evaluation of the $[C]^T [K^{nc}]^{-1} [C]$ term.

5.4 Construction of the Jacobian matrix associated with $\{F^c\}$

In order to simplify the presentation here we will assume a symmetric loading configuration such that the crack lies along the x -axis and the displacement and electric

potential along the crack faces satisfies $u_y^- = -u_y^+$ and $\phi^- = -\phi^+$. For this type of symmetry $\Delta u_n = 2u_y^+$ and $\Delta\phi = 2\phi^+$. The formulas to be presented in this section can be readily generalized to the non-symmetric cases. We begin with the scalar potential formulation. The nodal forces normal to the crack face and the nodal charges on the crack face are arranged into the vector $\{F^\phi\}$, where the superscript ϕ signifies the generalized forces associated with the scalar potential formulation. These forces can be calculated as

$$\{F^\phi\} = \int_S [N]^T \begin{Bmatrix} t_y \\ -\omega \end{Bmatrix} dS \quad (5.11)$$

where t_y is the normal traction on the top crack face and ω is the surface charge density on the top crack face. The array $[N]$ is a collection of the appropriate interpolation functions associated with the nodes along the crack face. For both the “exact” and energetically consistent boundary conditions the traction and surface charge density are dependent on the crack opening displacement and electric potential drop in a non-linear fashion. For a Newton-Rapshon solution procedure the incremental relationships between the generalized nodal forces and generalized nodal displacements are required. The incremental forces can be written as

$$\{ \delta F^\phi \} = \int_S [N]^T \begin{Bmatrix} \delta t_y \\ -\delta \omega \end{Bmatrix} dS = \underbrace{\int_S [N]^T \begin{bmatrix} \frac{\partial t_y}{\partial u_y} & \frac{\partial t_y}{\partial \phi} \\ \frac{\partial \omega}{\partial u_y} & \frac{\partial \omega}{\partial \phi} \end{bmatrix} [N] dS}_{[J_\phi]} \begin{Bmatrix} \delta \bar{u}_y \\ \delta \bar{\phi} \end{Bmatrix} \quad (5.12)$$

Here, the vector $\{ \delta \bar{u}_y \quad \delta \bar{\phi} \}$ is intended to represent the nodal opening displacements and electric potentials on the top crack face. The crack gap Jacobian matrices for the “exact” and energetically consistent (EC) boundary conditions are

$$[J_\phi^{Exact}] = \begin{bmatrix} 0 & 0 \\ -\frac{\Delta \phi}{\Delta u_y^2} \kappa_0 & \frac{1}{\Delta u_y} \kappa_0 \end{bmatrix} \quad \text{and} \quad [J_\phi^{EC}] = \begin{bmatrix} -\frac{\Delta \phi^2}{\Delta u_y^3} \frac{d^2 h_c}{dE_c^2} & \frac{\Delta \phi}{\Delta u_y^2} \frac{d^2 h_c}{dE_c^2} \\ \frac{\Delta \phi}{\Delta u_y^2} \frac{d^2 h_c}{dE_c^2} & -\frac{1}{\Delta u_y} \frac{d^2 h_c}{dE_c^2} \end{bmatrix} \quad (5.13)$$

Note that the crack gap Jacobian and hence the full finite element Jacobian is symmetric for the energetically consistent boundary conditions but not symmetric for the “exact” boundary conditions.

