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著者	進藤 裕英
journal or publication title	Journal of applied physics
volume	95
number	8
page range	4303-4309
year	2004
URL	<a href="http://hdl.handle.net/10097/35765">http://hdl.handle.net/10097/35765</a>

doi: 10.1063/1.1682693

# Finite element analysis of electric fracture properties in modified small punch testing of piezoceramic plates

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(Received 13 October 2003; accepted 20 January 2004)

The fracture behavior of a piezoelectric ceramic under applied electric fields has been the subject of recent studies. We have used finite element analysis to study experiments with the modified small punch (MSP) technique. Nonlinear three-dimensional finite element analysis was employed to calculate the MSP energy and maximum strain energy density. The effects of an applied electric field, 180° and 90° domain switching on the MSP energy, and maximum strain energy density are discussed, and the model predictions are compared with the results of the experiments. The polarization switching zones corresponding to combined mechanical and electrical loads are also obtained. © 2004 American Institute of Physics. [DOI: 10.1063/1.1682693]

## I. INTRODUCTION

Pb(Zr,Ti)O<sub>3</sub> (PZT) is widely used in piezoelectric devices, e.g., transducers, filters, sensors, and actuators. The high mechanical stresses and intense electric fields in the PZT ceramic may cause microcracks to develop which eventually lead to failure of the device. The fracture behavior of PZT under mechanical and electrical loads has been the subject of recent studies.<sup>1,2</sup> The single-edge precracked beam tests were performed on a commercial PZT ceramic, and these tests were simulated numerically with the finite element method.<sup>3</sup> Indentation fracture tests were also made on the PZT ceramics to estimate the fracture toughness, and a three-dimensional (3D) finite element analysis was employed to calculate the energy release rate and stress intensity factor.<sup>4</sup> The crack growth in a ferroelectric barium titanate ceramic was investigated under applied electric fields up to four times the coercive field strength by using the Vickers indentation technique, and the change in crack length and fracture toughness was discussed in connection with the influence of polarization switching on the crack generating stresses.<sup>5</sup> The Vickers indentation technique was also used to study the fracture behavior of poled ferroelectrics.<sup>6</sup> Direct observations of domain switching were made, which suggest that switching induced by the indenter itself plays an important role in determining the apparent fracture toughness.

In a series of articles, a model was developed to simulate the observed nonlinearities in material behavior.<sup>7,8</sup> The ceramics were considered as an aggregate of many grains which were modeled as single domain with switching. Investigated in Ref. 9 was the fracture toughness variation due to small-scale domain switching near the tip of a conducting crack. The shape of the switching zone around a crack tip was predicted by a work energy-based switching criterion. Hayashi *et al.*<sup>10</sup> investigated the displacement and polarization switching properties of piezoelectric laminated actuators theoretically, numerically, and experimentally. Shindo *et al.*<sup>11</sup>

examined the effects of applied voltage and polarization switching on the electroelastic field concentrations ahead of electrodes in multilayer piezoelectric actuators in a combined experimental and numerical investigation.

In the present article, fracture behavior of a piezoelectric ceramic under an applied electric field is discussed using the modified small punch (MSP) test technique. The purpose of the present article is also to present a model for such a MSP test. This is done with a nonlinear finite element analysis of the whole apparatus, which includes the punch, the piezoelectric plate specimen, and the specimen holder. To carry out the analysis, a polarization switching model is assumed for the specimen material. The MSP energy and maximum strain energy density are calculated to qualitatively account for the effect of electric field on fracture initiation load obtained by the MSP test.

## II. EXPERIMENTAL PROCEDURE

Commercially supplied P-7 (Murata Manufacturing Co., Ltd., Japan) piezoelectric ceramic was selected for the experiment. The material properties are listed in Table I. The coercive electric field  $E_c$  is 0.8 MV/m. At least 32 small, thin piezoceramic plate specimens of 10×10×0.5 mm used for the MSP tests were sliced. Poling was done along the axis of the 0.5 mm dimension, and silver electrodes were coated on the two 10 mm×10 mm surfaces.

All MSP tests were conducted using a screw-driven test machine. To generate electric fields, a power supply for voltages up to 1.25 kV/dc was used to apply positive and negative electric fields of 0.2, 0.4, 0.8, and 1.0 MV/m. Loads which caused fracture were measured for each set of specimens for various electric fields. For 0, ±0.4, ±0.8, and ±1.0 MV/m, four or five tests were performed.

## III. BASIC EQUATIONS AND PREDICTION OF POLARIZATION SWITCHING

In this section, the governing field equations for a ferroelectric will be summarized.

