ORAL/POSTER REFERENCE: ICF100923OR

ASYMPTOTIC MODE III AND MODE E CRACK TIP SOLUTIONS IN FERROELECTRIC MATERIALS

Chad M. Landis

Department of Mechanical Engineering and Materials Science, MS 321,
Rice University, P.O. Box 1892, Houston, TX, 77025
landis@rice.edu, ph: 713-348-3609, fax: 713-348-5423

ABSTRACT

Complete asymptotic solutions for the Mode III, longitudinal or anti-plane shear, and Mode E applied electric field cases are presented for idealized ferroelectric switching materials. The mathematical procedure required to solve these problems has been presented by Rice [1]. The purpose of this work is to compare and contrast the mechanical and electrical solutions. The constitutive behavior of the material is specified by an initial linear response, a segment of non-hardening switching behavior, i.e. perfect plasticity in the mechanical case, and finally a region where lock-up occurs. The crack tip solution is characterized by an outer solution with a standard $r^{-1/2}$ singularity that is not centered on the crack tip, a switching zone with the solution given by a simple radial slip line field, and an inner lock-up region which surrounds the crack tip.

KEYWORDS

Ferroelectric, dielectric, non-linear behavior, crack tip fields

1. INTRODUCTION

To reduce the mathematical complexity of analyzing the crack tip fields, the following assumptions are made. First, all electromechanical coupling effects including piezoelectricity are ignored. This assumption is not necessary for the purely mechanical anti-plane shear case. Second, the constitutive response, i.e. stress versus strain or electric field versus electric displacement, is taken to be completely reversible. This is to say that the stress or electric field is a unique function of the strain or electric displacement respectively. Borrowing the mechanics terminology, deformation theory plasticity is assumed. This assumption is used in preference to a more appropriate incremental theory in order to make the mathematics tractable.

The remainder of the paper will be devoted to presenting the equations governing the distributions of stress and strain or electric displacement and electric field and the solution to these equations very close to a crack tip. In order to emphasize the similarities between the mechanical and the electrical problems the equations will be presented concurrently.

2. GOVERNING EQUATIONS

Equilibrium and Gauss' law are given by

$$\frac{\partial \tau_x}{\partial x} + \frac{\partial \tau_y}{\partial y} = 0, \qquad \frac{\partial D_x}{\partial x} + \frac{\partial D_y}{\partial y} = 0 \tag{1}$$

where the shear stresses are $\tau_x = \tau_{xz}$ and $\tau_y = \tau_{yz}$, and the *x* and *y* components of the electric displacement are D_x and D_y.

The shear strains, $\gamma_x = \gamma_{xz}$ and $\gamma_y = \gamma_{yz}$, and electric field components, E_x and E_y, are derived from the gradient of the *z* displacement, w, or the electric potential, ϕ, respectively.

$$\gamma_x = \frac{\partial w}{\partial x} \text{ and } \gamma_y = \frac{\partial w}{\partial y}, \quad E_x = -\frac{\partial \phi}{\partial x} \text{ and } E_y = -\frac{\partial \phi}{\partial y} \tag{2}$$

Eqn. 2 implies the following compatibility condition for the shear strains and that the curl of the electric field is zero.

$$\frac{\partial \gamma_x}{\partial y} - \frac{\partial \gamma_y}{\partial x} = 0, \qquad \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} = 0 \tag{3}$$

The constitutive behavior of the material is assumed to be completely reversible, i.e. a deformation theory in mechanics terminology is used. For an isotropic material the stresses and strains or the electric field and electric displacement are collinear.

$$\frac{\tau_x}{\tau_y} = \frac{\gamma_x}{\gamma_y}, \qquad \frac{E_x}{E_y} = \frac{D_x}{D_y} \tag{4}$$

What remains is to specify the relationships between the magnitudes of the shear stress and shear strain and the magnitudes of the electric field and electric displacement. These magnitudes are given by

$$\tau = \left(\tau_x^2 + \tau_y^2\right)^{1/2} \text{ and } \gamma = \left(\gamma_x^2 + \gamma_y^2\right)^{1/2}, \quad E = \left(E_x^2 + E_y^2\right)^{1/2} \text{ and } D = \left(D_x^2 + D_y^2\right)^{1/2} \tag{5}$$

For the mechanical problem the stress is specified as a function of the strain and the electrical problem is characterized with the electric field as a function of the electric displacement.

$$\tau = \begin{cases} G\gamma & \text{for } \gamma \le \gamma_0 \\ \tau_0 & \text{for } \gamma_0 \le \gamma \le \gamma_L \\ \tau_0 + G(\gamma - \gamma_L) & \text{for } \gamma \ge \gamma_L \end{cases}, \qquad E = \begin{cases} D/\kappa & \text{for } D \le D_0 \\ E_0 & \text{for } D_0 \le D \le D_L \\ E_0 + (D - D_L)/\kappa & \text{for } D \ge D_L \end{cases} \tag{6}$$

