Chapter 4

A NONLINEAR FINITE ELEMENT SIMULATION ON THE CRACKING OF ELECTROSTRICTIVE CERAMIC MULTILAYER ACTUATORS

4.1 INTRODUCTION

The analytical solution discussed in last chapter is only valid under the small-scale saturation conditions, and is obtained under the condition that the stress field does not affect the electric field. To analyze the problem, with realistic device geometries and nonlinear electro-mechanical coupling, one has to do a nonlinear finite element analysis (Gong 1995; Gong and Suo 1996). The plan of this chapter is as follows. Section 4.2 formulates the finite element approach. Section 4.3 compares the last chapter's analytical solution with the finite element results and extends the finite element analysis to the actuators under large-scale saturation conditions. Section 4.4 draws the conclusion.

4.2 PROBLEM FORMULATION

We focus our attention on plane strain problems, which allow us to compare finite element results with existing analytical solutions. This section discusses details of the finite element formulation specific to nonlinear electrostrictive ceramics. Once the stress field is solved, we apply fracture mechanics to obtain the stress intensity factor.

Nonlinear Finite Element Method

We use eight-node quadratic isoparametric elements (Zienkiewicz 1977). Divide the physical plane x-y into many (possibly curved) quadrilaterals, and map every element to a square with side length 2 in the calculation plane ξ - η according to

$$x = \sum_{i=1}^{8} x_i N_i(\xi,\eta), \quad y = \sum_{i=1}^{8} y_i N_i(\xi,\eta), \tag{4.2.1}$$

where (x_i, y_i) are the nodal position vectors, and $N_i(\xi,\eta)$ are the interpolation functions. Denote the nodal values of the displacements and electric potential by u_i, v_i, ϕ_i. Approximate the field $u(x,y)$, $v(x,y)$, and $\phi(x,y)$ within an element in the same way as the position vectors, namely,

$$u(x,y) = \sum_{i=1}^{8} u_i N_i(\xi,\eta), \; v(x,y) = \sum_{i=1}^{8} v_i N_i(\xi,\eta), \; \phi(x,y) = \sum_{i=1}^{8} \phi_i N_i(\xi,\eta). \tag{4.2.2}$$

Write all the nodal values of u, v, and ϕ on the mesh by a column, $\boldsymbol{a}$, and assemble the above interpolation in matrix form

$$\begin{bmatrix} u(x,y) \\ v(x,y) \\ \phi(x,y) \end{bmatrix} = \mathbf{N}\boldsymbol{a}. \tag{4.2.3}$$

where $\mathbf{N}$ contains the interpolation functions for all the nodes of the entire mesh.

The basic field equations in Section 2 can be written as a weak statement:

$$\int \left(\sigma_{ij} \delta\gamma_{ij} - D_i \delta E_i \right) dv = \int \left(t_i \delta u_i - \omega \delta\phi \right) ds. \tag{4.2.4}$$

Here $\delta(\;)$ indicates small variations. Denote

$$\Sigma = \begin{bmatrix} \sigma_x \\ \sigma_y \\ \tau_{xy} \\ D_x \\ D_y \end{bmatrix}, \quad \Gamma = \begin{bmatrix} \gamma_x \\ \gamma_y \\ 2\gamma_{xy} \\ -E_x \\ -E_y \end{bmatrix}, \quad \mathrm{T} = \begin{bmatrix} t_x^0 \\ t_y^0 \\ -\omega^0 \end{bmatrix}. \tag{4.2.5}$$

Here t^0 is the traction prescribed on part of the boundary S_t, and ω^0 is the charge per unit area prescribed on part of the boundary S_ω. Taking gradients of the displacements and the electric potential according to (4.2.3), (3.1.1), and (3.1.4) one obtains that

$$\delta\Gamma = \mathbf{B}\delta\boldsymbol{a}, \tag{4.2.6}$$

where **B** is the matrix resulting from the differenciation. In the discretized form, (4.2.4) becomes

$$\delta\boldsymbol{a}^{\mathrm{T}}\int_{v}\mathbf{B}^{\mathrm{T}}\Sigma dv = \delta\boldsymbol{a}^{\mathrm{T}}\int_{S_t+S_\omega}\mathbf{N}^{\mathrm{T}}\mathbf{T}dS. \tag{4.2.7}$$

The superscript T stands for the transpose of a matrix. Since (4.2.7) holds true for arbitrarily chosen $\delta\boldsymbol{a}$, one concludes that

$$\int_{v}\mathbf{B}^{\mathrm{T}}\Sigma dv = \int_{S_t+S_\omega}\mathbf{N}^{\mathrm{T}}\mathbf{T}dS. \tag{4.2.8}$$