We now present the analogous matrices for the vector potential formulation. The generalized nodal forces for the vector potential formulation are given as

$$\{ F^\psi \} = \begin{Bmatrix} \int_S [N]^T t_y dS \\ -\int_S [B]^T \phi n_y dS \end{Bmatrix} \quad (5.14)$$

Here, $[N]$ are the appropriate shape functions associated with the crack surface, and $[B]$ are the derivatives of the shape functions with respect to the direction of the crack face. In a manner analogous to Equation (5.12) the increments of the generalized forces for the vector potential formulation can be written as

$$\{\delta F^\psi\} = \int_S [\bar{N}]^T [J_\psi] [\bar{N}] dS \begin{Bmatrix} \delta \tilde{u}_y \\ \delta \tilde{\psi} \end{Bmatrix} \quad \text{with} \quad [\bar{N}] = \begin{bmatrix} [N] & [0] \\ [0] & [B] \end{bmatrix} \quad (5.15)$$

where the crack gap Jacobian matrices for the “exact” and energetically consistent boundary conditions are

$$[J_\psi^{Exact}] = \begin{bmatrix} 0 & 0 \\ \frac{D_c}{\kappa_0} & -\frac{u_y}{\kappa_0} \end{bmatrix} \quad \text{and} \quad [J_\psi^{EC}] = \begin{bmatrix} 0 & E_c \\ E_c & -\frac{d^2 \tilde{u}_c}{dD_c^2} u_y \end{bmatrix} \quad (5.16)$$

Again notice that the crack gap Jacobian for the energetically consistent boundary conditions is symmetric but that for the “exact” boundary conditions is not. Also, for the vector potential formulation it is more useful to use the internal energy of the crack $\tilde{u}_c(D_c) = h_c + E_c D_c$, which is a function of the electric displacement within the gap. Then the electric field within the crack is simply $E_c = d\tilde{u}_c/dD_c$ and the traction on the crack surfaces is $\sigma_c = \tilde{u}_c$.

Using the finite element Jacobian matrices for the crack faces defined here, Equation (5.10) can be solved using a standard Newton-Raphson method. Again, the Newton-

Raphson Jacobian matrix will be symmetric for the energetically consistent boundary conditions, but not for the “exact” boundary conditions. Due to the condensation step, the matrix to be inverted at each Newton-Raphson iteration is fully dense but is only the size of twice the number of nodes on the crack face (for symmetric 2-D simulations). This reduction in the system size allows for relatively rapid computation which is very useful for the investigation of many different loading scenarios on a given crack geometry.

6. Calculation of fracture parameters

Once a given finite element solution is in hand, we are interested in obtaining several relevant fracture parameters including stress and electric displacement intensity factors and the energy release rates. Since the “exact” boundary conditions yield different results for the energy release rates we will make a distinction between $\mathcal{G}$ and $\mathcal{G}_{tip}$ based on the method of calculation. Where the energy release rate is computed based on the fields local to the crack tip, such a quantity will be referred to as the crack tip energy release rate $\mathcal{G}_{tip}$.

6.1 Numerical calculation of $\mathcal{G}_{tip}$ using K_I and K_D

Consider a crack in a linear piezoelectric body under mixed Mode I and Mode D (also called Mode IV) loading. The crack tip energy release rate can be given in terms of the intensity factors as

$$\mathcal{G}_{tip} = H_{11}K_I^2 + 2H_{12}K_IK_D + H_{22}K_D^2 \quad (6.1)$$

Here H_{11} , H_{12} and H_{22} are components of the Irwin matrix, which depend only on the material properties of the piezoelectric solid. The stress and electric displacement intensity factors characterize the near tip electromechanical fields and are defined such that on the plane directly ahead of the crack tip

$$\sigma_{yy} = \frac{K_I}{\sqrt{2\pi r}} \quad \text{and} \quad D_y = \frac{K_D}{\sqrt{2\pi r}} \quad \text{on} \quad \theta = 0 \quad (6.2)$$

Near the crack tip, the crack opening displacement and electric potential drop are given as

$$\begin{Bmatrix} \Delta u_y \\ \Delta \phi \end{Bmatrix} = 4\sqrt{\frac{2r}{\pi}} \begin{bmatrix} H_{11} & H_{12} \\ H_{12} & H_{22} \end{bmatrix} \begin{Bmatrix} K_I \\ K_D \end{Bmatrix} \quad (6.3)$$

The normal component of the electric displacement can be written from Equation (5.3). Note that in two-dimensional problems only the z -component of the vector potential exists and hence we will drop the subscript such that $\psi \equiv \psi_z$ and then (5.3) yields

$$D_y = -\frac{\partial \psi}{\partial x} \quad (6.4)$$

Equations (6.2) and (6.4) then imply that

$$K_D = -(\psi - \psi_0) \sqrt{\frac{\pi}{2r}} \quad (6.5)$$

where ψ_0 is the value of the vector potential at the crack tip and ψ is a value of the vector potential on the top crack face at a distance r from the crack tip.

