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On a Failure Related Problem of Linear Piezoelectricity

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1. Introduction

Piezoelectricity is a process of electromechanical interaction that occurs exclusively in anisotropic solids, thus found in most crystals. The piezoelectric effect, however, can also be induced in originally isotropic ceramics (such as barium titanate and lead titanate zirconate) through a process known as poling, which consist of subjecting the ceramic to a very high direct voltage for a certain amount of time.

Ceramics of these type are extensively used in electronic packaging, electromechanical devices, control systems and large flexible structures. In these applications the ceramic bodies are subjected to severe loading conditions as a result of which they may fail due to fracture or dielectric breakdown. Failure becomes even more eminent when the piezoelectric body has inherent manufacturing defects such as cracks, holes or impurities.

The purpose of this article is to present a brief account of a problem with strong practical connotations, namely a piezoelectric body containing a hole of elliptic shape, which in the limit is representative of a crack. A theoretical model is presented to analyze the behavior of the electro-elastic fields in the neighborhood of the cavity and crack.

2. Linear Piezoelectricity

We are concerned with deformable dielectric bodies lacking a center of material symmetry and,therefore, prone to exhibit piezoelectricity. The analysis

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of such bodies is carried out through the conjunction of continuum mechanics and electrodynamics theories, of which this section gives an account of the main equations for time-independent deformations. The piezoelectric body $\mathcal{B}$, with body forces and charge density neglected, is described in terms of a Cartesian coordinate system x_1, x_2, x_3. Denoting by T_{ij}, D_i, S_{ij}, u_i and E_i the components of stress, induction, strain, displacement and electric field, respectively, and by ϕ the electric potential, the governing equations reduce to elastic equilibrium and Gauss law, namely

$$\frac{\partial T_{ij}}{\partial x_j} = 0, \qquad \frac{\partial D_i}{\partial x_i} = 0 \tag{1a – b}$$

and the relations of strain-displacement and irrotationality of the electric field, that is

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \qquad E_i = -\frac{\partial \phi}{\partial x_i} \tag{2a – b}$$

where (2b) is a consequence of the quasi-electrostatic approximation. The set (1)-(2) represents 13 equations in 22 unknowns, which must be complemented by constitutive relations derived by means of thermodynamic potentials. One possible phenomenological description of a piezoelectric material is obtained by considering the electric enthalpy, namely

$$\boldsymbol{\Psi} = U(S_{ij}, D_i) - E_i D_i \tag{3}$$

from where the stress and induction are obtained through the relations

$$T_{ij} = \frac{\partial \boldsymbol{\Psi}}{\partial S_{ij}}, \quad D_i = -\frac{\partial \boldsymbol{\Psi}}{\partial E_i} \tag{4}$$

When strain and electric field are the independent variables, the most general, linear piezoelectric material is described by the following quadratic function:

$$\boldsymbol{\Psi} = \frac{1}{2} c_{ijkl}\, S_{ij}\, S_{kl} - \frac{1}{2}\epsilon_{ij}\, E_i\, E_j - e_{ijk}\, E_i\, S_{jk} \tag{5}$$

where c_{ijkl}, ϵ_{ij} and e_{ijk} are the components of the elastic, dielectric and piezoelectric tensors satisfying the following symmetry conditions:

$$c_{ijkl} = c_{ijlk} = c_{jikl} = c_{klij}; \quad e_{kij} = e_{kji}; \quad \epsilon_{ik} = \epsilon_{ki}$$

Hence, using (4) and (5) the constitutive relations for the linear material become

$$T_{ij} = c_{ijkl}\ S_{kl} - e_{kij}\ E_k$$
$$D_i = e_{ikl}\ S_{kl} + \epsilon_{ik}\ E_k \tag{6}$$

From (6) it is clear that when $e_{kij} = 0$ one obtains constitutive relations for the elastic and electrostatic problems independently of each other. Moreover, it should be pointed out that (6) is the most suitable equation for theoretical purposes. On the other hand, expressions in terms of stress and electric field as independent variables are mostly used for experimental purposes, while equations derived from a thermodynamic potential as function of stress and induction are convenient for two-dimensional analyses.