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TABLE I. Material properties of the P-7 piezoelectric ceramic.

Elastic stiffnesses ( $\times 10^{10}$ N/m <sup>2</sup> )					Piezoelectric coefficients ( $\times 10^{-12}$ m/V)			Dielectric constants ( $\times 10^{-10}$ C/Vm)	
$c_{11}$	$c_{33}$	$c_{44}$	$c_{12}$	$c_{13}$	$d_{31}$	$d_{33}$	$d_{15}$	$\epsilon_{11}$	$\epsilon_{33}$
13.0	11.9	2.5	8.3	8.3	-207	410	550	171	186

Newton's and Gauss' laws give

$$\sigma_{ji,j} = 0, \quad (1)$$

$$D_{i,i} = 0, \quad (2)$$

where  $\sigma_{ij}$  and  $D_i$  are the stress and electric displacement, and a comma followed by an index denotes partial differentiation with respect to a space coordinate  $x_i$  ( $i=1,2,3$ ). We have employed Cartesian tensor notation and the summation convention for repeated tensor indices. Quasistatic and small strain conditions are

$$E_i = -\phi_{,i}, \quad (3)$$

$$\epsilon_{ij} = \frac{1}{2}(u_{j,i} + u_{i,j}), \quad (4)$$

where  $E_i$  and  $\phi$  are the electric field and electric potential, and  $\epsilon_{ij}$  and  $u_i$  are the strain and displacement. In a ferroelectric, domain-wall motion within each grain leads to a change in the remanent strain  $\epsilon_{ij}^r$  and remanent polarization  $P_i^r$ . The total strain and electric displacement are given by

$$\epsilon_{ij} = \epsilon_{ij}^\ell + \epsilon_{ij}^r, \quad (5)$$

$$D_i = D_i^\ell + P_i^r, \quad (6)$$

where the superscript  $\ell$  refers to linear and

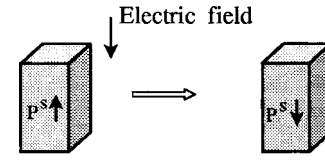
$$\epsilon_{ij}^\ell = s_{ijkl}\sigma_{kl} + d_{kij}E_k, \quad (7)$$

$$D_i^\ell = d_{ikl}\sigma_{kl} + \epsilon_{ik}^T E_k. \quad (8)$$

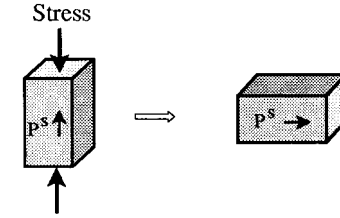
In Eqs. (7) and (8),  $s_{ijkl}$ ,  $d_{kij}$  and  $\epsilon_{ik}^T$  are the elastic compliance, direct piezoelectric constant, and dielectric permittivity at constant stress, which satisfy the following symmetry relations:

$$s_{ijkl} = s_{jikl} = s_{ijlk} = s_{jilk} = s_{klij}, \quad d_{kij} = d_{kji}, \quad \epsilon_{ik}^T = \epsilon_{ki}^T. \quad (9)$$

The direction of spontaneous polarization  $P^s$  of each grain can change by  $90^\circ$  or  $180^\circ$  for ferroelectric switching induced by a sufficiently large electric field. The  $90^\circ$  ferroelastic domain switching is induced by a sufficiently large stress field. Figure 1 shows the schematics of polarization switching for different types of external loading. The criterion states that a polarization switches when the electrical and mechanical work exceeds a critical value<sup>7</sup>



(a)  $180^\circ$  switching



(b)  $90^\circ$  switching

FIG. 1. Polarization switching induced by electrical and mechanical loads.

$$\sigma_{ij}\Delta\epsilon_{ij} + E_i\Delta P_i \geq 2P^s E_c, \quad (10)$$

where  $\Delta\epsilon_{ij}$  and  $\Delta P_i$  are the changes in the spontaneous strain and spontaneous polarization during switching, respectively, and  $E_c$  is the coercive electric field. The values of  $\Delta\epsilon_{ij}$  and  $\Delta P_i$  are given in Appendix A.

