# INFLUENCES OF DOMAIN SWITCHING AND DIPOLE DYNAMICS ON THE NORMAL MODE RESPONSES OF A FERROELECTRIC CERAMIC BAR

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Abstract—We consider in this paper the dynamic electromechanical responses of ferroelectric ceramics compatible with the normal mode experiment. In this experiment, the direction of wave propagation is normal to the direction of remanent polarization; and during the passage of the wave in such a ceramic, it dipoles, resulting in an electrical output in the external circuit which connects its electroded surfaces. We formulate the boundary–initial value problem corresponding to this experiment and present numerical results which exhibit the nature of its responses. Our formulation presupposes that the mechanical properties of the ceramic are elastic, but takes into account the transient responses of dipole moments and the consequences of domain switching. We also allow the depoled state of the ceramic to be transversely isotropic which differs from its isotropic virgin state and transversely isotropic poled state. On the basis of the numerical results we offer specific conjectures as to possible modes of failure of normal mode devices.

### 1. INTRODUCTION

One of the more useful applications of ferroelectric ceramics is that they are excellent power supplies of electricity. In such applications a poled specimen of a ceramic is subjected to dynamic mechanical loadings and the resulting electrical power in the external circuit which connects the electroded surfaces of the specimen can be quite adequate in supplying sufficiently high voltages or large amounts of current to other devices. It is generally believed that the dynamic mechanical loadings actually depole the specimen thereby giving rise to the electrical output. In this paper, it is our intent to examine the response of such a power supply.

When a poled specimen of a ceramic is subjected to dynamic mechanical loadings, it exhibits both mechanical and electrical responses depending also on the nature of the external circuit which connects its electroded surfaces. The mechanical and electrical responses are inter-related so that the mechanical, piezoelectric and dielectric properties of the ceramic must be taken into account in our examination of the problem.

The problem we have in mind corresponds to the normal mode experiment for which the direction of wave propagation is normal to the direction of remanent polarization[1]. We consider the boundary-initial value problem associated with a resistive external circuit. The constitutive relations for the stress and the electric displacement which we adopt presuppose that the mechanical properties of the ceramic are elastic, but they account for the transient responses of dipole moments and the consequences of the transient responses of domain switching.<sup>†</sup> These transient responses which are due to mechanical strain and electric field necessitate the specification of rate laws describing their behavior. Nevertheless, our intent is to consider the *simplest* non-trivial constitutive relations and rate laws which are sufficient to yield results comparable to experimental observables.

For the purpose of the current calculations we make use of the explicit finite difference algorithm for shocks developed by Bailey and Chen[4]. This algorithm treats the problem of shock evolution quite accurately in that it includes the usual jump conditions which must be satisfied across shock discontinuities. The usage of this algorithm thus enables us to capture more precisely the consequences of the rate laws.

<sup>&</sup>lt;sup>†</sup>The interested reader may consult the papers by Chen and Peercy[2], and Chen[3] concerning some of the arguments leading to these constitutive relations.

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First we consider the conditions of the normal mode experiment. It consists of a rectangular ferroelectric bar poled in the  $X_3$ -direction. Let  $l_1$ ,  $l_2$  and  $l_3$  denote, respectively, the thicknesses of the bar in the  $X_1$ -,  $X_2$ - and  $X_3$ -directions. The electroded  $X_3$ -surfaces are connected via a resistor, an inductor and/or a capacitor. Time-dependent mechanical loads are applied at the  $X_1 = 0$  surface. During the course of the experiment the voltage drop across the external circuit is recorded. This voltage drop is a manifestation of the electromechanical interaction occurring in the ferroelectric bar and the nature of the external circuit.

In order to capture the principal features of the problem and to simplify matters, we assume that the  $X_2$ - and  $X_3$ - surfaces are clamped so that the components  $u_2$  and  $u_3$  of the mechanical displacement **u** of these surfaces are constant for all time t, namely<sup>†</sup>

$$u_{2}(X_{1}, 0, X_{3}, t) = \text{const.}, \qquad u_{2}(X_{1}, l_{2}, X_{3}, t) = \text{const.}, u_{3}(X_{1}, X_{2}, 0, t) = \text{const.}, \qquad u_{3}(X_{1}, X_{2}, l_{3}, t) = \text{const.}$$
(1)

Constraints (1) necessarily imply that the motion is one dimensional and the only non-zero component of the mechanical displacement is  $u_1$  such that

$$u_1 = u_1(X_1, X_2, X_3, t) = u_1(X_1, t)$$
<sup>(2)</sup>

for all  $(X_2, X_3)$ . This assumption together with the observation that the surfaces associated with the  $X_3$ -direction are equipotential surfaces also implies that the  $X_3$ -component  $E_3$  of the electric field **E** depends on time t alone.