Notice Σ is a function of Γ, and therefore a function of $\boldsymbol{a}$. Equation (4.2.8) is a set of nonlinear equations for nodal variables $\boldsymbol{a}$. They are solved incrementally by linear equations

$$\mathbf{K}\Delta\boldsymbol{a}=\Delta\lambda\mathbf{R} \tag{4.2.9}$$

Here $\Delta\boldsymbol{a}$ is the increment, $\Delta\lambda$ is a parameter that controls the loading increment, **K** is the tangential stiffness matrix,

$$\mathbf{K} = \int_{v}\mathbf{B}^{\mathrm{T}}\mathbf{C}^{-1}\mathbf{B}dv, \tag{4.2.10}$$

and **R** is the equivalent load,

$$\mathbf{R} = \int_{S_t+S_m} \mathbf{N}^{\mathrm{T}}\mathbf{T}\,dS. \qquad (4.2.11)$$

The matrix **C** contains the differentical coefficients of the constitutive equations, namely,

$$\mathrm{d}\boldsymbol{\Gamma}=\mathbf{C}\mathrm{d}\boldsymbol{\Sigma}. \qquad (4.2.12)$$

The matrix **C** is symmetric, but in general not positive-definite.

Nonlinear Dielectric Response Function $f(D)$

Figure 3.1 shows two *D-E* relations in the absence of stress. The relation used by Gong (1994), Hom and Shankar (1994) and Gong (1995) in the finite element analysis is written as

$$f(D) = \frac{E_s}{2} ln\left(\frac{1+D/D_s}{1-D/D_s}\right). \qquad (4.2.13)$$

Here D_s is the saturated electric displacement, E_s is a characteristic electric field. When E is small, D is linearly proportional to E, and the slope defines the dielectric permittivity ε. One can confirm that

$$E_s = D_s / \varepsilon. \qquad (4.2.14)$$

When $E << E_s$, the ceramic is linear. When $E > E_s$, D is maintained at the constant saturation value D_s.

Notice that when the electric displacement saturates, the electrostrictive strain also saturates. This introduces another important parameter in actuator design,

$$\gamma_s = QD_s^2, \tag{4.2.15}$$

which is the saturation strain along the electric field direction in the absence of stress. The saturation strain transverse to the electric field is $-qQD_s^2$.

Boundary Conditions

Figure 4.1 shows the boundary conditions appropriate for a multilayer actuator. Place the origin of the Cartesian coordinate *x-y* at a terminated electrode edge. Because of the symmetry, only half of an individual layer needs to be analyzed. Along the upper electrode, the vertical displacement is constant

$$v(x,H) = constant. \tag{4.2.16a}$$

The value of the constant is to be determined as a part of the solution. The electric field potential equals the applied electric voltage,

$$\phi(x,H) = V_{\text{appl}}. \tag{4.2.16b}$$

When no external stress is applied on the actuator, the shear stress and the vertical resultant force vanish, namely,

$$\sigma_{xy} = 0, \qquad \int_{-L_2}^{L_1} \sigma_{yy}(x,H)dx = 0. \tag{4.2.16c}$$

The lower electrode is connected to the ground, so that

$$\phi(x,0) = 0, \qquad -L_2 \le x \le 0. \tag{4.2.16d}$$

The vertical displacement and the shear stress vanish on both the electrode and its front plane due to the symmetry,

$$v(x,0)=0, \quad \sigma_{xy}=0, \quad -L_2 \le x \le L_1. \tag{4.2.16e}$$

In front of the lower electrode plane, due to symmetry, the vertical electric displacement vanishes,

$$D_y(x,0)=0, \quad 0<x<L_1. \tag{4.2.16f}$$

At the end of the actuator and its vertical symmetric plane, tractions and horizontal electric displacement vanish,

$$\sigma_{xx}=0, \quad \sigma_{xy}=0, \quad D_x=0. \tag{4.2.16g}$$

To avoid rigid body motion, we constrain the horizontal motion at the left lower corner,

$$u(-L_2,0)=0. \tag{4.2.16h}$$

Stress far away from the Electrode Edge

We will use finite element program to analyze a special case that both L_1 and L_2 are much larger than H. Although this configuration is different from a typical actuator, it emphasizes the conditions around the electrode edge with minimum complications from the external boundaries. The more realistic complication $L_2 >> L_1$, $L_1 \approx H$ will be studied elsewhere.