The shear modulus and dielectric permittivity are G and κ, the shear yield stress and coercive field are τ_0 and E_0, and the lock-up strain and electric displacement are γ_L and D_L. The parameters γ_0 and D_0 are related to the yield stress and coercive field by

$$\gamma_0 = \frac{\tau_0}{G}, \qquad D_0 = \kappa E_0 \tag{7}$$

3. THE CRACK TIP

The crack tip solutions presented here along with the solution for a conducting crack are discussed in further detail by Landis [2]. Consider a semi-infinite crack with faces lying along the negative *x*-axis and tip at the origin. It is assumed that the size of the switching zone, as yet to be determined, is much smaller than the crack length or any other characteristic length in the geometry of the problem. In the mechanical case the crack faces are traction free. For the electrical case it is assumed that the permittivity of free space is zero and there is no normal component of electric displacement along the crack faces. The boundary conditions are then that

$$\text{for } y = 0,\ x < 0 \quad \tau_y = 0, \quad D_y = 0 \tag{8}$$

The solutions for the full fields with lock-up are now presented. The reader is referred to Rice [1] for the mathematical details of the solution procedure. For both the mechanical and electrical problems the switching regions are circles and the radii of the switching regions for the mechanical and electrical cases are

$$R_\tau = \frac{1}{2\pi}\left(\frac{K_{\mathrm{III}}}{\tau_0}\right)^2, \qquad R_E = \frac{1}{2\pi}\left(\frac{K_{\mathrm{E}}}{E_0}\right)^2 \tag{9}$$

The lock-up zones are also circular, surround the crack tip and are embedded within the switching zones. The radii of the lock-up zones are,

$$R_\tau^L = \frac{\gamma_0}{\gamma_L} R_\tau, \qquad R_E^L = \frac{D_0}{D_L} R_E \tag{10}$$

The solutions outside the switching region are given by

$$\text{mechanical} \begin{cases} \tau_y + i\tau_x = \dfrac{K_{\mathrm{III}}}{\left[2\pi\left(x - X_\tau + iy\right)\right]^{1/2}}, \ \text{for } \left|x - X_\tau + iy\right| \geq R_\tau \\ X_\tau = R_\tau\left[1 - 2\dfrac{\gamma_L/\gamma_0 - 1 + \ln\left(\gamma_0/\gamma_L\right)}{\left(\gamma_L/\gamma_0 - 1\right)^2}\right] \end{cases} \tag{11}$$

$$\text{electrical} \begin{cases} E_y + iE_x = \dfrac{K_{\mathrm{E}}}{\left[2\pi\left(x - X_E + iy\right)\right]^{1/2}}, \ \text{for } \left|x - X_E + iy\right| \geq R_E \\ X_E = R_E\left[2\dfrac{D_L/D_0 - 1 + \ln\left(D_0/D_L\right)}{\left(D_L/D_0 - 1\right)^2} - 1\right] \end{cases} \tag{12}$$

Here X_τ and X_E represent the *x* coordinate of the centers of the switching zones. The solution in the switching region is a radial slip line field. The solutions in these regions are

$$\text{mechanical}\ \begin{cases} \tau_{\bar\theta} = \tau_0,\ \tau_{\bar r} = \gamma_{\bar r} = 0,\ \gamma_{\bar\theta} = \dfrac{2R_\tau \gamma_0}{\bar r}\cos\bar\theta, \ \text{for}\ \ 2R_\tau^L \cos\bar\theta \le \bar r \le 2R_\tau \cos\bar\theta \\ \bar r = \sqrt{\left(x - X_\tau + R_\tau\right)^2 + y^2}, \quad \bar\theta = \arctan\dfrac{y}{x - X_\tau + R_\tau} \end{cases} \tag{13}$$

$$\text{electrical}\ \begin{cases} E_{\bar r} = E_0,\ E_{\bar\theta} = D_{\bar\theta} = 0,\ D_{\bar r} = \dfrac{2R_E D_0}{\bar r}\cos\bar\theta, \ \text{for}\ \ 2R_E^L \cos\bar\theta \le \bar r \le 2R_E \cos\bar\theta \\ \bar r = \sqrt{\left(x - X_E - R_E\right)^2 + y^2}, \quad \bar\theta = \arctan\dfrac{y}{x - X_E - R_E} \end{cases} \tag{14}$$

As drawn in Figure 1 and as indicated by the region of validity for Eqn. 13 and Eqn. 14 the lock-up zone is circular and it is tangent to the boundary of the switching zone. This point of tangency lies on the crack faces in the mechanical case and in front of the crack tip in the electrical case. The solution within the lock-up zone cannot be written in simple closed form with stresses or electric fields as functions of coordinates as in Eqns. 11-14. Instead the solution is given for the coordinates as a function of the strain or electric field components.