The constitutive relations for the stress and the electric displacement which describe the mechanical, piezoelectric and dielectric responses of the ceramic are quite complex. First, we suppose that in the virgin or thermally depoled state the mechanical properties of the ceramic are elastic, and it behaves like a normal dielectric exhibiting no piezoelectric effect. In such a state the material of the specimen is regarded to be isotropic and homogeneous. Second, the material of a poled specimen of the ceramic is transversely isotropic with respect to the poling direction, namely the  $X_3$ -direction, and whose properties depend on the number of aligned dipoles in this direction. Third, we need to account for the transient response of domain switching which alters the number of aligned dipoles. Fourth, the additional transient responses of the dipole moment also give rise to rate effects involving the mechanical, piezoelectric and dielectric properties of the ceramic.

In view of these observations we see that the derivation of the constitutive relations can be quite lengthy and tedious and is beyond the scope of this paper.<sup>‡</sup> We, therefore, simply list the relations which are of interest in the present context. The central assumption concerning these relations is that the direction of polarization does not alter, but that the number of aligned dipoles in this direction may change, thereby altering its magnitude.

For our present purposes we need the normal components of the stress T and the  $X_3$ component of the electric displacement D. Thus, in the standard condensed notation, we
have§

$$T_{1} = (C_{11} + a_{11}N)S_{1} + (C_{12} + a_{12}N)S_{L} + (C_{12} + a_{13}N)S_{P} + (b_{1k} + d_{1k}N)\mu_{Sk} - e_{31}NE_{3} - g_{31}N\mu_{E3} + h_{1}N$$
(3)<sub>1</sub>

$$T_{2} = (C_{12} + a_{12}N)S_{1} + (C_{11} + a_{11}N)S_{L} + (C_{12} + a_{13}N)S_{P} + (b_{2k} + d_{2k}N)\mu_{Sk} - e_{31}NE_{3} - g_{31}N\mu_{E3} + h_{1}N$$
(3)<sub>2</sub>

†In practice, however, the ferroelectric bar is potted in impedance matching epoxy so that this assumption seems quite reasonable.

<sup>‡</sup>In this regard, refer to Chen[3].

Since we are considering the depolarization of the rectangular bar, we presume that all the switchable dipoles are parallel ones.

$$T_3 = (C_{12} + a_{13}N)S_1 + (C_{12} + a_{13}N)S_1 + (C_{11} + a_{33}N)S_P$$

$$+ (b_{3k} + d_{3k}N)\mu_{sk} - e_{33}NE_3 - g_{33}N\mu_{E3} + h_3N$$
(3)<sub>3</sub>

and

$$D_{3} = e_{31}NS_{1} + e_{31}NS_{L} + e_{33}NS_{P} + j_{3i}N\mu_{Si} + (\varepsilon + \varepsilon_{33}N)E_{3} + (\delta + \delta_{33}N)\mu_{E3} + k_{3}N.$$
(4)

In eqns (3) and (4), N is the number of the aligned dipoles in the  $X_3$ -direction,  $S_L$  is the remanent lateral strain and  $S_P$  is the remanent polar strain due to poling<sup>†</sup>

$$S_1 = \frac{\partial}{\partial X_1} u_1 \tag{5}$$

is the normal component of strain S in the  $X_1$ -direction, and  $\mu_S$  and  $\mu_E$  are, respectively, the transient responses of the dipole moment due to strain and electric field. In addition, we have the rate laws

$$\dot{N} + \alpha_N (S_1 - S_L, E_3) N = \beta_N (S_1 - S_L, E_3)$$
(6)

$$b_{1k}\dot{\mu}_{sk} + \alpha b_{1k}\mu_{sk} = \beta_{b_{11}}S_1 + \beta_{b_{12}}S_L + \beta_{b_{13}}S_P \tag{7}$$

$$b_{2k}\dot{\mu}_{sk} + \alpha b_{2k}\mu_{sk} = \beta_{b_{1}2}S_{1} + \beta_{b_{1}1}S_{L} + \beta_{b_{1}3}S_{P}$$
(7)<sub>2</sub>

$$b_{3k}\dot{\mu}_{5k} + \alpha b_{3k}\mu_{5k} = \beta_{b_13}S_1 + \beta_{b_13}S_L + \beta_{b_33}S_P \tag{7}$$