When $L_1 >> H$ and $L_2 >> H$, one can readily determine the stresses in the actuator far away from the electrode, where the electric field is uniform, vanishing in the inactive part, and equal to the applied electric field in the active part. The only nonzero stress component is σ_{yy}, which is tensile ahead of the electrode edge, and compressive behind, due to the global mismatch between the active part and the inactive part. Denote the stress far ahead of the electrode edge by σ^+ and the stress far behind the electrode edge by σ^-. The resultant force vanishes,

$$L_1\sigma^+ + L_2\sigma^- = 0. \tag{4.2.17a}$$

The vertical displacement is the same in both parts,

$$\frac{1-\nu^2}{Y}\sigma^- + (1-\nu q)QD^2 = \frac{1-\nu^2}{Y}\sigma^+. \tag{4.2.17b}$$

These two equations solve the two stresses, giving

$$\sigma^+ = \frac{L_2}{L_1+L_2}\frac{1-\nu q}{1-\nu^2}YQD^2, \tag{4.2.18a}$$

$$\sigma^- = -\frac{L_1}{L_1+L_2}\frac{1-\nu q}{1-\nu^2}YQD^2. \tag{4.2.18b}$$

For example, taking $L_2 = L_1$, $Y = 10^{11}\mathrm{N/m^2}$, $QD^2 = 10^{-3}$, $\nu = q = 0.3$, one finds that the tensile stress $\sigma^+ = 50\mathrm{MPa}$. We emphasize that the stresses σ^+ and σ^- are valid far away from the electrode edge. The stress field in general must be determined by using the finite element analysis.

Computing the Stress Intensity Factor

Once the stress field is obtained from the finite element calculation, the stress intensity factor can be evaluated by means of the fracture mechanics. Consider a crack-like flaw of length *a*, taken to be much smaller than the layer thickness, *i.e.*, $a/H \ll 1$. The stress normal to the crack surface, σ_n, induces a stress intensity factor (Tada *et al.* 1985)

$$K_I = \sqrt{\frac{2}{\pi a}}\int_0^a \sigma_n(x)\sqrt{\frac{x}{a-x}}dx. \tag{4.2.19}$$

We evaluate this integral numerically.

Introduce a dimensionless parameter

$$\alpha = \frac{QD_s Y\gamma_s}{E_s} = \frac{Y\gamma_s^2}{\varepsilon E_s^2}, \tag{4.2.20}$$

which is a material constant that measures the relative magnitude of mechanical and electrical energy. Its mathematical significance can be appreciated as follows. For a ceramic under uniaxial stress σ and electric displacement D, the longitudinal strain γ and electric field E are

$$\gamma = \frac{\sigma}{Y} + QD^2, \quad E = -2QD\sigma + \frac{E_s}{2} ln\left(\frac{1 + D / D_s}{1 - D / D_s}\right). \tag{4.2.21}$$

Normalize the strain by γ_s, the stresse by $Y\gamma_s$, the electric displacement by D_s, and the electric field by E_s, so that (4.2.21) takes a dimensionless form

$$\gamma = \sigma + D^2, \quad E = -2\alpha D\sigma + \frac{1}{2} ln\left(\frac{1 + D}{1 - D}\right). \tag{4.2.22}$$

Similar relation for the multiaxial loading state can also be deduced from (3.2.6) and (3.2.7). Consequently, when $\alpha = 0$, the stresses do not affect electric fields. The approximation $\alpha = 0$ has been made in most previous publications, which we will verify in this paper.

The stress intensity factor takes the dimensionless form

$$\frac{K_I}{Y\gamma_s\sqrt{H}} = k\left(\frac{a}{H}, \frac{E_{appl}}{E_s}, \alpha, \nu, q\right). \tag{4.2.23}$$

Function k is to be determined from the finite element calculation.

4.3 RESULTS AND DISCUSSIONS

This section compares the previous analytical solution with our finite element results and extends the conclusion to large scale saturation.

Comparison of the Finite Element Calculation with the HGS Solution

We compare the analytical solution of previous chapter with the finite element results in this section. In all numerical calculations, we set $\nu = 0.26$, $q = 0.38$, and $L_1 = L_2 = 40H$. We use a small loading level $E_{appl} / E_s = 0.08$ to represent the small-scale saturation conditions. Figure 4.2 compares the electric field distribution along the x-axis. The solid line is the HGS solution; the electric field vector lies in the x direction ahead of the electrode edge, and in the y direction behind of the electrode edge. The finite element results for $\alpha = 0$ and $\alpha = 0.02$ are indicated. As mentioned before, α defined in (4.2.20) affects the ability of the stress field to influence the electric field. In most existing analytical solutions, this parameter has been set to zero to simplify the analysis. Figure 4.2 shows that a realistic value, $\alpha = 0.02$, does not change the electric field substantially, and both sets of results agree with the HGS solution.

Figure 4.3 compares the electric displacement distribution. Again, the two cases $\alpha = 0$ and $\alpha = 0.02$ give similar results. The difference between the finite element results and the analytical solution is caused by different *D-E* relations used in the calculations (shown in Fig. 3.1). This is confirmed by comparing the finite element results with the existing analytical solutions in Appendix B.