While each grain obeys the constitutive relations (7) and (8), the direct piezoelectric constant in the constitutive relations depends on the orientation of the polarization vector in the ceramic. The components of the piezoelectricity tensor during switching are

$$d'_{ikl} = \left\{ d_{33}n_i n_k n_l + d_{31}(n_i \delta_{il} - n_i n_k n_l) + \frac{1}{2}d_{15}(\delta_{ik}n_l - 2n_i n_k n_l + \delta_{il}n_k) \right\}, \quad (11)$$

where  $n_i$  is the unit vector in the poling direction,  $\delta_{ij}$  is the Kronecker delta, and  $d_{33} = d_{333}$ ,  $d_{31} = d_{311}$ , and  $d_{15} = 2d_{131}$  are the direct piezoelectric constants when the piezoelectric ceramic is completely poled in the  $x_3$  direction. The primed quantities denote the piezoelectric constants associated with the original coordinate system during the polarization switching.  $\sigma_{ij}$  and  $D_i^\ell$  during polarization switching are related to  $\epsilon_{ij}^\ell$  and  $E_k$  by

$$\sigma_{ij} = c_{ijkl}\epsilon_{kl}^\ell - e'_{kij}E_k, \quad (12)$$

$$D_i^\ell = e'_{ikl}\epsilon_{kl}^\ell + \epsilon_{ik}E_k, \quad (13)$$

where  $c_{ijkl}$  and  $e'_{ikl}$  are the elastic and piezoelectric constants,  $\epsilon_{ik}$  is the dielectric permittivity at constant strain, and

$$c_{ijkl} = c_{jikl} = c_{ijlk} = c_{jilk} = c_{klij}, \quad e'_{kij} = e'_{kji}, \quad \epsilon_{ik} = \epsilon_{ki}. \quad (14)$$

For the  $180^\circ$  switching, the coercive field is obtained as

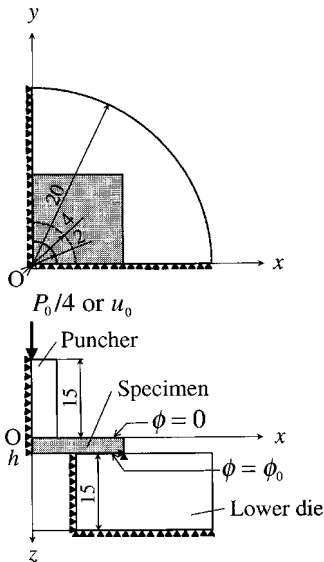


FIG. 2. Finite element model of the MSP test.

$$E_3 = -E_c, \tag{15}$$

which is not affected by the applied stress. However, according to the criterion in Ref. 12, the coercive field for 180° switching is

$$E_3 = - \frac{E_c}{1 - (2d_{33}/P^s)\sigma_{33}}. \tag{16}$$

It is noted that the second term in the denominator includes the normal stress effect as a result of piezoelectricity, and the coercive field increases or decreases depending on the magnitude and direction of the stress  $\sigma_{33}$ .

**VI. FINITE ELEMENT ANALYSIS**

We performed 3D finite element calculations to determine the MSP energy and maximum strain energy density for the PZT specimens. A rectangular Cartesian coordinate system (x,y,z) is used with the z axis coinciding with the poling direction. The analytical model is shown in Fig. 2. A mechanical load was produced by the application of either a prescribed force  $P_0$  or a prescribed displacement  $u_0$  along the z direction. For electrical loads, a negative or positive electric potential  $\phi_0$  was added on the surface,  $z=h$ . The surface  $z=0$  is grounded. We used the commercial finite element code ANSYS. Eight-node 3D space solid was used in the analysis. The contact between the specimen and the lower die was modeled using contact elements. Young’s modulus and Poisson’s ratio of the puncher and lower die are taken to be  $E=206$  GPa and  $\nu=0.3$ . Because of the double symmetry of the body and loading, only one-quarter of the body was modeled. The total number of nodes and elements in the finite element calculations were 6445 and 15 057, respectively. Each 3D finite element consists of about 10 000 grains.

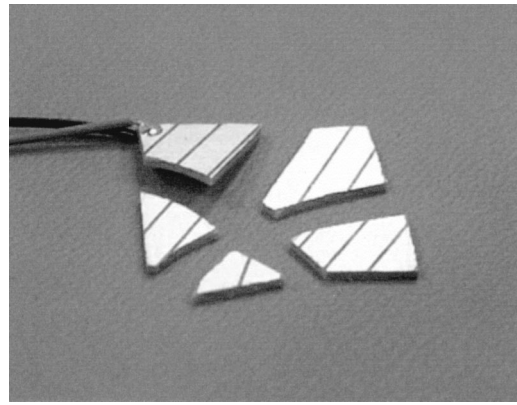


FIG. 3. Fracture appearance of MSP specimen.