$$d_{1k}\dot{\mu}_{Sk} + \alpha d_{1k}\mu_{Sk} = \beta_{d_{1}1}S_1 + \beta_{d_{1}2}S_L + \beta_{d_{1}3}S_P \tag{8}$$

$$d_{2k}\dot{\mu}_{Sk} + \alpha d_{2k}\mu_{Sk} = \beta_{d_12}S_1 + \beta_{d_11}S_L + \beta_{d_13}S_P \tag{8}$$

$$d_{3k}\dot{\mu}_{5k} + \alpha d_{3k}\mu_{5k} = \beta_{d_1\,3}S_1 + \beta_{d_1\,3}S_L + \beta_{d_3\,3}S_P \tag{8}$$

$$\dot{\mu}_{\mathrm{E3}} + \alpha \mu_{\mathrm{E3}} = \beta_{\mathrm{E3}} E_3 \tag{9}$$

$$j_{3i}\mu_{Si} + \alpha j_{3i}\mu_{Si} = \beta_{j31}S_1 + \beta_{j31}S_L + \beta_{j33}S_P.$$
(10)

We require

$$g_{31}\beta_{E3} = \beta_{j31}, \qquad g_{33}\beta_{E3} = \beta_{j33}$$
 (11)

so as to ensure compatibility of the piezoelectric coupling terms for all time.

The interpretations of the constitutive relations and the rate laws should be quite evident in view of the discussions given by Chen[3] in the general context. Here, however, the constitutive relations and the rate laws are more restrictive. In particular, they describe the responses of a poled ferroelectric bar subjected to conditions (1) and (2) and they account for the transient effects due to domain switching and dipole dynamics. The depoled state need not be the virgin state. In fact, we require it to be transversely isotropic via the specifications of the parameters of the right-hand members of the rate laws, eqns (7) and (8). We further presume that the mechanical displacement of the depoled state from the virgin state is uniform.

The state of the poled rectangular bar is defined by

$$T_1 = T_2 = T_3 = 0,$$
  
 $D_3 = D_P, \quad E_3 = 0,$   
 $S_1 = S_L, \quad N = N_P.$ 
(12)

†Cf. Chen[5].

For convenience, we may normalize N with respect to the poled state, namely

$$N_{\rm P} = 1. \tag{13}$$

The values of  $h_1$  and  $h_3$  depend on the specification of the depoled state. It follows from eqns (3), (7) and (8) that at the poled state defined by eqn (12)

$$\left( C_{11} + a_{11}N_{\rm P} + C_{12} + a_{12}N_{\rm P} + \frac{\beta_{b11}}{\alpha} + \frac{\beta_{b12}}{\alpha} + \frac{\beta_{d11}}{\alpha}N_{\rm P} + \frac{\beta_{d12}}{\alpha}N_{\rm P} \right) S_{\rm L} + \left( C_{12} + a_{13}N_{\rm P} + \frac{\beta_{b13}}{\alpha} + \frac{\beta_{d13}}{\alpha}N_{\rm P} \right) S_{\rm P} + h_1 N_{\rm P} = 0$$
 (14)

$$2\left(C_{12} + a_{13}N_{\rm P} + \frac{\beta_{b13}}{\alpha} + \frac{\beta_{d13}}{\alpha}N_{\rm P}\right)S_{\rm L} + \left(C_{11} + a_{33}N_{\rm P} + \frac{\beta_{b33}}{\alpha} + \frac{\beta_{d33}}{\alpha}N_{\rm P}\right)S_{\rm P} + h_3N_{\rm P} = 0.$$
(15)

Formulae (14) and (15) yield the values of  $h_1$  and  $h_3$  for known values of  $S_L$  and  $S_P$ .

By eqns (4) and (10), we have at the poled state defined by eqn (12)

$$D_{\rm P} = 2\left(e_{31} + \frac{\beta_{j31}}{\alpha}\right) N_{\rm P} S_{\rm L} + \left(e_{33} + \frac{\beta_{j33}}{\alpha}\right) N_{\rm P} S_{\rm P} + k N_{\rm P}.$$
 (16)

Therefore, the value of k follows from eqn (16) for known values of  $S_L$ ,  $S_P$  and  $D_P$ .