Stress distributions along the *x*-axis are plotted in Fig. 4.4 and Fig. 4.5. The small differences between the analytical solution and the finite element calculation suggest that the stress singularity does not change when using a slightly different *D-E* relations in Fig. 3.1. It also suggests that a similar stress intensity factor should be obtained. Consequently, details in the shape of the *D-E* relation plays little role as far as cracking condition is concerned.

Since the stress contributes negligibly to the electric field. Our finite element calculation under the large-scale saturation conditions will focus on the case $\alpha = 0$.

Large-Scale Saturation

When the applied electric loading approaches the saturation electric field, the saturation zone size becomes comparable to the layer thickness. The electric field in the ceramic is no longer $\sqrt{r}$ distributed around the electrode edge. Consequently, the electric field intensity factor, K_E, is no longer meaningful, nor is the saturation cylinder radius, r_s. Nevertheless, we can normalize lengths in the similar manner as in the small-scale saturation case by a characteristic length, still written as r_s, but defined by

$$r_s = \frac{HE_{\mathrm{appl}}^2}{\pi E_s^2}. \tag{4.3.1}$$

This definition is motivated by combining (3.3.9) and (2.2.2), although neither holds the original physical meaning. Figures 4.6 and 4.7 plot the stresses along x-axis at different applied electric field. The solid lines are the stress distributions under the small-scale conditions. It may be instructive to think of the stress field as a combination of the local logarithmic singular stress field and the global uniform stress field. Near the electrode edge, the stress distributions are similar to those under the small-scale saturation conditions. Far away from the electrode edge, the stress is uniform, compressive behind the edge and tensile ahead of the edge, (4.2.18).

Once the stress field is determined, the stress intensity factor K_I is evaluated for a small flaw from (4.2.19). The value of K_I depends on the position, orientation and size of the flaw introduced in the calculation. Such information on flaws is in general unavailable, or at the best, imprecise. We assume that the length of the crack-like flaw, a, is on the order of grain diameter, much smaller than the layer thickness, H. To be definite, we place the flaw along the x-axis, with one tip of the flaw at the point behind the electrode edge, where the normal stress changes from compression to tension. Figure 4.8 shows the calculated stress intensity factor at different applied electric field. They all peak when the other flaw tip is at the electrode edge, and reaches similar value. The peak value of K_{I} is written as

$$(K_{\mathrm{I}})_{\max} \cong 0.25 Y \gamma_s \sqrt{2H} \frac{E_{appl}}{E_s}. \tag{4.3.2}$$

It is noted from Fig. 4.8 that the prefactor varies with the load level E_{appl} / E_s, but only by a small amount. A larger value is chosen to write (4.3.2) for conservative design. No flaw will grow if $(K_{\mathrm{I}})_{\max} < K_{\mathrm{Ic}}$. Equation (4.3.2) defines a critical layer thickness

$$H_c = 8\left(\frac{K_{\mathrm{Ic}} E_s}{Y \gamma_s E_{appl}}\right)^2. \tag{4.3.3}$$

No flaw will grow if every individual layer of the actuator is thinner than H_c. The form of the above expression is identical to the small-scale saturation approximation, (2.2.6). The prefactor in (4.3.3), however, depends on the load level E_{appl} / E_s. The value used in (4.3.3) belongs to $E_{appl} / E_s = 0.2$, which serves as a conservative approximation, judging from Fig. 4.8.

The above cracking condition is derived under the assumption that small flaws are available in a size range, and the flaw that maximizes K_{I} is critical. Consequently, the cracking condition so derived does not depend on the flaw size. If, however, the flaw size a is known from processing, a different cracking condition can be formulated. Figure 4.9 shows crack driving force for three flaw sizes as a function of applied electric loads. For large flaws, K_{I} keeps increasing as the applied loading increases. For small flaws, K_I peaks at certain applied load. The peak values are basically the same as one obtained from Fig. 4.8. Based on this behavior, we construct a maximum crack driving force verses normalized flaw sized curve in Fig. 4.10. Below this curve, flaws cannot grow at any electrical loads.

4.4 CONCLUSION

The finite element calculation indicates that the crack nucleation condition deduced from the small-scale saturation is still approximately valid when the applied electric field approaches the saturation field. More acurate cracking conditions under the large-scale saturation conditions can also be obtained in similar forms, but with different numerical coefficients. Stress induced by electrostriction consists of two parts: a uniform stress induced by the overall strain mismatch far behind and far ahead of the electrode edge, and a nonuniform stress induced by the electric field concentration near the electrode end. For the particular geometry we have analyzed in the paper, the second part plays the dominant role in crack nucleation. For a typical actuator, where the gap between the internal electrode edge and the actuator end (L_2 in Fig. 1.1) is comparable to the layer thickness H, a further study on actuator geometry dependence of the cracking criterion is discussed in Chapter 6.