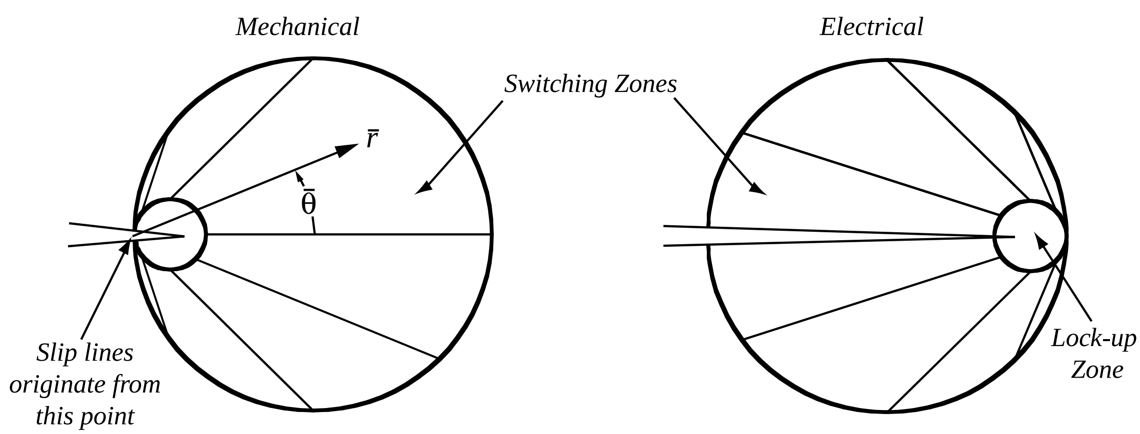

Figure 1: The switching and lock-up regions around a crack tip for the mechanical and electrical cases.

The crack tip solutions within the lock-up zones can be represented by contours of constant strain or electric field magnitude. The constant strain or electric field contours are circles that are not centered on the crack tip. The *x* and *y* coordinates along a given contour are then

$$x = X + R\cos 2\alpha \tag{15}$$

$$y = R\sin 2\alpha \tag{16}$$

where *X* is the *x* coordinate of the center of the contour and *R* is the radius of the contour. The angle 2α is the angle between a line drawn to a point along the contour and the *x*-axis. Then the components of shear strain or electric field at this point along the contour are

$$\text{mechanical:}\ \ \gamma_x = -\gamma\sin\alpha, \quad \gamma_y = \gamma\cos\alpha \tag{17}$$

$$\text{electrical:}\ \ E_x = -E\sin\alpha, \quad E_y = E\cos\alpha \tag{18}$$

The parameters $R(\gamma)$ and $X(\gamma)$ for the mechanical case will be presented first. For a given strain magnitude the radius and the *x* coordinate of the center of this circle are

$$\text{mechanical}\begin{cases} R(\gamma) = R_\tau \dfrac{1}{\gamma/\gamma_0\left(1+\gamma/\gamma_0-\gamma_L/\gamma_0\right)} \\ X(\gamma) = 2R_\tau\left[\dfrac{1-\gamma_L/\gamma_0+\gamma/\gamma_0\ln\left(\dfrac{\gamma/\gamma_0}{1+\gamma/\gamma_0-\gamma_L/\gamma_0}\right)}{\gamma/\gamma_0\left(\gamma_L/\gamma_0-1\right)^2}\right]-R(\gamma) \end{cases} \quad \text{for } \gamma\geq\gamma_L \tag{19}$$

For the electrical problem the radius of a constant electric field contour and the *x* coordinate of its center are,

$$\text{electrical}\begin{cases} R(E) = R_E \dfrac{1}{E/E_0\left(E/E_0+D_L/D_0-1\right)} \\ X(E) = 2R_E\left[\dfrac{D_L/D_0-1+E/E_0\ln\left(\dfrac{E/E_0}{E/E_0+D_L/D_0-1}\right)}{E/E_0\left(D_L/D_0-1\right)^2}\right]-R(E) \end{cases} \quad \text{for } E\geq E_0 \tag{20}$$

4. DISCUSSION AND IMPLICATIONS FOR NUMERICAL METHODS

The analyses presented in Section 3 are most applicable to initially unpoled ferroelectric ceramics. The analysis of poled ferroelectrics and in general full electromechanical coupling is beyond the scope of this work. The inclusion of coupling in the electrical and mechanical fields requires more detailed constitutive relations. Hence, due to the complexity that this type of coupling introduces it is likely that the solution to the crack tip problem will rely on numerical methods. The features appearing in the simple solutions of Section 3 will almost certainly appear in the more complicated fully coupled problem as well. For example, at the point of tangency between the switching and lock-up regions there is a large gradient of strain in the mechanical case and electrical displacement in the electrical case. This is an interesting issue for a numerical solution since from a mathematical standpoint, Eqn. 1 and Eqn. 3, these field variables are not equivalent. Hence, a standard finite element formulation that interpolates displacement and electric potential may be inferior to a mixed or hybrid formulation. At the very least the solutions presented in Section 3 offer an analytical check for any numerical method designed to solve field problems in ferroelectrics.

REFERENCES

1. Rice, J.R. (1967) *Journal of Applied Mechanics*, 34, 287-298.

2. Landis, C.M. (2001) submitted to *Engineering Fracture Mechanics*.