3. A Piezoelectric Body with a Hole

The problem under consideration is the following: $\boldsymbol{\mathcal{B}}$ is unbounded and assumed transversely isotropic with respect to a coordinate system x, y, z such that the axis of material symmetry(perpendicular to the isotropic plane) is in z-direction. Examples of materials with this particular symmetry are furnished by poled ferroelectric ceramics with their polarization vector along z and hexagonal crystals of the 6mm class with their 6th fold axis again parallel to z.

Material is extracted from the body to produce a volumetric hole in the form of an infinitely long cylinder with elliptic face of dimensions $2a$ and $2b$ $(a > b)$, such that the generator of the cylinder is perpendicular to y while the major and minor axes of the ellipse remain along coordinates x and z, respectively. When $b = 0$ the generator of the cylinder becomes the leading edge (or front) of a slit crack. Under the assumption of plane strain conditions along the generator, a two-dimensional analysis of the elliptic hole contained in the anisotropic plane can be carried out in closed form. Despite the fact that such configuration is two-dimensional, the problem gives rise to the most general condition of electro-elastic coupling effects, thus being a valuable source to withdraw information regarding the effects of defects in piezoelectric materials.

Furthermore, the elliptic hole (whose contour we shall denote by Γ) is assumed to be filled with a homogeneous gas, most likely air of dielectric constant (or permittivity) ϵ_0, and is free of forces and electric surface charge. On the other hand, mechanical and electrical loads in the form of forces, displacements, charge or voltages are applied to the body at remote distances, inducing, in general, stresses, electric fields, etc. in the body and hole. Naturally, in the latter no mechanical fields are present. Finding the electric variables permeating the hole reduces to the solution of Laplace's equation for the electric potential ϕ^c in the cavity, that is $\nabla^2\phi^c = 0$.

In contrast, the solution in matter is a much more difficult problem which requires first to define an appropriate set of constitutive equations. As mentioned before, a set in terms of stress and induction is the most convenient when the analysis is carried out in two dimensions, in which case we have [1]

$$\begin{Bmatrix} S_{xx} \\ S_{zz} \\ 2S_{xz} \end{Bmatrix} = \begin{Vmatrix} a_{11} & a_{12} & 0 \\ a_{12} & a_{22} & 0 \\ 0 & 0 & a_{33} \end{Vmatrix} \begin{Bmatrix} T_{xx} \\ T_{zz} \\ T_{xz} \end{Bmatrix} + \begin{Vmatrix} 0 & b_{21} \\ 0 & b_{22} \\ b_{13} & 0 \end{Vmatrix} \begin{Bmatrix} D_x \\ D_y \end{Bmatrix} \tag{7a}$$

$$\begin{Bmatrix} E_x \\ E_z \end{Bmatrix} = - \begin{Vmatrix} 0 & 0 & b_{13} \\ b_{21} & b_{22} & 0 \end{Vmatrix} \begin{Bmatrix} T_{xx} \\ T_{zz} \\ T_{xz} \end{Bmatrix} + \begin{Vmatrix} c_{11} & 0 \\ 0 & c_{22} \end{Vmatrix} \begin{Bmatrix} D_x \\ D_z \end{Bmatrix} \tag{7b}$$

where a_{ij}, b_{ij} and c_{ii} are the elements of the reduced (or effective) elastic compliance, piezoelectric and impermittivity matrices, respectively.

The two-dimensional versions of (1) and (2) in conjunction with (7) must be solved subject to boundary conditions stating that Γ is traction free and that the normal component of the induction and the electric potential are continuous. Thus

$$\begin{aligned} & t_x = 0\ ; \quad t_z = 0; \\ & D_n = -\epsilon_0 \frac{\partial \phi^c}{\partial n}; \qquad \text{on } \Gamma \\ & \phi = \phi^c \end{aligned} \tag{8a-d}$$

where the variables to the left of the equal signs are calculated in matter, t_x and t_z are the Cartesian components of the stress vector and n is the unit outward normal vector to Γ. We refer to (8) as the exact set of boundary conditions.

