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NORMAL MODE RESPONSES OF LINEAR PIEZOELECTRIC MATERIALS WITH HEXAGONAL SYMMETRY

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Abstract—We consider in this paper the dynamic electromechanical responses of linear piezoelectric materials with hexagonal symmetry in the normal mode configuration. In particular, we formulate the coupled transient problem and obtain numerical results to illustrate the nature of the electrical outputs of rectangular specimens of these materials subjected to time dependent mechanical boundary loads.

1. INTRODUCTION

In this paper we consider the dynamic coupled electromechanical responses of linear piezoelectric materials which have the symmetry of a hexagonal crystal in class C_{6v}. Such a material has five independent elastic constants, three independent piezoelectric constants, and two independent dielectric constants. Hence rather complex coupling phenomena may occur depending on the conditions of the problem and the nature of the external electrical circuit. Here, we consider a particular problem which is consistent with the conditions of the normal or transverse mode experiment[1], and the boundary-initial conditions are such that the mechanical problem is one dimensional. As we shall see, our results illustrate clearly the nature of the electromechanical interaction occurring in the normal mode experiment.

Our motivation for this study is that polarized ferroelectric ceramics effectively have the symmetry of a hexagonal crystal. In addition to being piezoelectric, ferroelectric ceramics also exhibit rate dependent effects when depolarization occurs under the action of high stress loadings. Hence the constitutive relations which we adopt do not adequately describe their responses in the latter situation, but we feel that our results do give excellent qualitative insight regarding the solution of the problem when rate dependent effects are included. Further, a special case of our results holds for the situation when a ferroelectric ceramic undergoes complete depolarization immediately behind the shock front.

2. BASIC EQUATIONS

The constitutive relations of a linear piezoelectric material are, in general,

$$T_{ij} = \mathscr{C}^E_{ijkl} S_{kl} - e_{kij} E_k, \qquad D_i = e_{ijk} S_{jk} + \epsilon^S_{ij} E_j, \tag{2.1}$$

where T_{ij} is the stress, S_{ij} the strain, E_i the electric field, and D_i the electrical displacement. The strain is defined by the relation

$$S_{ij} = \tfrac{1}{2}(u_{i,j} + u_{j,i}) \tag{2.2}$$

with u_i being the mechanical displacement. In (2.1) $\mathscr{C}^E_{ijkl}$ is the elastic constant, e_{ijk} the piezoelectric constant, and ϵ^S_{ij} the permittivity. The appropriate field equations are balance of linear momentum

$$T_{ij,i} = \rho \ddot{u}_j, \tag{2.3}$$

where ρ is the reference mass density, and Gauss' law

$$D_{i,i} = 0. \tag{2.4}$$

Clearly, the field equations (2.3) and (2.4) and the constitutive relations (2.1) with the strain-displacement relations (2.2) yield a system of equations for the determination of the mechanical displacement u_i and the electric field E_i which is given by the gradient of the electric potential φ in that it obeys the relation

$$\operatorname{curl} \boldsymbol{E} = \boldsymbol{O}. \tag{2.5}$$

For a hexagonal crystal, the constitutive relations (2.1) with (2.2) reduces to[2]

$$\begin{aligned}
T_{11} &= \mathscr{C}^E_{1111}u_{1,1} + \mathscr{C}^E_{1122}u_{2,2} + \mathscr{C}^E_{1133}u_{3,3} - e_{311}E_3,\\
T_{22} &= \mathscr{C}^E_{1122}u_{1,1} + \mathscr{C}^E_{1111}u_{2,2} + \mathscr{C}^E_{1133}u_{3,3} - e_{311}E_3,\\
T_{33} &= \mathscr{C}^E_{1133}u_{1,1} + \mathscr{C}^E_{1133}u_{2,2} + \mathscr{C}^E_{3333}u_{3,3} - e_{333}E_3,\\
T_{12} &= T_{21} = \tfrac{1}{2}(\mathscr{C}^E_{1111} - \mathscr{C}^E_{1122})(u_{1,2} + u_{2,1}),\\
T_{23} &= T_{32} = \mathscr{C}^E_{2323}(u_{2,3} + u_{3,2}) - e_{113}E_2,\\
T_{13} &= T_{31} = \mathscr{C}^E_{2323}(u_{1,3} + u_{3,1}) - e_{113}E_1,
\end{aligned} \tag{2.6}$$

and

$$\begin{aligned}
D_1 &= e_{113}(u_{1,3} + u_{3,1}) + \epsilon^S_{11}E_1,\\
D_2 &= e_{113}(u_{2,3} + u_{3,2}) + \epsilon^S_{11}E_2,\\
D_3 &= e_{311}u_{1,1} + e_{311}u_{2,2} + e_{333}u_{3,3} + \epsilon^S_{33}E_3.
\end{aligned} \tag{2.7}$$