The rate laws, eqns (7)–(10), are rather straightforward. However, the rate law, eqn (6), characterizing the consequences of domain switching due to strain in the presence of electric field merits some comment. First, domain switching due to strain depends non-linearly on the strain, and we expect extensive domain switching to occur only if the strain from the poled state is compressive. We expect that, for fixed  $E_3$ ,  $\alpha_N$  is a positive monotonically increasing function of  $|S_1 - S_L|$ , and, for fixed  $S_1 - S_L$ ,  $\alpha_N$  is a positive decreasing function of  $E_3$  if sgn  $E_3 = \text{sgn } N$  or a positive increasing function of  $E_3$  if sgn  $E_3 = -\text{sgn } N$ . The equilibrium values of N are given by the values of  $\beta_N/\alpha_N$  such that sgn  $N = \text{sgn } \beta_N/\alpha_N$ . We expect that, for fixed  $S_1 - S_L$ ,  $|\beta_N/\alpha_N|$  is a monotonically decreasing function of  $|S_1 - S_L|$ , and, for fixed  $S_1 - S_L$ ,  $|\beta_N/\alpha_N|$  is a monotonically decreasing function of  $|S_1 - S_L|$ , and, for fixed  $S_1 - S_L$ ,  $|\beta_N/\alpha_N|$  is a monotonically decreasing function of  $|S_1 - S_L|$ , and, for fixed  $S_1 - S_L$ ,  $|\beta_N/\alpha_N|$  is a monotonically decreasing function of  $|S_1 - S_L|$ , and, for fixed  $S_1 - S_L$ ,  $|\beta_N/\alpha_N|$  is a monotonically decreasing function of  $|S_1 - S_L|$ , and, for fixed  $S_1 - S_L$ ,  $|\beta_N/\alpha_N|$  is a monotonically decreasing function of  $|S_1 - S_L|$ , and, for fixed  $S_1 - S_L$ ,  $|\beta_N/\alpha_N|$  is a monotonically decreasing function of  $|S_1 - S_L|$ , and, for fixed  $S_1 - S_L$ ,  $|\beta_N/\alpha_N|$  is a monotonically decreasing function of  $|S_1 - S_L|$ , and, for fixed  $S_1 - S_L$ ,  $|\beta_N/\alpha_N|$  is a monotonically decreasing function of  $|S_1 - S_L|$ , and, for fixed  $S_1 - S_L$ ,  $|\beta_N/\alpha_N| = -\text{sgn } E_3$ . Further, for compressive strain from the poled state, the rate law, eqn (6), is valid if and only if at any time t

$$|N(t)| > |\beta_N / \alpha_N| \tag{17}$$

otherwise eqn (6) should be replaced by  $\dot{N} = 0$ .

For expansive strain from the poled state, we presume that  $\alpha_N$  and  $\beta_N$  are essentially constant functions of  $S_1 - S_L$ . Here, we expect that  $\alpha_N$  is a positive even function of  $E_3$  and increases monotonically with  $|E_3|$ , and that  $\beta_N/\alpha_N$  is an odd function of  $E_3$  such that sgn  $\beta_N/\alpha_N = \text{sgn } E_3$  and whose magnitude increases monotonically with  $|E_3|$ . Further, for expansive strain from the poled state, the rate law, eqn (6), is valid if and only if at any time t

$$\operatorname{sgn} N(t) \neq \operatorname{sgn} \beta_N / \alpha_N \tag{18}$$

or

sgn 
$$N(t) = \operatorname{sgn} \beta_N / \alpha_N$$
 and  $|N(t)| < |\beta_N / \alpha_N|$  (19)

otherwise eqn (6) should be replaced by  $\dot{N} = 0$ .

#### 3. THE BOUNDARY-INITIAL PROBLEM OF THE NORMAL MODE EXPERIMENT

For our present purpose we restrict our attention to the case when the electroded  $X_3$ -

surfaces are connected via a resistor. As we shall see, it is not difficult to extend the formulation to the case of an arbitrary external circuit.

In addition to the equation of balance of linear momentum appropriate to the current situation, i.e.

$$\frac{\partial T_1}{\partial X_1} = \rho_{\mathsf{R}} \ddot{u}_1 \tag{20}$$

where  $\rho_R$  is the reference mass density, we need to derive the governing differential equation of the component  $E_3$  of the electric field. To this end, we consider a Gaussian element with exterior unit normal enclosing the electrode of the  $X_3 = l_3$  surface. The global form of Gauss' law implies that for the Gaussian element of interest

$$Q = -l_2 \int_0^{l_1} D_3 \, \mathrm{d}X_1 \tag{21}$$

where Q is the total free charge of the electrode. Since the current i in the external circuit is given by

$$i = -\dot{Q} \tag{22}$$

and since  $E_3$  is a function of t alone, it follows from eqns (4) and (9) that