For the scalar potential formulation the values of the crack opening and potential drop are computed as nodal quantities at every node along the crack face. Then for any distance r behind the crack tip, Δu_y and $\Delta \phi$ are known and the intensity factors K_I and K_D can be computed by inverting Equation (6.3). For two nodes sufficiently close to the crack tip this procedure should yield similar results for K_I and K_D and any differences can be used as a measure of the error in the procedure.

For the vector potential formulation the opening displacement and vector potential ψ are computed from the finite element solution at each crack face node. From ψ Equation (6.5) offers a direct method for calculating K_D and then K_I can be calculated using Equation (6.3) as

$$K_I = (\frac{1}{4} \sqrt{\frac{\pi}{2r}} \Delta u_y - H_{12} K_D) / H_{11} \quad (6.6)$$

Finally, the crack tip energy release rate can be calculated from (6.1).

Figure 3. The contour used for analyzing the relationship between the J -integral and the energy release rate. The crack is parallel to the x direction and the contour Γ intersects the top and bottom crack faces at the same x position x^Γ .

6.2 Evaluation of $\mathcal{G}_{tip}$ using the J -integral

The relationship between the J -integral and the crack tip energy release rate $\mathcal{G}_{tip}$ has been discussed by Landis [6] and derived for the energetically consistent boundary conditions. For a crack parallel to the x -direction as shown in Figure 3, the J -integral J_Γ yields the amount of energy entering the contour Γ per unit of virtual advance of the contour Γ and the crack in the x -direction. J_Γ is given as

$$J_\Gamma = \int_\Gamma (h n_x - \sigma_{ji} n_j u_{i,x} + D_i n_i E_x) d\Gamma \quad (6.7)$$

Here n_i are the components of unit vector normal to the contour and pointing to the right along the contour.

For a closed contour Γ that contains no singularities, no body force, and no body charge, J_Γ is equal to zero. When the solid is reversible and the region between the crack faces cannot store or remove energy from the system, $J_\Gamma = \mathcal{G}_{tip}$ and J_Γ is independent of the path Γ . However, for the energetically consistent or “exact” crack face boundary conditions, the region between the crack faces can store energy and there are tractions on the crack faces and the normal component of electric displacement is non-zero. In such cases, J_Γ is not equal to $\mathcal{G}_{tip}$ and it is path dependent. However, relationships between J_Γ and $\mathcal{G}_{tip}$ can be determined for both the energetically consistent $\mathcal{G}_{tip}^{EC}$ and “exact” $\mathcal{G}_{tip}^{Exact}$ boundary conditions as

$$\mathcal{G}_{tip}^{EC} = J_\Gamma - h_c(x^\Gamma) \Delta u_y(x^\Gamma) \quad (6.8)$$

$$\mathcal{G}_{tip}^{Exact} = J_\Gamma - \int_{x^\Gamma}^0 \kappa_0 \frac{\Delta \phi}{\Delta u_y} \frac{d(\Delta \phi)}{dx} dx \quad (6.9)$$

Here, $h_c(x^\Gamma)$ represents the electrical enthalpy density of the crack gap and $\Delta u_y(x^\Gamma)$ represents the crack opening displacement evaluated at the intersection of the J -contour with the crack surfaces, x^Γ .