Formulae (2.6) and (2.7) indicate that a hexagonal crystal has 5 elastic constants, 3 piezoelectric constants and 2 dielectric constants. A poled ferroelectric ceramic with x_3 being the poling direction effectively has the symmetry of a hexagonal crystal. However, poled ferroelectric ceramics also exhibit rate dependent effects when depolarization occurs under the action of high stress loadings so that in this situation (2.6) and (2.7) do not fully describe their responses[3]. In any case we shall consider in the sequel the consequences of (2.6) and (2.7) within the context of the normal or transverse mode experiment. We believe that our results will give excellent qualitative insight with regard to the problem when the rate dependent effects are included.

3. THE NORMAL MODE EXPERIMENT AND THE GOVERNING EQUATIONS

Let us first consider the conditions of the normal or transverse mode experiment whose geometrical configuration is illustrated graphically in Fig. 1. In this experiment conducting electrodes are deposited on the x_3 faces of a polarized ferroelectric ceramic bar with rectangular cross section. The electrodes are connected via a resistor, inductor and/or capacitor. Time dependent loads are then applied at the $x_2 = 0$ face. During the course of the experiment

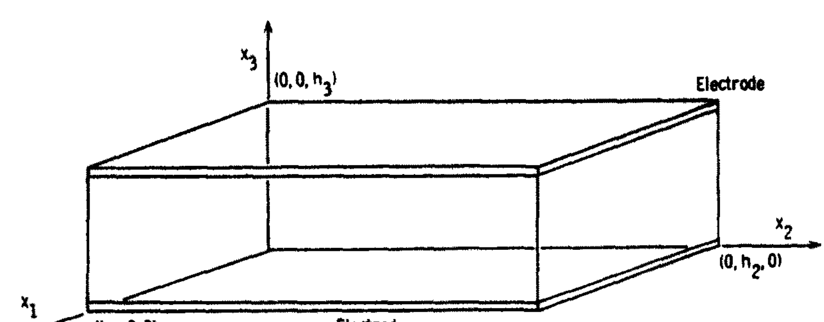

Fig. 1. Geometry of the problem.

the voltage drop across the external circuit element is recorded. This voltage drop is a manifestation of the electromechanical interaction occurring in the ceramic.

In order to capture the principle features of the problem and to simplify matters, we assume that

$$\begin{aligned} u_1 &= u_1(0, x_2, x_3, t) = u_1(h_1, x_2, x_3, t) = 0, \\ u_3 &= u_3(x_1, x_2, 0, t) = u_3(x_1, x_2, h_3, t) = 0. \end{aligned} \tag{3.1}$$

The constraints (3.1) necessarily imply that the motion is one dimensional and the only nonzero component of the mechanical displacement is u_2 such that

$$\begin{aligned} u_2 &= u_2(x_1, x_2, x_3, t) \\ &= u_2(x_2, t) \end{aligned} \tag{3.2}$$

for all (x_1, x_3). In view of $(3.2)_2$ we see that the constitutive relations (2.6) of the stress components become

$$\begin{aligned} T_{11} &= \mathscr{C}^E_{1122} u_{2,2} - e_{311} E_3, \\ T_{22} &= \mathscr{C}^E_{1111} u_{2,2} - e_{311} E_3, \\ T_{33} &= \mathscr{C}^E_{1133} u_{2,2} - e_{333} E_3, \\ T_{12} &= T_{21} = 0, \\ T_{23} &= T_{32} = -e_{113} E_2, \\ T_{13} &= T_{31} = -e_{113} E_1, \end{aligned} \tag{3.3}$$

and the constitutive relations (2.7) of the electrical displacement components reduces to

$$\begin{aligned} D_1 &= \epsilon^S_{11} E_1, \\ D_2 &= \epsilon^S_{11} E_2, \\ D_3 &= e_{311} u_{2,2} + \epsilon^S_{33} E_3. \end{aligned} \tag{3.4}$$