4. Electro-Elastic Fields in Matter

Exact expressions for the elastic and electric variables induced in $\mathcal{B}$ by the applied loads were found recently by Sosa and Khutoriansky [1] by means of complex variables analysis and will not be repeated here. Instead we concentrate on the values taken by the fields on Γ, from where important information regarding the behavior of $\mathcal{B}$ can be deduced. To this end, it is convenient to express the fields in terms of components normal (n) and tangent (s) to Γ, where the only independent variable is the angle $0 \leq \theta < 2\pi$ measured over the curve in counter clockwise sense. For example, we can show that the normal and tangential components of the electric field are given by

$$E_n(\theta) = \frac{1}{\Theta}\left(\alpha E_x^\infty \cos\theta + E_z^\infty \sin\theta\right) + \frac{2}{\Theta}\Re\sum_{k=1}^{3}(\alpha\cos\theta + \mu_k \sin\theta)\kappa_k F_k$$

$$E_s(\theta) = \frac{1}{\Theta}\left(\alpha E_z^\infty \cos\theta - E_x^\infty \sin\theta\right) + \frac{2}{\Theta}\Re\sum_{k=1}^{3}(\alpha\mu_k\cos\theta - \sin\theta)\kappa_k F_k \qquad \text{(9a-b)}$$

where E_x^∞, E_z^∞ are the prescribed values of the field at infinity,

$$\alpha = \frac{b}{a}\ ; \quad \Theta = \sqrt{\alpha^2\cos^2\theta + \sin^2\theta}\ ; \quad F_k = \frac{a_k(\sin\theta + i\cos\theta)}{a\sin\theta - \mu_k b\cos\theta}\ ;$$

and a_k are three coefficients that depend on the material properties of the body and gas enclosed within the hole and on the applied loads. Moreover, μ_k are three complex roots (with positive imaginary parts) satisfying the characteristic equation

$$a_{11}c_{11}\ \mu^6 + \left[a_{11}c_{22} + 2a_{12}c_{11} + a_{33}c_{11} + b_{21}^2 + b_{13}^2 + 2b_{21}b_{13}\right]\ \mu^4$$
$$\left[a_{22}c_{11} + 2a_{12}c_{22} + a_{33}c_{22} + 2b_{21}b_{22} + 2b_{13}b_{22}\right]\ \mu^2 + a_{22}c_{22} + b_{22}^2 = 0$$

and

$$\kappa_k = \frac{b_{13}c_{22}\mu_k - c_{11}\mu_k(b_{21}\mu_k^2 + b_{22})}{c_{11}\mu_k^2 + c_{22}}.$$

As far as the elastic variables is concerned, we have that on Γ the stress vector vanishes, thus $T_{nn} = T_{ns} = 0$. However, a hoop stress can, in general, be induced, whose value is given by

$$T_{ss}(\theta) = \frac{1}{\Theta^2}\left[T_{xx}^\infty \sin^2\theta + T_{zz}^\infty\alpha^2\cos^2\theta - 2T_{xz}^\infty\alpha\cos\theta\sin\theta\right]$$
$$+ \frac{2}{\Theta^2}\Re\sum_{k=1}^{3}(\mu_k\sin\theta + \alpha\cos\theta)^2 F_k \qquad (10)$$

where T_{xx}^{∞}, etc. are normal and shear stresses prescribed at remote distances from the hole. From (9) and (10) we derive the following results:

RESULT 1: Comparison between exact and impermeable models.

When $\mathcal{B}$ is subjected to a field $\mathbf{E}^{\infty} = E_0\ \mathbf{e}_z$, where $\mathbf{e}_z$ is a unit vector in z-direction, the field induced on the boundary of a slender elliptic hole has very different characteristics according to the nature of the electric boundary conditions prescribed on Γ. Indeed, from (9b) it is found that

$$E_s(\theta) = \frac{(\alpha\gamma + 2c_{11}c_{22}^{-1})E_0\alpha\cos\theta}{(\alpha\gamma + 2\epsilon_0 c_{11})\Theta} \tag{11}$$

where $1 < \gamma < 2$ is a material parameter. The so-called *impermeable* model, is based on an approximation consisting of neglecting the domain interior to the hole, or equivalently setting $\epsilon_0 = 0$. In such a case, the two electric boundary conditions given by (8c-d) are replaced by simply $D_n = 0$. The physical argument behind such approximation relies upon the fact that the dielectric constants of $\mathcal{B}$ are usually much larger than ϵ_0. As we shall see such an argument has limitations imposed by the geometry of the hole. Letting $E_s^A(\theta)$ be the field due to the impermeable approximation as found from (11) when $\epsilon_0 = 0$, we have

$$\frac{E_s^A(\theta)}{E_s(\theta)} = 1 + \frac{2\epsilon_0 c_{11}}{\alpha\gamma} \tag{12}$$