$$i = l_2 I + l_2 I_z \dot{E}_3 + l_2 (I_z + I_\delta \beta_{E3}) E_3 + l_2 (I_\delta - I_\delta \alpha) \mu_{E3}$$
(23)

where

$$I = \int_{0}^{t_{1}} (e_{31}N(S_{1} + S_{L}) + e_{33}NS_{P} + j_{3i}N\mu_{Si} + k_{3}N) \, \mathrm{d}X_{1}$$
(24)

$$I_{t} = \int_{0}^{I_{1}} (\varepsilon + \varepsilon_{33}N) \,\mathrm{d}X_{1}$$
<sup>(25)</sup>

and

$$I_{\delta} = \int_{0}^{I_{1}} \left(\delta + \delta_{33}N\right) dX_{1}.$$
 (26)

The voltage drop across the external resistor is, of course, equal to the voltage drop across the electrodes, so that

$$iR = -l_3 E_3 \tag{27}$$

where R is the resistance. Combining eqns (23) and (27), we obtain

$$l_{2}I_{\varepsilon}\dot{E}_{3} + \left\{\frac{l_{3}}{R} + l_{2}(\dot{I}_{\varepsilon} + I_{\delta}\beta_{E3})\right\}E_{3} + l_{2}(\dot{I}_{\delta} - I_{\delta}\alpha)\mu_{E3} = -l_{2}\dot{I}.$$
(28)

Formula (28) is the external circuit equation for the determination of the  $E_3$ -component of the electric field. It is clear, of course, that it may be readily generalized to the case of an arbitrary external circuit. We simply need to equate the voltage drop across the external circuit to that across the electrodes of the ferroelectric bar.

The solution of the normal mode problem with a resistive external circuit thus entails the simultaneous solution of the equation of balance of linear moment, eqn (20), with the constitutive relation for  $T_1$ , eqn (3), the external circuit equation, eqn (28), and the rate laws, eqns (6)-(10). The appropriate boundary-initial conditions are

$$u_{1}(X_{1}, 0) = u_{0} + S_{L}X_{1}, \qquad \dot{u}_{1}(X_{1}, 0) = 0$$

$$T_{1}(0, t) = f(t), \qquad u_{1}(l_{1}, t) = 0$$

$$E_{3}(0) = 0$$

$$N(X_{1}, 0) = 1$$

$$b_{1k}\mu_{Sk}(0) = b_{2k}\mu_{Sk}(0) = b_{3k}\mu_{Sk}(0) = 0$$

$$d_{1k}\mu_{Sk}(0) = d_{2k}\mu_{Sk}(0) = d_{3k}\mu_{Sk}(0) = 0$$

$$\mu_{E3}(0) = 0$$

$$j_{3i}\mu_{Si}(0) = 0$$

where  $u_0$  is a constant. The system of equations and the boundary-initial conditions are sufficiently complex so as to require numerical solution techniques. As we have remarked earlier, we make use of the explicit finite difference algorithm developed by Bailey and Chen[4] in the solution of these equations. This algorithm is capable of treating the problem of shock evolution quite accurately. Upon obtaining the solution of the system of equations, we may also determine the values of the stress components  $T_2$  and  $T_3$  via the evaluation of the constitutive relations, eqns (3)<sub>2</sub> and (3)<sub>3</sub>.

In closing, we note as a matter of interest that the initial conditions corresponding to the components  $u_2$  and  $u_3$  of the mechanical displacement **u** are

$$u_2(X_1, X_2, X_3, 0) = S_L X_2$$
$$u_3(X_1, X_2, X_3, 0) = S_P X_3.$$

## 4. AN EXAMPLE

We present here the numerical results of an example problem in order to illustrate the responses of the normal mode experiment. It is clear that these results cannot be exhaustive in view of the complexities of the governing equations. Our intention is to illustrate its essential features and to present certain representative results.

The material we have in mind is the ferroelectric ceramic PZT65/35. This is a ceramic for which we have comparatively a fair amount of information to permit us to define its material properties corresponding to the constitutive relations and rate laws laid down in the previous sections. It should be mentioned that the material properties are based on information obtained from numerous sources and they are quite representative qualitatively.<sup>†</sup> This is because the properties of ferroelectric ceramics depend to some extent on the manner in which they are made. In addition, the necessary experiments required to completely characterize a particular ceramic are rather difficult and quite numerous, although some of which are currently underway.