For the energetically consistent boundary conditions the crack tip energy release rate can be calculated simply from J_Γ , $h_c(x^\Gamma)$ and $\Delta u_y(x^\Gamma)$, but for the “exact” boundary conditions an additional integral along the crack faces is required. The accurate computation of these integrals can be accomplished using the domain integral technique. Note that this method for the calculation of $\mathcal{G}_{tip}$ requires the field solutions in the material and not just along the crack faces. Hence, while this method for computing $\mathcal{G}_{tip}$ tends to be more accurate than the method outlined in Section 6.1, it requires a recovery of the finite element solution for the nodes bounding a ring of elements, which can be a computationally expensive process.

Figure 4. The geometry of the four-point bend specimen. The actual geometry analyzed has dimensions, $d_1 = 10 \text{ mm}$, $d_2 = 20 \text{ mm}$, $L = 28 \text{ mm}$, $b = 4 \text{ mm}$ and $a = 0.5 - 3.5 \text{ mm}$.

7. The four point bend specimen

Consider a linear piezoelectric four-point bend specimen as illustrated in Figure 4. Plane strain conditions will be assumed in the out-of-plane direction and the material properties are characteristic of PIC-151 and are given in the Appendix. Due to the symmetry of the specimen geometry and the symmetry of the electromechanical loading with respect to the x -axis, only the right half of the beam needs to be analyzed. Figure 5 illustrates the details of the finite element mesh that has been used to compute the results. Over most of the body standard eight-noded quadrilateral elements are used. Near the crack tip region, the mesh is refined and the elements attached to the crack tip are standard quarter-point elements.

Figure 5. The schematic of the finite element meshing of the specimen. Eight-noded elements are used with quarter-point elements at the crack tip. Around the crack tip the mesh is refined.

The first sets of results to be presented are for the two types of linear boundary conditions, permeable and impermeable. For these boundary conditions the stress and electric displacement intensity factors can be given as

$$K_I = \sigma \sqrt{\pi a} \left(1 - \frac{a}{b}\right)^{-3/2} F(a/b) + \frac{H_{12}}{H_{11}} D \sqrt{\pi a} \left(1 - \frac{a}{b}\right)^{-3/2} G(a/b) \quad (7.1)$$

$$K_D = -\frac{H_{12}}{H_{22}} \sigma \sqrt{\pi a} \left(1 - \frac{a}{b}\right)^{-3/2} S(a/b) + D \sqrt{\pi a} \left(1 - \frac{a}{b}\right)^{-3/2} T(a/b) \quad (7.2)$$

where

$$\sigma = \frac{6M}{tb^2} = \frac{3P(d_2 - d_1)}{tb^2} \quad \text{and} \quad D = \kappa_{33}^\sigma E = \kappa_{33}^\sigma \frac{\Delta V}{L} \quad (7.3)$$

Figures 6a-b present the dimensionless functions F , G , S and T associated with the stress and electric displacement intensity factors in Eqs. (7.1) and (7.2) for the four-point bend specimen illustrated in Figure 4. Also included on these figures are thin black and dashed black lines representing the dimensionless functions F and T for the analogous isotropic elastic and dielectric specimens respectively. Note that, for the permeable boundary conditions, S is equal to F . Using K_I and K_D , the energy release rate, either total or crack tip, can be computed using Eq. (6.1).

Figure 6. The dimensionless functions for the stress and electric displacement intensity factors as defined in Eqs. (7.1) and (7.2). Note that $S(a/b)$ is equal to $F(a/b)$ for the permeable boundary conditions. Also, both $G(a/b)$ and $T(a/b)$ are equal to zero for the permeable boundary conditions.

Next we investigate the effects of the two types of non-linear boundary condition types, energetically consistent and “exact”, on the fracture parameters for the four-point bend specimen. For the “exact” and energetically consistent boundary conditions the crack gap is assumed to behave in a linear dielectric manner such that electrical discharge is not allowed to occur. Figures 7a-b plot K_I and K_D as functions of the applied electric field, $E = \Delta V/L$, for a mechanical loading of 2000N and a crack length of 1mm for the four different crack face boundary condition types.