Now, for most piezoelectric materials $\epsilon_0 c_{11} \sim 10^{-4}$ and $\gamma \sim 1$. Therefore, for relatively "open" holes, that is when $\alpha >> \epsilon_0 c_{11}$, exact and approximate models yield the same answer. On the other hand, when the ellipse is very slender, such that $\alpha \sim \epsilon_0 c_{11}$ it is found that $E_s^A(\theta) > E_s(\theta)$, and in the limit, when $\alpha \to 0$ one obtains $E_s^A(\theta) \to \infty$. This last result says that the field becomes singular everywhere in the slit crack (and in particular at its tip), a result found by other authors whose works were based precisely on impermeable boundary conditions ([2, 3, 4, 5, 6]).

RESULT 2: Field-defect interactions using (9).

Within the realm of exact boundary conditions, the case of a slit crack subjected to $\mathbf{E}^{\infty} = E_0\ \mathbf{e}_z$ gives for $\theta = 0$

$$\lim_{\alpha\to 0} E_s(0) = \frac{E_0}{\epsilon_0 c_{22}} \tag{13}$$

That is, use of conditions (8) predicts at the tip of the crack a bounded field. From a practical point of view, however, this result still places strong restrictions on the magnitudes of the applied field E_0. This is so because for most ceramics $\epsilon_0 c_{22} \sim 10^{-4}$. Since most poled ferroelectric ceramics loose their piezoelectric properties when subjected to fields of order 10^6 V/m applied in a direction opposite to the inherent polarization vector, it is clear that under prescribed fields of only 100 V/m the material will degrade permanently. In other words, the material fails electrically.

RESULT 3: Stresses induced by electric fields.

The case of a piezoelectric body subjected to a remote electric field, in addition to mechanical forces, has consequences that we would like to consider here. It is interesting to note that some experimental observations and analytical models have speculated that an electric field may enhance or retard crack propagation initiated by the application of mechanical forces. Therefore, let us study the case when $\mathcal{B}$ is subjected to a field in z-direction, and draw our attention to the behavior of the stress component T_{ss} on Γ at the point $\theta = 0$. Thus, from (10) we have

$$T_{ss}(0) = \frac{K\ (c_{22}^{-1} - \epsilon_0)\ E_0}{\alpha\gamma + 2\epsilon_0 c_{11}} \tag{14}$$

where K is a positive, real number. If the piezoelectric solid is, in addition, subjected to remote forces, the corresponding stresses can be added to (14) according to the principle of superposition. On this point, it is useful to note that the sign of $T_{ss}(0)$ in (14) depends solely on the sign of E_0, since the rest of the expression is positive. Thus, the electric field can increase or reduce the intensity of the normal stress generated by say tensile forces applied in an independent manner. Due to the implications of this effect it seems appropriate to investigate the order of magnitude of the stress induced only by E_0. To this end, we note that for piezoelectric ceramics, the quantities involved in (14) have the following orders of magnitude: $c_{11}, c_{22} \sim 10^8$, $\epsilon_0 \sim 10^{-12}$, $\gamma \sim 1$ and $K \sim 10^8 - 10^9$. Hence, according to these values, the stress induced by the field for aspect ratios in the range say $10^{-2} < \alpha < 1$ is given (in its most critical condition) by

$$T_{ss}(0) \sim \frac{10 \times E_0}{\alpha} \tag{15}$$

That is, the slender the ellipse, the larger the stress in accordance to physical intuition. In some cases the value given by (15) may have a substantial incidence in the overall value of the hoop stress. For example, a field of 10^5 V/m applied alone could induce a stress of up to 100 MPa if the axes of the ellipse are in the ratio 1/100. Such value of stress is clearly detrimental in view of the fact that most piezoceramics have tensile strengths of approximately 80 MPa.

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