A Phenomenological Constitutive Law for Ferroelastic Switching and a Resulting Asymptotic Crack Tip Solution

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ABSTRACT: An isothermal, multiaxial, phenomenological constitutive law for ferroelastic switching in polycrystalline ceramics is developed. The law is valid for unpoled ferroelectric ceramics loaded by mechanical stress but no electric fields or other materials in which permanent deformation accumulates by a similar volume conserving twinning mechanism. The initial switching behavior of the material is described using perfectly plastic $J_2$ flow theory. Unlike metal plasticity in which dislocations are generated by sources, deformation as a result of twinning is limited by a finite transformation strain. Hence, special yield surfaces and associated flow rules are introduced to account for plastic deformation in the two possible "lock-up" states of the material. To demonstrate the constitutive law we have analyzed the stress and displacement fields occurring in the lock-up regime asymptotically close to a crack tip under mode I loading.

1. INTRODUCTION

Ferroelastic behavior is defined by a material's ability to exhibit a spontaneous strain in its stress-strain behavior. This behavior is similar to the magnetization versus magnetic field response of ferromagnetic materials thus revealing the source of the term "ferro"elastic. In general, ferroelasticity can be exhibited in both the volumetric and deviatoric shape changes of the material, as for example in phase transformation toughened zirconia (McMeeking and Evans, 1982). However, even when a material does not sustain a phase transformation, ferroelasticity can occur in the deviatoric strains as a result of a lattice twinning process. This deviatoric type of twinning occurs in both ferroelectric ceramics and shape memory alloys. Hereafter we will focus only on volume conserving ferroelastic behavior and on the mechanisms responsible for ferroelasticity in ferroelectric ceramics.

Ferroelectric ceramics are commonly made from lead based perovskite oxides such as lead titanate and lead zirconate (Jaffe, Cook and Jaffe, 1971). Above the Curie temperature they are cubic and paraelectric. When they are cooled down through the Curie temperature, they undergo a displacive phase transformation, most commonly to a tetragonal structure (see Figure 1). Due to an asymmetric arrangement of ions in the crystal structure, the resulting unit cell possesses an electrical dipole moment which is aligned with the $c$-axis of the tetragonal crystallography. As a consequence, the lattice has a spontaneous electrical polarization and, compared with the cubic state, a spontaneous strain with the electrical polarization aligned with the maximum principal spontaneous strain. In this state, the lattice is also piezoelectric.

When a polycrystalline ferroelectric is cooled down through the Curie temperature without any applied electric field and transforms to tetragonal symmetry, different regions of each single crystal in the ceramic will polarize electrically in one of the six possible directions for tetragonality. These regions, called domains, are separated by domain walls and form a complicated pattern within the single crystal. It is likely that each single grain in the polycrystal has about equal volumes of each of the six possible domain types. As a consequence, the electrical polarization of the single crystal, defined as the average dipole moment per unit volume, is nearly zero. Furthermore, the average strain of the single crystal (with the cubic state as a datum) is nearly zero as well. Averaged over the entire polycrystalline sample, the electrical polarization and the strain are zero.

In the absence of a biasing electric field, the application of mechanical stress to an unpoled, polycrystalline ferroelectric sample will only create a macroscopic change in remanent strain but no change in polarization. These processes actually occur by domain wall motion, allowing favorably oriented domains to absorb the space occupied by unfavorably oriented ones (Jaffe, Cook and Jaffe, 1971). At the domain level polarization switching will occur, however approximately equal volumes of both positive and negative polarization will accumulate leaving the polycrystal unpolarized on average, see Figure 1. Consequently, the material can be treated as

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purely ferroelastic when the behavior is averaged over many domains.

It is of interest to model the multiaxial constitutive behavior of these materials such that stress and strain fields can be computed around structural features such as holes or crack tips. Some constitutive laws have been developed based on averaging over the response of single crystallites or single domains in the polycrystal (Chan and Hagood, 1994; Hwang, Lynch and McMeeking, 1995; Hwang et al., 1998; Hwang and McMeeking, 1999; Huber et al., 1999). These models postulate a simple behavior for individual crystallites and derive their fidelity to physical behavior by averaging over many hundreds of grains. This makes them computationally slow and often impractical for use in the simulation of the inhomogeneous response of the ferroelectric in a complex device. Therefore, a more efficient phenomenological constitutive law is desired which will lend itself to rapid computation in, say, finite element analysis. The development of such a law can benefit from guidance from the shape memory alloy literature, since twinning and detwinning in such materials is analogous to polarization switching in ferroelectrics (Brinson and Lammering, 1992; Sun and Hwang, 1993; Boyd and Lagoudas, 1996; Rengarajan, Krishna Kumar and Reddy, 1998).