The polarization of each grain initially aligns as closely as possible with the z direction. The constitutive Eqs. (12) and (13) for PZT poled in the z direction are found in Appendix B. The polarization switching is defined for each element in a material. Boundary loads are applied, and the electroelastic fields of each element are computed from the finite element analysis. The switching criterion of Eq. (10) is checked for every element to see if switching will occur. After all possible polarization switches have occurred, the piezoelectricity tensor of each element is rotated to the polarization direction. The piezoelectric constant  $e'_{ikl}$  of each element is given in Appendix C. The electroelastic fields are recalculated, and the process is repeated until the solution converges. The macroscopic response of the material is determined by the finite element model, which is an aggregate of elements. The spontaneous polarization  $P^s$  and strain  $\gamma^s$  are assigned representative values of  $0.3$  C/m<sup>2</sup> and  $0.004$ , respectively.

**V. RESULTS AND DISCUSSION**

Figure 3 shows the fracture appearance of piezoelectric ceramic P-7. All specimens failed in a brittle manner. Table II shows the average fracture initiation loads  $P_c$  and the statistically determined standard deviations under different electric fields  $E_0$  obtained from the experiment. At low electric field levels, positive electric fields increase the fracture initiation load. A decrease in the fracture initiation load at  $E_0 = 1.0$  MV/m is considered to occur because of dielectric

TABLE II. Average fracture initiation loads and statistical standard deviations under electric fields for MSP specimens.

$E_0$ (MV/m)	$P_c$ (N)	
	Average	Standard deviation
-1.0	17.7	5.0
-0.8	15.5	2.8
-0.4	13.9	1.6
-0.2	11.9	...
0.0	13.7	0.49
+0.2	15.0	...
+0.4	16.6	2.0
+0.8	17.5	0.35
+1.0	4.79	1.0

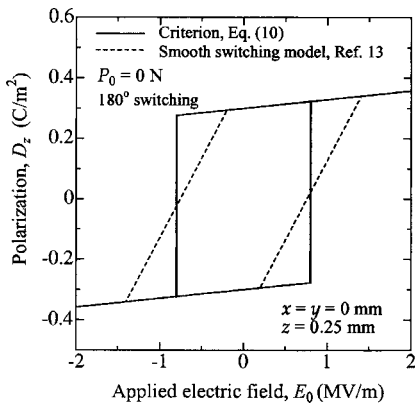


FIG. 4. Polarization vs applied electric field for  $P_0 = 0$  N.

breakdown and irreversible damage of the PZT. When the electric-field level in the negative direction reaches coercive field,  $E_0 = -0.8$  MV/m, the direction of polarization of the stress-free sample switches. At  $E_0 = -1.0$  MV/m, the polarization has reversed and is now aligned with the negative electric field. Also, the effective coercive field under applied stress changes as a function of mechanical load. The behavior of the fracture initiation load for approximately  $E_0 = -0.4$  MV/m leading to  $E_0 = -1.0$  MV/m is expected to be very complicated because of all of these phenomena.

Figure 4 shows the polarization  $D_z$  at  $x = y = 0$  mm,  $z = h/2 = 0.25$  mm versus electric field  $E_z$  for  $P_0 = 0$  N. The model was used to predict macroscopic nonlinear response involving  $180^\circ$  switching, and simulations were carried out with the assumption that the value of saturation polarization is  $0.3$  C/m<sup>2</sup>. The hysteresis loop for  $P_0 = 0$  N shows that switching commences when  $E_0 = \pm 0.8$  MV/m and changes rapidly as the electric-field magnitude increases. The curves generated by the model are also compared with a smooth switching model<sup>13</sup> (see Appendix D). When the smooth switching modeling type is used, the shape of polarization–electric-field curve is changed. However, the strain–electric field curves for the MSP specimens are almost the same for these two models (not shown).

Shindo et al.<sup>14</sup> used the small punch (SP) test to characterize the elastic–plastic fracture toughness  $J_{IC}$  of structural

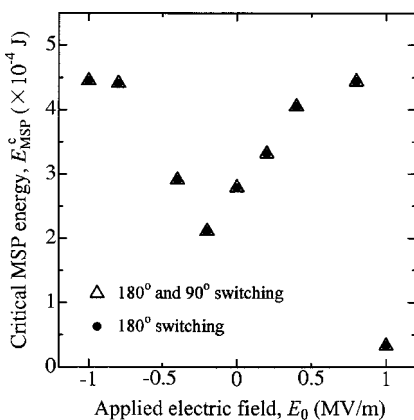


FIG. 5. Critical MSP energy vs applied electric field.