The symmetry of the problem also dictates that the electric field E_i can depend at most on (x_2, t) independent of (x_1, x_3). Now, Gauss' law (2.4) with $(3.2)_2$ and (3.4) implies that E_2 is independent of x_2; and, since $(x_1, x_2, 0)$ and (x_1, x_2, h_3) are equipotential surfaces, E_3 is also independent of x_2 and is given by

$$E_3 = E_3(t). \tag{3.5}$$

We are now in the position to derive the governing equations of the coupled dynamic problem. It follows directly from (2.3), (3.2), (3.3) and (3.5) that

$$\mathscr{C}^E_{1111} \frac{\partial^2 u_2}{\partial x_2^{\,2}} = \rho \ddot{u}_2. \tag{3.6}$$

Formula (3.6) is, of course, the usual wave equation. However, its solution need not be straightforward because its boundary conditions depend, in general, on E_3 (consider, for instance, the condition $T_{22} = 0$ at $x_2 = h_2$). This necessitates the derivation of the governing equation of E_3. As we shall see, this equation depends, in particular, on the nature of the external circuit.

To begin with, let us refer to the Gaussian element as illustrated in Fig. 2, and consider the global form of Gauss' law, viz.,

$$Q = \oint_A \boldsymbol{D} \cdot \boldsymbol{n} \, \mathrm{d}A, \tag{3.7}$$

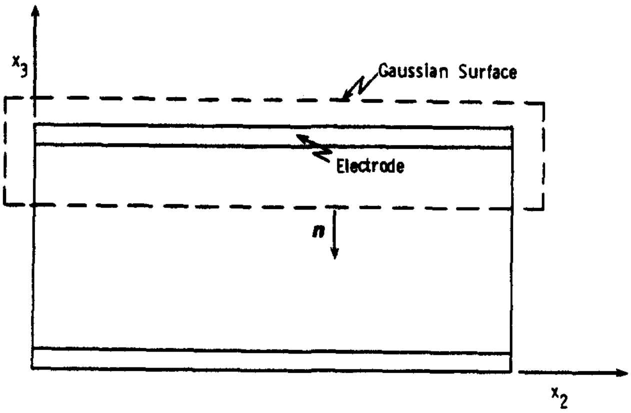

Fig. 2. Projection of the Gaussian surface on the x_2, x_3-plane.

where Q is the total free charge within the closed surface A with outward unit normal n. It follows directly from (3.7) that for the Gaussian element of interest, we have

$$Q = -\int_0^{h_1}\int_0^{h_2} D_3\, dx_1\, dx_2. \tag{3.8}$$

Here Q is the total free charge of the electrode. The current i in the external circuit is, of course, given by

$$i = -\frac{dQ}{dt}. \tag{3.9}$$

Hence, formula (3.8) with $(3.2)_2$, $(3.4)_3$, (3.5) and (3.9) yields

$$h_1 h_2 \epsilon_{33}^{S} \frac{dE_3}{dt} - i = -h_1 e_{311} \frac{d}{dt}\int_0^{h_2} u_{2,2}\, dx_2. \tag{3.10}$$

Resistive external circuit

When the external circuit consists of a resistor with resistance R, the voltage drop $\mathcal{V}$ across it is given by

$$\mathcal{V} = iR.$$

But this voltage drop is equal to the voltage drop across the electrodes. Hence, we have

$$iR = -h_3 E_3. \tag{3.11}$$

Substituting (3.11) into (3.10) yields the equation

$$h_1 h_2 \epsilon_{33}^{S} \frac{dE_3}{dt} + \frac{h_3}{R} E_3 = -h_1 e_{311} \frac{d}{dt}\int_0^{h_2} u_{2,2}\, dx_2 \tag{3.12}$$

for the determination of E_3. Notice that this equation depends on the nature of the mechanical disturbance; hence simultaneous solution of (3.6) and (3.12) is necessary.