Of considerable interest is the fact that the permeable, impermeable and “exact” boundary conditions yield very similar results for K_I that are relatively *independent* of

the level of the applied electric field. However, the energetically consistent boundary conditions predict a distinct dependence of the stress intensity factor on the applied electric field. Given that the electrical boundary conditions are very similar for the energetically consistent and the “exact” boundary conditions, it becomes apparent that the additional mechanical crack face traction associated with the energetically consistent boundary conditions, Eqs. (4.7) and (4.8), is responsible for this dependence of K_I on the applied electric field. Figure 7b illustrates the dependence of K_D on the applied electric field, with K_D being constant for the permeable boundary conditions and K_D being linearly dependent on the applied electric field for the impermeable crack face boundary conditions. The effects of the crack gap’s ability to support electric fields can be ascertained by comparing the results for the “exact” and energetically consistent boundary conditions to those for the impermeable boundary conditions. Furthermore, the effects of the crack face traction associated with the energetically consistent boundary conditions are apparent for positive levels of electric field where the results for the “exact” and energetically consistent boundary conditions diverge.

Figure 7. (a) Stress and (b) electric displacement intensity factors for the four boundary condition types for a given mechanical load as a function of the applied electric field. Note that the “exact”, permeable and impermeable lines are indistinguishable from one another in (a).

While the results for K_I and K_D are of interest, they are only of use within a fracture criterion in conjunction with an energetic constraint. Specifically, unless the fracture process itself can *supply* energy to the surrounding material, crack growth can only occur if the amount of energy entering the crack tip is positive. Hence, when the fracture process consumes energy, the fracture criterion must at the very least require the inequality $\mathcal{G}_{tip} > 0$. Figure 8 plots the energy release rates as a function of the applied electric field for the same set of mechanical loading and as in Figures 7a-b but a crack length of 0.75mm. For each of the boundary condition types the solid lines represent the crack tip energy release rate as computed from Eq. (6.1), and the dots represent the “total” or “global” energy release rate as computed from Eq. (2.8) using a Δa of 0.5mm. We note that when there is no dissipation in either the material or its surroundings there can be no difference between these two measures of energy release rate. Hence, any difference that does arise represents a failure of the modeling procedure to generate physically consistent results. The results shown on Figure 8 demonstrate that of the four crack face boundary condition types, only the “exact” boundary conditions generate a significant (non-numerical) difference between the crack tip and total energy release rates. Furthermore, the crack tip energy release rate for the “exact” boundary conditions is significantly greater than the total energy release rate. Also, the total energy release rate

from the “exact” boundary conditions is similar (but always less than) the energy release rate for the energetically consistent boundary conditions. This observation leads to the conclusion that the total energy release rate from the “exact” boundary conditions is a reasonable approximation for the energy release rate for the energetically consistent boundary conditions. Similar observations and conclusions have been made by Landis[6] in the analysis of the center-cracked plate problem.

Figure 8. The energy release rates for the four different boundary condition types for a given mechanical loading of 2000N as a function of electric field. Solid lines represent the results as computed from Eq. (6.1) and the dots are results computed from Eq. (2.8) using a Δa of 0.5mm.

In addition to the approximations used to model the crack face boundary conditions, it is also useful to note the approximations applied to the constitutive model for linear