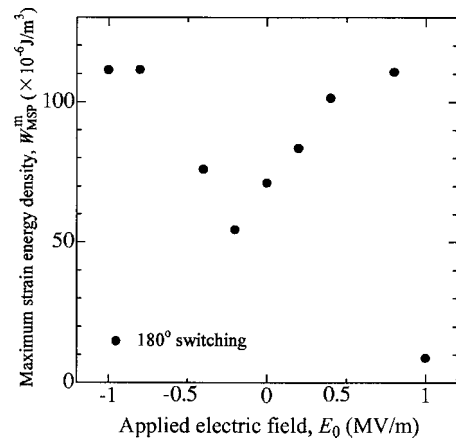


FIG. 6. Maximum strain energy density vs applied electric field.

alloys and weldments for superconducting magnets, and assessed correlation between SP energy and  $J_{IC}$ . Fracture properties measured using this miniature specimen testing approach have been shown to reasonably accurate for a wide range of metals, but have yet to be explored for piezoelectric ceramics. Figure 5 presents the critical MSP energy  $E_{MSP}^c$  including  $180^\circ$  and  $90^\circ$  switching effects (open triangle) for various electric fields  $E_0$ . The load–displacement curves were drawn up to the average fracture initiation load  $P_c$  using the finite element method, and the  $E_{MSP}^c$  was calculated from the area under the curve (energy to failure). It is interesting to note that the MSP energies for  $E_0 = +0.8$  MV/m and  $E_0 = -0.8$  MV/m have very nearly the same values. A similar phenomenon was observed for  $E_{MSP}^c$  without  $90^\circ$  switching effect (solid circle), and the  $90^\circ$  switching has no effect on the critical MSP energy. Figure 6 shows the maximum strain energy density  $W_{MSP}$  versus  $E_0$ . The  $W_{MSP}$  as a function of applied load is computed via finite element analysis without  $90^\circ$  switching effect. The  $W_{MSP}^m$  occurs at the observed crack initiation location.

Figure 7 shows the MSP energy  $E_{MSP}$  of the finite element solutions without the  $90^\circ$  switching effect under an average fracture initiation load for zero electric field  $P_0 = 13.7$  N and different electric fields  $E_0$ , where the result has been normalized by the MSP energy  $E_{MSP0}$  for  $E_0$

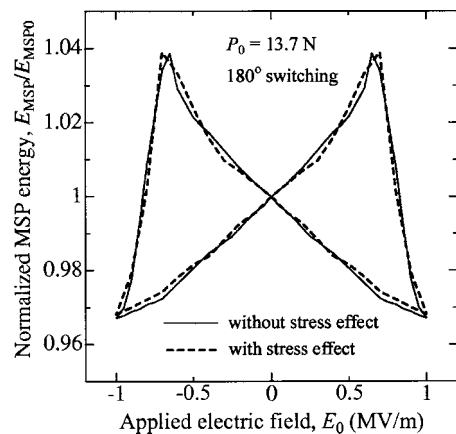


FIG. 7. MSP energy under various electric fields for applied force.



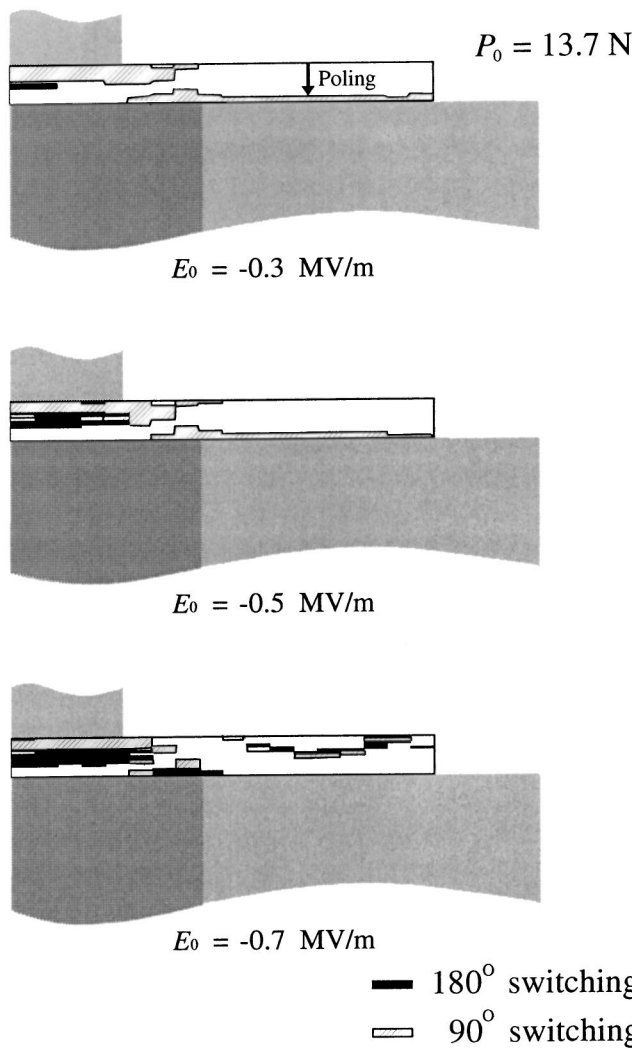


FIG. 8. Polarization switching zone induced by applied force and electric field.