Specifically, we have the following:

$$\rho_{\rm R} = 7.826 \times 10^3 \,\rm kg \,m^{-3}$$
  
 $C_{11} = 1.823 \times 10^{11} \,\rm Pa, \quad C_{12} = 8.287 \times 10^{10} \,\rm Pa$ 
  
 $|a_{11}| = 1.0 \times 10^9 \,\rm Pa \qquad with \, {\rm sgn} \, a_{11} N = 1$ 

<sup>†</sup>The equilibrium properties of PZT65/35 have been determined by Chen[5].

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$$|a_{12}| = 2.1 \times 10^{9} \text{ Pa} \quad \text{with sgn } a_{12}N = 1$$

$$|a_{13}| = 2.2 \times 10^{9} \text{ Pa} \quad \text{with sgn } a_{13}N = -1$$

$$|a_{33}| = 3.73 \times 10^{10} \text{ Pa} \quad \text{with sgn } a_{33}N = -1$$

$$\frac{\beta_{b11}}{\alpha} = -1.75 \times 10^{10} \text{ Pa}, \qquad \frac{\beta_{b12}}{\alpha} = -7.93 \times 10^{9} \text{ Pa}$$

$$\frac{\beta_{b13}}{\alpha} = -1.21 \times 10^{10} \text{ Pa}, \qquad \frac{\beta_{b33}}{\alpha} = -3.05 \times 10^{10} \text{ Pa}$$

$$\frac{\beta_{411}}{\alpha} = -6.4 \times 10^{9} \text{ Pa}, \qquad \frac{\beta_{412}}{\alpha} = -3.19 \times 10^{9} \text{ Pa}$$

$$\frac{\beta_{413}}{\alpha} = 1.56 \times 10^{9} \text{ Pa}, \qquad \frac{\beta_{433}}{\alpha} = 1.16 \times 10^{10} \text{ Pa}$$

$$\frac{\beta_{E3}}{\alpha} = 1.0$$

$$e_{31} = -7.046 \text{ Cm}^{-2}, \qquad g_{31} = \frac{\beta_{131}}{\alpha} = 0.919 \text{ Cm}^{-2}$$

$$e_{33} = 12.32 \text{ Cm}^{-2}, \qquad g_{33} = \frac{\beta_{133}}{\alpha} = -1.61 \text{ Cm}^{-2}$$

$$e = 3.120 \times 10^{-9} \text{ Fm}^{-1}, \qquad \delta = 2.552 \times 10^{-9} \text{ Fm}^{-1}$$

$$|\epsilon_{33}| = 1.886 \times 10^{-9} \text{ Fm}^{-1} \qquad \text{with sgn } \epsilon_{33}N = -1$$

$$|\delta_{33}| = 1.543 \times 10^{-9} \text{ Fm}^{-1} \qquad \text{with sgn } \delta_{33}N = -1$$

and in Figs 1 and 2 we illustrate the graphical representations of the function  $\alpha_N$  and  $|\beta_N/\alpha_N|$  for zero electric field and as functions of  $E_3$ , respectively. These representations are for compressive strain from the poled state. As a matter of interest, the functions corresponding to Fig. 2 are

$$\alpha_N = \begin{cases} 10^3 \exp\left(-7.5 \times 10^{-9} E_3\right), & A \ge 0\\ (10^3 - 2 \times 10^8 A (1 - \exp\left(6.5 \times 10^{-2} A\right))\right) \exp\left(-7.5 \times 10^{-9} E_3\right), & A < 0 \end{cases}$$

where

$$A = -2(S_1 - S_L - B)/B$$
  
$$B = -5 \times 10^{-3} \exp(7.5 \times 10^{-9} E_3)$$

and

$$\frac{\beta_N}{\alpha_N} = \begin{cases} 1 - \frac{1}{2} \exp\left(-C\right), & C \ge 0\\ \frac{1}{2} \exp C, & C < 0 \end{cases}$$



Fig. 1. Properties of  $\alpha_N$  and  $\beta_N/\alpha_N$  as functions of  $S_1 - S_L$  at  $E_3 = 0.0$  V m<sup>-1</sup>. The three curves of  $\alpha_N$  correspond to three different depoling rates: top curve corresponds to fastest depoling rate, middle curve corresponds to intermediate depoling rate and bottom curve corresponds to slowest depoling rate.