Inductive external circuit

For the case when the external circuit is an inductor with inductance L, we have

$$\mathcal{V} = L\frac{di}{dt},$$

and

$$L\frac{\mathrm{d}i}{\mathrm{d}t} = -h_3E_3. \tag{3.13}$$

Formulae (3.10) and (3.13) yield

$$h_1h_2\epsilon_{33}^S\frac{\mathrm{d}^2E_3}{\mathrm{d}t^2} + \frac{h_3}{L}E_3 = -h_1e_{311}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\int_0^{h_2} u_{2,2}\,\mathrm{d}x_2. \tag{3.14}$$

Capacitative external circuit

For a capacitative external circuit with capacitance C, we have

$$\mathcal{V} = \frac{1}{C}\int_0^t i(\tau)\,\mathrm{d}\tau,$$

and

$$\frac{1}{C}\int_0^t i(\tau)\,\mathrm{d}\tau = -h_3E_3. \tag{3.15}$$

In this instance, E_3 is given by the simple formula

$$E_3 = -\frac{h_1e_{311}}{h_1h_2\epsilon_{33}^S + h_3C}\int_0^{h_2} u_{2,2}\,\mathrm{d}x_2. \tag{3.16}$$

It is clear from the preceding analyses that we may also derive the governing equation of E_3 for more complex circuits. In these instances we first derive via Kirchoff's law the circuit equation for the current i in terms of E_3, and the solution of the problem entails the simultaneous solution of (3.6), (3.10) and the circuit equation. Since the procedure is quite apparent, we will not dwell on this matter. Instead, we shall consider, among other things, certain interesting implications of (3.12) in the next section.

4. MOTION CONTAINING A SHOCK

We now assume that the motion $(3.2)_2$ contains a shock moving with velocity

$$u_n = \frac{\mathrm{d}y}{\mathrm{d}t}, \tag{4.1}$$

where $x_2 = y(t)$ gives the position of the shock at time t. Across the shock u_2 is continuous, but

$$[\![\dot{u}_2]\!] \neq 0, \quad [\![u_{2,2}]\!] \neq 0, \tag{4.2}$$

where $[\![\cdot]\!]$ denotes the jump, i.e. $[\![f]\!] = f^- - f^+$ with $f^\mp = \lim_{x_2 \to y(t)^\mp} f(x_2, t)$.

Since the electric field is lamellar, it follows immediately that [4, Sec. 175]

$$[\![E_1]\!] = [\![E_3]\!] = 0, \quad [\![E_2]\!] \neq 0. \tag{4.3}$$

On the other hand, the electrical displacement is a solenoidal field, and we have [4, Sec. 175]

$$[\![D_2]\!] = 0, \quad [\![D_1]\!] \neq 0, \quad [\![D_3]\!] \neq 0. \tag{4.4}$$

In view of (4.3) and (4.4), we see that $(3.4)_{1,2}$ imply

$$\begin{aligned} D_1 = D_2 = 0, \\ E_1 = E_2 = 0, \end{aligned} \tag{4.5}$$

otherwise we would have a contradiction. Also, (3.4)$_3$, (4.3) and (4.4) yield

$$[D_3] = e_{311}[u_{2,2}], \tag{4.6}$$

which gives the jump in D_3 in terms of the jump in strain.

We now examine the implications of (3.12) when the motion contains a shock. It follows immediately from (3.12) that

$$h_1h_2\epsilon_{33}^S\frac{\mathrm{d}E_3}{\mathrm{d}t}+\frac{h_3}{R}E_3 = -h_1e_{311}u_n[u_{2,2}] - h_1e_{311}\int_0^{y(t)}\frac{\partial}{\partial t}u_{2,2}\,\mathrm{d}x_2 - h_1e_{311}\int_{y(t)}^{h_2}\frac{\partial}{\partial t}u_{2,2}\,\mathrm{d}x_2. \tag{4.7}$$

If the material is initially at rest in a homogeneous configuration and if the strain loading corresponds to a step function S so that

$$[u_{2,2}] = u_{2,2}^- = S, \tag{4.8}$$

then (4.7) has the reduced form

$$h_1h_2\epsilon_{33}^S\frac{\mathrm{d}E_3}{\mathrm{d}t}+\frac{h_3}{R}E_3 = -h_1e_{311}u_nS \tag{4.9}$$

for times less than wave front transit time. Formula (4.9) together with the initial condition $E_3(0)=0$ may be readily integrated, and we have the solution

$$E_3(t) = -\frac{Rh_1e_{311}u_n}{h_3}S\left\{1-\exp\left(-\frac{h_3}{Rh_1h_2\epsilon_{33}^S}t\right)\right\}. \tag{4.10}$$