=0 MV/m. Also shown are the prediction with stress effect for the MSP specimen by Eq. (16). The curve rises at first when the electric field  $E_0$  is reduced starting at zero. As the electric field  $E_0$  continues to be reduced, polarization switching commences at approximately  $E_0 = -0.5$  MV/m and since

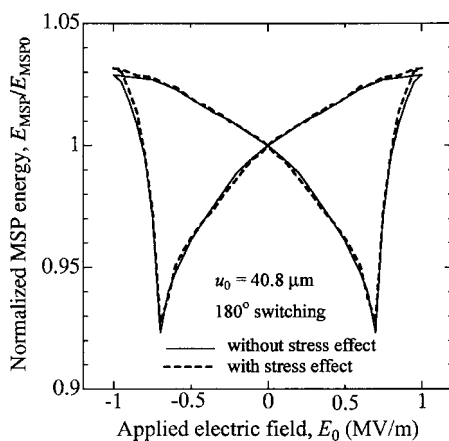


FIG. 9. MSP energy under various electric fields for applied displacement.

the remanent polarization is now diminishing, the MSP energy falls. The electric field in the  $z$  direction is now increased again toward 1.0 MV/m. The results show that switching recommences at approximately  $E_0 = 0.5$  MV/m to eliminate the existing negative remanent polarization. This is completed by the time the field reaches approximately 0.7 MV/m. As the field is cycled between approximately  $-1.0$  MV/m and 1.0 MV/m, the hysteresis curve is reproduced. In addition, it is noted that the results using either Eqs. (15) or (16) are almost the same for the thin piezoelectric plates. Figure 8 shows the  $180^\circ$  and  $90^\circ$  switching zones of the specimen under  $P_0 = 13.7$  N and  $E_0 = -0.3, -0.5,$  and  $-0.7$  MV/m. The size of the switching zone increases with increasing negative electric field.

Using a reaction at  $x=0, z=0$  for  $P_0 = 13.7$  N and  $E_0 = 0$  MV/m, the applied displacement,  $u_0 = 40.8 \mu\text{m}$ , was obtained. Figure 9 shows the normalized MSP energy  $E_{\text{MSP}}/E_{\text{MSP0}}$  of the finite element solutions without the  $90^\circ$  switching effect under a constant displacement  $u_0 = 40.8 \mu\text{m}$  and different electric fields  $E_0$ . For a given displacement, the MSP energy decreases at first when the electric field  $E_0$  is reduced starting at zero. As the electric field  $E_0$  continues to be reduced, a negative remanent polarization develops in the portion of the specimen and the MSP energy rises steeply. As the field is cycled between approximately  $-1.0$  MV/m and 1.0 MV/m, the butterfly loop is repeated. The numerical results under a constant displacement are in contrast to those under an applied force. Fracture mechanism is due to the additional stress induced by the applied electric field.

## VI. CONCLUSIONS

The fracture behavior of piezoelectric ceramic P-7 was investigated under mechanical and electrical loads utilizing the MSP technique. A finite element model was developed to simulate the relation between MSP energy and applied electric field. The strain energy density was also computed. These results have four important consequences: (i) Measured fracture initiation loads and calculated maximum strain energy density are sensitive to the change in the applied electric field and polarization switching. (ii) At low electric field levels, a negative (positive) electric field introduced starting at zero increases (decreases) the computed values of MSP energy for applied load. For applied displacement, the negative (positive) electric field decreases (increases) the MSP energy, at first. (iii) The increase of the negative electric field causes the switched area to grow, and the MSP energy versus electric-field curves show the nonlinear behavior. (iv) For the piezoelectric thin plates, the  $180^\circ$  switching dominates the nonlinear material response, and the  $90^\circ$  switching can be neglected.