Fig. 2. Properties of  $\alpha_N$  (corresponding to intermediate depoling rate) and  $\beta_N/\alpha_N$  as functions of  $S_1 - S_L$  at (i)  $E = 0.0 \text{ V m}^{-1}$ , (ii)  $E_3 = 1.5 \times 10^7 \text{ V m}^{-1}$ , and (iii)  $E_3 = 3.0 \times 10^7 \text{ V m}^{-1}$ .

where

$$C = -5(S_1 - S_L - B)/B.$$

It will be quite apparent that  $E_3$  is always positive, and, in view of the initial condition  $N(X_1, 0) = 1$ , neither eqns (17), (18) nor (19) is satisfied ahead of the shock. Therefore, it is not necessary to specify the properties of  $\alpha_N$  and  $\beta_N/\alpha_N$  for expansive strain from the poled

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state. Finally, the values of  $S_L$ ,  $S_P$  and  $D_P$  as determined experimentally are

$$S_1 = -8.600 \times 10^{-4}$$
,  $S_P = 1.857 \times 10^{-3}$ ,  $D_P = 0.3654 \,\mathrm{C \,m^{-2}}$ .

These values permit the determination of  $h_1$ ,  $h_3$  and k via eqns (14)-(16), and we have

$$h_1 = 7.036 \times 10^7 \text{ Pa}, \quad h_3 = -1.140 \times 10^8 \text{ Pa}, \quad k = 0.3350 \text{ C m}^{-2}.$$

The preceding material parameters, as specified, merit some comments. First, we note that the value of  $\alpha$ , which characterizes the time scale of dipole dynamics, may be assigned independently. This is as it should be, and permits its determination via the comparison of appropriate numerical results and experimental data. Second, the equilibrium depoled state is transversely isotropic. Denoting the parameters of the depoled state by the subscript D, we have, in particular

$$C_{11D} = C_{11} + \frac{\beta_{b11}}{\alpha} = 1.648 \times 10^{11} \text{ Pa}$$

$$C_{12D} = C_{12} + \frac{\beta_{b12}}{\alpha} = 7.494 \times 10^{10} \text{ Pa}$$

$$C_{13D} = C_{12} + \frac{\beta_{b13}}{\alpha} = 7.077 \times 10^{10} \text{ Pa}$$

$$C_{33D} = C_{11} + \frac{\beta_{b33}}{\alpha} = 1.518 \times 10^{11} \text{ Pa}.$$

These parameters should be compared to those of the virgin state which is, of course, isotropic.<sup>†</sup> Third, at the equilibrium poled state the elastic, piezoelectric and dielectric constants are precisely those given by Chen[5]. Finally, the material parameters are such that it exhibits elastic and piezoelectric relaxations, and dielectric creep. The physical justifications for these responses are due to the wave propagation experiments reported by Dick and Vorthman[6], and the electrical pulsing experiments reported by Bailey and Chen[7].

For the purposes of the current example, we consider the rectangular bar with dimensions

$$l_1 = 2.2 \times 10^{-2} \text{ m}, \quad l_2 = 3.0 \times 10^{-3} \text{ m}, \quad l_3 = 1.0 \times 10^{-2} \text{ m}$$

and we let the boundary condition  $T_1(0, t)$  be given by

$$T_1(0,t) = -1.5 \times 10^9 \,\mathrm{Pa}.$$

Our intent is to obtain the solutions of the boundary-initial value problem for three different depoling rates due to strain by considering the field dependent counterparts of the three curves of  $\alpha_N$  given in Fig. 1, and three values of external resistance. We exhibit some of the essential features of these solutions so as to demonstrate the nature of the responses of the normal mode experiment.

In Fig. 3 we illustrate the resulting dipole alignment N as functions of position for the three depoling rates due to strain. Clearly, changes in dipole alignment become more abrupt as depoling rate increases. Figure 4 shows the corresponding profiles of the stress component  $T_1$ . Notice that the stress profiles are also affected by the depoling rates. In particular, the two-wave structure, most clearly exhibited by the profiles corresponding to the fastest depoling rate, is substantiated by the experimental results of Dick and Vorthman[6] who

†Cf. Chen[5].



Fig. 3. Dipole alignment as function of position at three different times. Top curves correspond to slowest depoling rate, middle curves correspond to intermediate depoling rate, and bottom curves correspond to fastest depoling rate. The resistance of the external circuit is  $10^6 \Omega$ . Note that changes in dipole alignment are small at each depoling rate; they are, however, quite noticeable among the different rates.



Fig. 4. Stress component  $T_1$  as function of position at three different times. Top curves correspond to slowest depoling rate, middle curves correspond to intermediate depoling rate, and bottom curves correspond to fastest depoling rate. The resistance of the external circuit is  $10^4 \Omega$ .

consider the depoling of PZT95/5 in the normal mode experiment.<sup>†</sup> Notice also that the stress component  $T_1$  is tensile ahead of the shock. This is due to the presence of the electric field component  $E_3$  and conventional piezoelectric coupling. In Fig. 5, we exhibit the profiles of the stress components  $T_1$ ,  $T_2$  and  $T_3$  corresponding to the fastest depoling rate. Ahead of the shock  $T_1$  and  $T_2$  are equal, and  $T_3$  is compressive.