piezoelectric materials, Eqs. (3.8) and (3.9). Most piezoelectric materials of technological interest are polarized ferroelectric materials. Hence, the constitutive equations (3.8) and (3.9) are valid for the *changes* of strain and polarization with respect to the remanently poled state. For the case of the strain, this distinction plays no role in the physical situation since any initial stress-free strain state can be set as the reference state and identified as zero strain. However, the same change of reference state cannot be made with the polarization and electric displacement. Hence, taking the impermeable boundary conditions as an example, when the electrical boundary conditions on the crack faces are stated as $D_i n_i = 0$, this actually should be read as $\Delta D_i n_i = 0$. Furthermore, these conditions implicitly assume that a surface free charge density equal in magnitude to the remanent polarization is left on the crack faces as the crack grows. If the remanent polarization is accounted for in the constitutive law and the crack face boundary conditions $D_i n_i = 0$ are applied, then such a model predicts that the electric field within the crack gap, $-\Delta\phi/\Delta u_y$, will be enormous even for zero applied electrical loading. Even under the standard assumptions, which are more closely approximated as $\Delta D_i n_i = 0$, the electric field within the crack gap can grow to be very large for even very modest applied electrical loadings. Certainly, the electric field within the crack gap cannot increase indefinitely and eventually some type of electrical discharge will occur. A very simple model for electrical discharge (perhaps the simplest) was proposed in Eqs. (4.10) and (4.11). It is assumed that the crack gap behaves in a linear dielectric manner up to an electric field of E_d . Once this discharge field is reached charge is allowed to transfer between the crack faces in an amount such that the electric field within the crack gap remains at E_d . We note that this idealized model for the crack gap discharge requires the

vector potential finite element method for its solution. Figure 9 illustrates the effects of electrical discharge on the energy release rate predicted using the energetically consistent boundary conditions, and applied load of 4000N and a crack length of 0.75mm. Again, the lines represent the calculation of the energy release rate based on Eq. (6.1), and the dots are computed using Eq. (2.8) using a Δa of 0.5mm. These calculations indicate that, to within numerical error, the crack tip and “global” procedures for computing the energy release rate are in agreement for the energetically consistent boundary conditions. Of greater interest is the effect of the electrical discharge. Notice that as the critical electric field level for discharge, E_d , decreases the effects of the applied electric field are diminished and the energy release rate increases. In the limit as $E_d \rightarrow 0$ the results for the permeable crack face boundary conditions are recovered. Therefore, when the dielectric strength of the crack gap medium is low, it becomes reasonable to apply the electrically permeable crack assumption to the fracture problem.

Figure 9. The energy release rate as a function of applied electric field under a constant load using energetically consistent boundary conditions and different levels of the critical discharge field within the crack gap. Solid lines represent the results as computed from Eq. (6.1) and the dots are results computed from Eq. (2.8) using a Δa of 0.5mm.

8. Discussion

To date there remains controversy over the appropriate electromechanical fracture criteria for piezoelectric and ferroelectric materials. The development of a mature understanding of electromechanical fracture has been hindered by a number of complex and coupled processes that are both difficult to model and measure. These processes include the effects of domain switching, electrical discharge, and the material separation process at the crack tip. There exist several excellent studies concerning the levels of electromechanical loading required to propagate cracks in different electromechanical materials, but to date no experimental measurements have been carried out to directly measure the energy release rate for a given sample geometry and loading. Hence, the developments of fracture criteria have relied on various modeling efforts to predict the prevailing energetics when fracture proceeds. On this situation, one point should be made clear; the prediction of the energy release rate is very sensitive to the assumptions about the crack face boundary conditions. This fact is illustrated in Section 7 of this paper for the specific example of the 4-point bend specimen. Instead of relying on the imaginations of the modelers, a more robust approach would be to measure the energy release rates directly so that the unreasonable models can be debunked. The purpose of

Section 2 of this paper is to outline the measurements that need to be performed in such an experiment. Specifically, the load-displacement and charge-voltage response of two specimens that differ in their crack lengths must be measured, and then the energy release rate for that geometry and environment can be determined.