Formula (4.10) indicates that $|E_3(t)|$ increases monotonically with time to the steady value

$$|E_3(\infty)| = \left|\frac{Rh_1e_{311}u_n}{h_3}S\right|, \tag{4.11}$$

and which depends, in particular, on the magnitude of the strain. Notice also that the rate of increase of $E_3(t)$ depends on the RC time constant of the circuit with $h_1h_2\epsilon_{33}^S/h_3$ being the capacitance of the specimen and which depends on its geometry.

It suffices to point out at this juncture that in the linear context an equation analogous to (4.9) is also valid in the limiting case when a polarized ceramic undergoes complete rapid depolarization immediately behind the shock regardless of the nature of the wave structure. In this situation ϵ_{33}^S is the equilibrium value, e_{311} is the instantaneous value and the strain S is identified as the shock strength and it may depend on time if the shock evolves as it propagates. Further, for times greater than the wave front transit time, we have the homogeneous equation

$$h_1h_2\epsilon_{33}^S\frac{\mathrm{d}E_3}{\mathrm{d}t}+\frac{h_3}{R}E_3 = 0, \tag{4.12}$$

so that the magnitude of the electric field decays exponentially from its value at transit time.

5. EXAMPLES WITH RESISTIVE EXTERNAL CIRCUIT

It would be interesting to consider certain solutions of the coupled problem for the case of a resistive external circuit and to illustrate, in particular, the influences of the boundary condition at $x_2 = h_2$ and the resistive load on the electrical response.

The material which we use in our sample problem is a ferroelectric ceramic called PZT 5H, and the appropriate properties relevant to our present considerations are [5]

$$\mathscr{C}_{1111}^E = 12.6\times10^{11}\,\text{dyne/cm}^2,$$

$$e_{311} = -6.5\times10^{-4}\,\text{coul/cm}^2,$$

$$\epsilon_{33}^S = 1.3\times10^{-10}\,\text{farad/cm},$$

$$\rho = 7.5\,\text{gm/cm}^3;$$

The geometrical dimensions of the specimen are taken to be

$$h_1 = 0.318\,\text{cm}, \quad h_2 = 2.22\,\text{cm}, \quad h_3 = 0.953\,\text{cm},$$

and the resistances of the external circuit are

$$R = 10{,}000\,\text{ohm},$$
$$R = 50{,}000\,\text{ohm}.$$

The coupled problem, namely (3.6) and (3.12), together with the initial conditions

$$u_2(x_2, 0) = 0, \quad \dot{u}_2(x_2, 0) = 0, \quad E_3(0) = 0$$

are solved numerically using a modification of the computer code WONDY IV for the following three cases [6]:

(i)

$$T_{22}(0, t) = 6.3 \times 10^9\,\text{dyne/cm}^2,$$
$$T_{22}(h_2, t) = 0;$$

(ii)

$$T_{22}(0, t) = \begin{cases} 4.67 \times 10^9\,\text{t dyne/cm}^2, & t < 1.35\,\mu\text{sec}, \\ 6.3 \times 10^9\,\text{dyne/cm}^2, & t > 1.35\,\mu\text{sec}, \end{cases}$$
$$T_{22}(h_2, t) = 0;$$

(iii)

$$T_{22}(0, t) = \begin{cases} 4.67 \times 10^9\,\text{t dyne/cm}^2, & t < 1.35\,\mu\text{sec}, \\ 6.3 \times 10^9\,\text{dyne/cm}^2, & t > 1.35\,\mu\text{sec}, \end{cases}$$
$$u_2(h_2, t) = 0.$$

In Fig. 3 we illustrative graphically the current, i.e. $i = -h_3E_3/R$, of cases (i) and (ii) for 3 wave front transit times. Note that the gradual initial rise of the current is due not only to the nature of the boundary condition at $x_2 = 0$ but also the RC time constant of the circuit. Also, the current begins to drop at approximately the first wave front transit time. This is a direct result of the stress free boundary condition at $x_2 = h_2$. It is also of interest to point out that because of electromechanical coupling and the stress free boundary condition a wave also