## APPENDIX A

The values in  $\Delta \epsilon_{kl}$  and  $\Delta P_i$  for  $180^\circ$  switching can be expressed as

$$\begin{aligned} \Delta \varepsilon_{11} &= 0, & \Delta \varepsilon_{22} &= 0, & \Delta \varepsilon_{33} &= 0, \\ \Delta \varepsilon_{12} &= 0, & \Delta \varepsilon_{23} &= 0, & \Delta \varepsilon_{31} &= 0, \end{aligned} \tag{A1}$$

$$\Delta P_1 = 0, \quad \Delta P_2 = 0, \quad \Delta P_3 = -2P^s. \tag{A2}$$

For 90° switching in the  $x_2x_3$  plane, there results

$$\begin{aligned} \Delta \varepsilon_{11} &= 0, & \Delta \varepsilon_{22} &= \gamma^s, & \Delta \varepsilon_{33} &= -\gamma^s, \\ \Delta \varepsilon_{12} &= 0, & \Delta \varepsilon_{23} &= 0, & \Delta \varepsilon_{31} &= 0, \end{aligned} \tag{A3}$$

$$\Delta P_1 = 0, \quad \Delta P_2 = \pm P^s, \quad \Delta P_3 = -P^s, \tag{A4}$$

where  $\gamma^s$  is the spontaneous strain. For 90° switching in the  $x_3x_1$  plane,

$$\begin{aligned} \Delta \varepsilon_{11} &= \gamma^s, & \Delta \varepsilon_{22} &= 0, & \Delta \varepsilon_{33} &= -\gamma^s, \\ \Delta \varepsilon_{12} &= 0, & \Delta \varepsilon_{23} &= 0, & \Delta \varepsilon_{31} &= 0, \end{aligned} \tag{A5}$$

$$\Delta P_1 = \pm P^s, \quad \Delta P_2 = 0, \quad \Delta P_3 = -P^s. \tag{A6}$$

**APPENDIX B**

For piezoceramics which exhibit the symmetry of a hexagonal crystal of class 6 mm with respect to the principal  $x$ ,  $y$ , and  $z$  axes, the constitutive relations can be written in the following form:

$$\begin{aligned} \begin{Bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{zx} \\ \sigma_{xy} \end{Bmatrix} &= \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{66} \end{bmatrix} \begin{Bmatrix} \varepsilon_{xx}^\ell \\ \varepsilon_{yy}^\ell \\ \varepsilon_{zz}^\ell \\ 2\varepsilon_{yz}^\ell \\ 2\varepsilon_{zx}^\ell \\ 2\varepsilon_{xy}^\ell \end{Bmatrix} \\ &- \begin{bmatrix} 0 & 0 & e'_{31} \\ 0 & 0 & e'_{31} \\ 0 & 0 & e'_{33} \\ 0 & e'_{15} & 0 \\ e'_{15} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{Bmatrix} E_x \\ E_y \\ E_z \end{Bmatrix}, \end{aligned} \tag{B1}$$

$$\begin{aligned} \begin{Bmatrix} D_x^\ell \\ D_y^\ell \\ D_z^\ell \end{Bmatrix} &= \begin{bmatrix} 0 & 0 & 0 & 0 & e'_{15} & 0 \\ 0 & 0 & 0 & e'_{15} & 0 & 0 \\ e'_{31} & e'_{31} & e'_{33} & 0 & 0 & 0 \end{bmatrix} \begin{Bmatrix} \varepsilon_{xx}^\ell \\ \varepsilon_{yy}^\ell \\ \varepsilon_{zz}^\ell \\ 2\varepsilon_{yz}^\ell \\ 2\varepsilon_{zx}^\ell \\ 2\varepsilon_{xy}^\ell \end{Bmatrix} \\ &+ \begin{bmatrix} \varepsilon_{11} & 0 & 0 \\ 0 & \varepsilon_{11} & 0 \\ 0 & 0 & \varepsilon_{33} \end{bmatrix} \begin{Bmatrix} E_x \\ E_y \\ E_z \end{Bmatrix}, \end{aligned} \tag{B2}$$

where

$$\left. \begin{aligned} c_{11} &= c_{1111} = c_{2222}, & c_{12} &= c_{1122}, & c_{13} &= c_{1133} = c_{2233}, & c_{33} &= c_{3333} \\ c_{44} &= c_{2323} = c_{3131}, & c_{66} &= c_{1212} = \frac{1}{2}(c_{11} - c_{12}) \end{aligned} \right\}, \tag{B3}$$

$$\left. \begin{aligned} e'_{15} &= e'_{131} = e'_{223} = d_{15}c_{44}, & e'_{31} &= e'_{311} = e'_{322} = d_{31}(c_{11} + c_{12}) + d_{33}c_{13} \\ e'_{33} &= e'_{333} = 2d_{31}c_{13} + d_{33}c_{33} \end{aligned} \right\}. \tag{B4}$$