The remainder of the paper was devoted to comparing the predictions for the stress and electric displacement intensity factors and energy release rates from the different crack face boundary conditions, permeable, impermeable, “exact” and energetically consistent. Additionally, the proposed experimental method for determining the energy release rate is carried out numerically in order to demonstrate the accuracy of the method and to expose an inconsistency in the “exact” boundary conditions. Calculations using the finite element method were performed on a 4-point bend specimen relevant to recent fracture measurements. For the two linear boundary conditions types, permeable and impermeable, the stress and electric displacement factors were reported as a function of crack length. The results indicate that the contributions to K_I from the mechanical loading and to K_D from the electrical loading for the PZT material are very similar to those for an isotropic material. Next, a condensation technique was applied within the finite element simulations in order to allow for the computationally efficient solution of the non-linear boundary condition types. This numerical method was employed to investigate the effects of electric field on the predicted fracture parameters for the four boundary condition types. The results clearly show that the crack face boundary conditions significantly affect the predictions for the influence of the applied electric field on the energy release rate and the stress and electric displacement intensity factors.

Furthermore, the results show very clearly that the crack tip energy release rate differs from the global energy release rate when the “exact” boundary conditions are used. This result is entirely unsatisfactory since these two quantities must be equal to one another when there is no (realized) dissipation in the system. Therefore, the only reasonable conclusion is that future modeling efforts must abandon the use of such energetically inconsistent boundary conditions.

Finally, the effects of dielectric breakdown within the crack gap were investigated within the context of the energetically consistent boundary conditions. Experimental evidence of such dielectric breakdown certainly exists, but an understanding of the effects on fracture is not well understood. In this paper a simple model for dielectric breakdown in the crack gap was applied and it was shown that as the breakdown strength of the gap decreases the predictions of the energetically consistent boundary conditions approaches those of the permeable boundary conditions. This is a very appealing result since it offers a physical explanation for how the crack can be open but the effects of the applied electric field on the energy release rate can be greatly (or almost entirely) diminished.

Appendix

The material properties used for numerical results are characteristic of PIC-151.

The Irwin matrix for this material under plane strain conditions is

$$\begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} = \begin{bmatrix} 1.119 \times 10^{-11} \text{ m}^2 / \text{N} & 9.901 \times 10^{-3} \text{ m}^2 / \text{C} \\ 9.901 \times 10^{-3} \text{ m}^2 / \text{C} & -3.110 \times 10^7 \text{ Vm} / \text{C} \end{bmatrix}$$

where the plane strain material properties used to derive this matrix are

in h -form:

$$\begin{aligned} c_{11}^D &= 122 \text{ GPa}, \quad c_{13}^D = 44.8 \text{ GPa}, \quad c_{33}^D = 130.2 \text{ GPa}, \quad c_{44}^D = 34.7 \text{ GPa} \\ h_{31} &= -1.27 \times 10^9 \text{ V/m}, \quad h_{33} = 2.00 \times 10^9 \text{ V/m}, \quad h_{15} = 1.22 \times 10^9 \text{ V/m} \\ \beta_{11}^\epsilon &= 1.108 \times 10^8 \text{ Vm/C}, \quad \beta_{33}^\epsilon = 1.326 \times 10^8 \text{ Vm/C} \end{aligned}$$

or in d -form

$$\begin{aligned} s_{11}^E &= 1.45 \times 10^{-11} \text{ m}^2 / \text{N}, \quad s_{13}^E = -9.27 \times 10^{-12} \text{ m}^2 / \text{N}, \\ s_{33}^E &= 1.59 \times 10^{-11} \text{ m}^2 / \text{N}, \quad s_{44}^E = 5.00 \times 10^{-11} \text{ m}^2 / \text{N} \\ d_{31} &= -2.79 \times 10^{-10} \text{ m/V}, \quad d_{33} = 3.30 \times 10^{-10} \text{ m/V}, \quad d_{15} = 6.00 \times 10^{-10} \text{ m/V} \\ \kappa_{11}^\sigma &= 1.70 \times 10^{-8} \text{ C/Vm}, \quad \kappa_{33}^\sigma = 1.52 \times 10^{-8} \text{ C/Vm} \end{aligned}$$

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