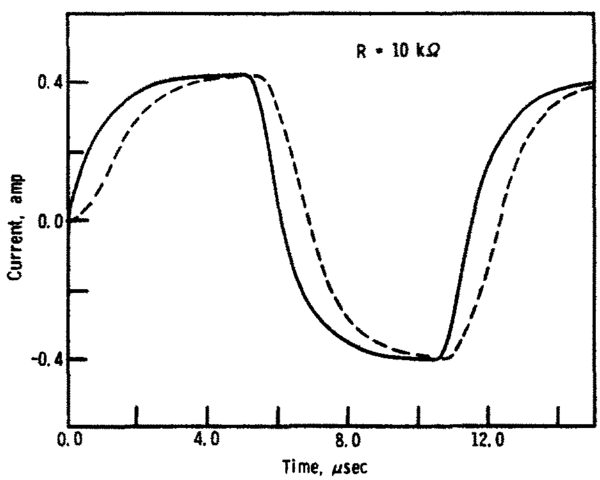

Fig. 3. Output current versus time for R = 10,000 ohm. Solid line refers to case (i), and dashed line refers to case (ii) (see text).

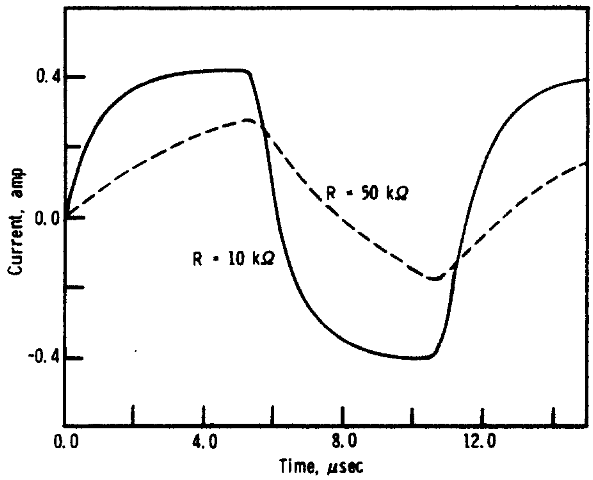

Fig. 4. Output current versus time for $R = 10{,}000$ ohm and $R = 50{,}000$ ohm for case (i) (see text).

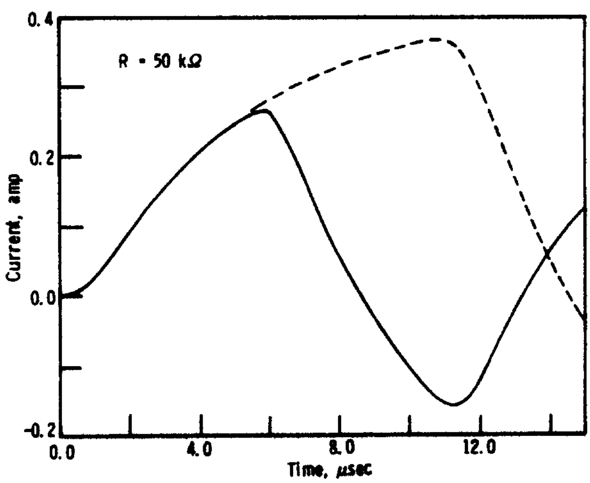

Fig. 5. Output current versus time for $R = 50{,}000$ ohm. Solid line refers to case (ii) and dashed line refers to case (iii) (see text).

originates at $x_2 = h_2$. Indeed, it follows from $(3.3)_2$ that

$$u_{2,2}(h_2, t) = \frac{e_{311}}{\mathscr{C}^E_{1111}} E_3(t).$$

In Fig. 4 we illustrate the influence of the external resistive load on the current for case (i). Clearly, these results show the influence of the RC time constant of the circuit on the nature of the electrical response.

In Fig. 5 we illustrate the corresponding results of cases (ii) and (iii). Note that in case (iii) the current continues to rise even after the first wave front transit time, and is quite different from that of case (ii). This is because of the fact that the boundary at $x_2 = h_2$ is held fixed. At approximately twice the wave front transit time the current begins to decrease.

The results which we have presented here are indicative of the complicated nature of electromechanical interactions, and the boundary conditions are of utmost importance in these considerations. Unfortunately, there are no definitive experimental results available for comparison with our predictions at this time.

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