†Virgin or thermally depoled PZT95/5 does not exhibit two-wave structure under otherwise identical conditions.



Fig. 5. Stress components  $T_1$ ,  $T_2$  and  $T_3$  as functions of position corresponding to fastest depoling rate. The resistance of the external circuit is  $10^4 \Omega$ .



Fig. 6. Stress components  $T_1$ ,  $T_2$  and  $T_3$  ahead of the shock as functions of time: (i) slowest depoling rate, (ii) intermediate depoling rate, and (iii) fastest depoling rate. The resistance of the external circuit is  $10^4 \Omega$ .

The nature of the stress due to conventional piezoelectric coupling is more clearly illustrated in Fig. 6 as a function of time. Notice that the rise time of the stress components decreases as depoling rate increases. The magnitudes of the stress components depend, of course, on the magnitude of the electric field component  $E_3$  which, in turn, depends on the value of the external resistance. In Fig. 7 we exhibit graphically the solutions of the electric field component  $E_3$  and the stress components  $T_1$  and  $T_2$  ahead of the shock as functions of time for three values of external resistance. Notice that the magnitudes of these quantities increase quite markedly for higher values of external resistance. Similar results are valid for the stress component  $T_3$ ; it is, however, compressive.



Fig. 7. Electric field component  $E_3$  and stress components  $T_1$  and  $T_2$  ahead of the shock as functions of time: (i)  $10^3 \Omega$ , (ii)  $10^4 \Omega$ , and (iii)  $10^5 \Omega$ . These results correspond to intermediate depoling rate.

#### 5. CLOSURE

The preceding example illustrates the complexities of the responses of the normal mode experiment. It does, however, lead to certain interesting conjectures. The stress components are compressive behind the shock. Ahead of the shock  $T_1$  and  $T_2$  are tensile, and  $T_3$  is compressive. We may, therefore, offer two conjectures as to possible modes of failure, resulting in the diminution of electrical output. These conjectures need not be mutually exclusive, however.

First, for the situation of rapid depoling and high external resistance the magnitude of  $T_1$  ahead of the shock is large and rises very rapidly; the magnitude of the gradient of  $T_1$  behind the shock is also large. Failure may, therefore, occur in the region around the shock because of the significant stress differential across it. We know that for ceramics whose properties smooth the wave profile and/or for low external resistance failure is less apt to occur. We suspect that this mode of failure will occur at early times.

Second, for the situation of high external resistance the state of piezoelectric stress ahead of the shock is quite complex with  $T_1$  and  $T_2$  being tensile and  $T_3$  being compressive. This complex state of stress may cause failure. If, in addition, the ceramic depoles rapidly, then we suspect failure will occur near certain weaknesses of the bar, which is liable to happen at any time.

In closing, we note that for ceramics which degrade the wave profile, depoling occurs less rapidly. The first mode of failure is, therefore, less likely, and the second mode of failure may occur at later times.

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#### REFERENCES

- 1. J. E. Besancon, J. David and J. Videl, Ferroelectric transducers. In Proceedings of the Conference on Megagauss Magnetic Field Generation by Explosives and Related Experiments, Frascati, Italy, 21-23 Sept., 1985. Euratom, Brussels (1966).
- P. J. Chen and P. S. Peercy, One dimensional dynamic electromechanical constitutive relations of ferroelectric materials. Acta Mechanica 31, 231-241 (1979).
- P. J. Chen, Three dimensional dynamic electromechanical constitutive relations for ferroelectric materials. Int. J. Solids Structures 16, 1059-1067 (1980).
- 4. P. B. Bailey and P. J. Chen, An accurate explicit finite difference algorithm for shocks in non-linear wave propagation-one dimension. *Wave Motion* 6, 279-287 (1984).
- 5. P. J. Chen, Three dimensional constitutive relations for ferroelectric materials in the presence of quasi-static domain switching. Acta Mechanica 48, 31-42 (1983).

- 6. J. J. Dick and J. E. Vorthman, Effect of electrical state on mechanical and electrical response of a ferroelectric
- ceramic PZT95/5 to impact loading. J. Appl. Phys. 49, 2494–2948 (1978).
  P. B. Bailey and P. J. Chen, Transient electromechanical responses of ferroelectric ceramics to impulsive electric fields. Int. J. Solids Structures 17, 471–478 (1981).