**APPENDIX C**

The piezoelectric constant  $e'_{ikl}$  is related to the elastic and direct piezoelectric constants by

$$\begin{aligned} e'_{111} &= d'_{111}c_{11} + d'_{122}c_{12} + d'_{133}c_{13}, & e'_{211} &= d'_{211}c_{11} + d'_{222}c_{12} + d'_{233}c_{13}, \\ e'_{122} &= d'_{111}c_{12} + d'_{122}c_{11} + d'_{133}c_{13}, & e'_{222} &= d'_{211}c_{12} + d'_{222}c_{11} + d'_{233}c_{13}, \\ e'_{133} &= d'_{111}c_{13} + d'_{122}c_{13} + d'_{133}c_{33}, & e'_{233} &= d'_{211}c_{13} + d'_{222}c_{13} + d'_{233}c_{33}, \\ e'_{123} &= 2d'_{123}c_{44}, & e'_{223} &= 2d'_{223}c_{44}, \\ e'_{131} &= 2d'_{131}c_{44}, & e'_{231} &= 2d'_{231}c_{44}, \\ e'_{112} &= 2d'_{112}c_{66}, & e'_{212} &= 2d'_{212}c_{66}, \\ e'_{311} &= d'_{311}c_{11} + d'_{322}c_{12} + d'_{333}c_{13}, & e'_{311} &= d'_{311}c_{11} + d'_{322}c_{12} + d'_{333}c_{13}, \\ e'_{322} &= d'_{311}c_{12} + d'_{322}c_{11} + d'_{333}c_{13}, & e'_{322} &= d'_{311}c_{12} + d'_{322}c_{11} + d'_{333}c_{13}, \end{aligned} \tag{C1}$$

$$e'_{333} = d'_{311}c_{13} + d'_{322}c_{13} + d'_{333}c_{33},$$

$$e'_{323} = 2d'_{323}c_{44},$$

$$e'_{331} = 2d'_{331}c_{44},$$

$$e'_{312} = 2d'_{312}c_{66}.$$

### APPENDIX D

In this Appendix, the smooth switching model is outlined. Kamlah and Tsakmakis<sup>13</sup> postulated the existence of a region of reversible behavior, such that sufficiently small changes of the electric field cause no change of the remanent polarization  $P_3^r$ . Only the normal strain  $\epsilon_{33}$  and electric displacement

$D_3$  were considered. For this case, the normal strain  $\epsilon_{33}$  and electric displacement  $D_3$  during 180° switching are

$$\epsilon_{33} = s_{13}\sigma_{11} + s_{13}\sigma_{22} + s_{33}\sigma_{33} + d'_{33}E_3, \tag{D1}$$

$$D_3 = d'_{31}\sigma_{11} + d'_{31}\sigma_{22} + d'_{33}\sigma_{33} + P_3(E_3), \tag{D2}$$

$P_3(E_3)$  is given by

$$P_3(E_3) = \begin{cases} \epsilon_{33}^T E_3 - P_{\text{sat}} & 0 \leq E_3 < E_c \\ (1/c^p + \epsilon_{33}^T)E_3 - E_c/c^p & E_c \leq E_3 < E_c + c^p P_{\text{sat}} \\ \epsilon_{33}^T E_3 + P_{\text{sat}} & E_c + c^p P_{\text{sat}} \leq E_3 \end{cases} \tag{D3}$$

and

$$P_3(E_3) = \begin{cases} \epsilon_{33}^T E_3 + P_{\text{sat}} & -E_c + c^p P_{\text{sat}} < E_3 < 0 \\ (1/c^p + \epsilon_{33}^T)E_3 + E_c/c^p & -E_c - c^p P_{\text{sat}} < E_3 \leq -E_c + c^p P_{\text{sat}} \\ \epsilon_{33}^T E_3 - P_{\text{sat}} & E_3 \leq -E_c - c^p P_{\text{sat}} \end{cases} \tag{D4}$$

where  $P_{\text{sat}}$  is saturation polarization and  $c^p$  is non-negative material constant.  $P_{\text{sat}} = 0.3 \text{ C/m}^2$  and  $c^p = 2.0 \text{ MV m/C}$  are used to get  $\epsilon_{33}$  and  $D_3$ .

### ACKNOWLEDGMENTS

This work was supported by the Ministry of Education, Culture, Sports, Science, and Technology of Japan under a Grant-in-Aid for Scientific Research (B) and a Grant-in-Aid for Exploratory Research.

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