In this paper, a phenomenological law for the ferroelastic switching behavior of unpoled ferroelectric ceramics below the Curie temperature will be developed. Although our thinking is guided by the phenomena that take place in tetragonal materials, we believe the resulting constitutive description is valid also for other symmetries such as rhombohedral and orthorhombic. In addition, some materials are composed of more than one phase, say tetragonal and rhombohedral together. This is the case with materials such as PZT and PLZT with compositions close to the morphotropic phase boundary, chosen for their attractive piezoelectric properties (Jaffe et al., 1971). Such materials can undergo a stress driven phase transformation involving a volume change. Apart from this phenomenon, which is not present in our model, we expect that our constitutive law is valid for these materials as well. It is likely, however, that our constitutive framework is most suitable for soft materials with compositions away from the morphotropic phase boundary. Although some modifications of our proposed law may be necessary to take the model into account with a particular material, we believe it provides a good basis for ferroelastic constitutive laws in general.

After a preliminary section describing the elastic response of the material we will develop a constitutive model for volume conserving ferroelastic switching which will include a simple method for handling the lock-up conditions. Thereafter, the mode I asymptotic crack tip solution for a material governed by the proposed constitutive law is given.

2. PRELIMINARIES

We consider the ceramic to be a homogenous continuum with properties representing the average state of strain of many grains within the polycrystal. Let the remanent, i.e., plastic strain be $e_{ij}^R$ where the unpoled state is the datum. The expression for the total strain, $e_{ij}$, is

$$e_{ij} = S_{ijkl} \sigma_{kl} + e_{ij}^R$$  \hspace{1cm} (2.1)$$

where $S_{ijkl}$ is the tensor of elastic compliances and $e_{ij}$ is the mechanical stress. The elastic compliances in Equation (2.1) depend on the remanent strain state. When is $e_{ij}^R$ is zero, $S_{ijkl}$ has an isotropic form given by

$$S_{ijkl} = L_{ijkl} = \frac{1}{4\mu} (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) - \frac{v}{2\mu(1+v)} \delta_{ij}\delta_{kl}$$  \hspace{1cm} (2.2)$$

where $\mu$ is the isotropic shear modulus, $v$ is the isotropic Poisson's ratio, $\delta_{ij}$ is the Kronecker delta, and $L_{ijkl}$ will be used to represent the isotropic elastic compliance tensor. When the material is strained by a large uniaxial tensile stress such that the remanent strain reaches its maximum, the elastic compliance becomes transversely isotropic about the tensile axis. If the tensile axis is $x_3$, the remanent strain is
\[ \varepsilon_R^e = \varepsilon_o (3\delta_{ij3} \delta_{j3} - \delta_{ij}) \]

Here \( \varepsilon_R^e \) is the magnitude of the maximum remanent strain that can be achieved in compression which will be explained in the next paragraph. When the material is in the maximum tensile remanent strain state the constitutive law is

\[ \varepsilon_R^e = \hat{S}_{ijkl} \sigma_{kl} + \varepsilon_o (3\delta_{ij3} \delta_{j3} - \delta_{ij}) \]

(2.3)

where \( \hat{S}_{ijkl} \) is elastic compliance tensor of the axially strained material. This elastic compliance tensor is transversely isotropic about the \( x_3 \) axis and has non-zero components, \( \hat{S}_{3333}, \hat{S}_{1111} = \hat{S}_{2222}, \hat{S}_{1113} = \hat{S}_{1233}, \hat{S}_{1122}, \hat{S}_{3313} = \hat{S}_{3233}, \hat{S}_{1212} = (\hat{S}_{1111} - \hat{S}_{1122})/2. \) Also note that \( \hat{S}_{ijkl} = \hat{S}_{ijkl} = \hat{S}_{ikjl} \) and \( \hat{S}_{ijkl} = \hat{S}_{jikl}. \)

Given the properties of the isotropic, unstrained material and the transversely isotropic, strained material we now propose a method to determine the linear properties of a material in an arbitrary remanent strain state. We define three new internal state variables, \( f_i, f_{II}, \) and \( f_{III}, \) hereafter referred to as coordinate volume fractions, such that

\[ f_i = \frac{1}{3} \left( \varepsilon_R^{e_i} + 1 \right) \]

(2.4a)

\[ f_{II} = \frac{1}{3} \left( \varepsilon_R^{e_{II}} + 1 \right) \]

(2.4b)

and

\[ f_{III} = \frac{1}{3} \left( \varepsilon_R^{e_{III}} + 1 \right) \]

(2.4c)

where \( \varepsilon_R^{e_i}, \varepsilon_R^{e_{II}}, \) and \( \varepsilon_R^{e_{III}} \) are the principal remanent strains. Here and throughout the paper we will not assume that \( \varepsilon_R^{e_i} \geq \varepsilon_R^{e_{II}} \geq \varepsilon_R^{e_{III}}. \) Using this restriction is not necessary and may make numerical implementation more difficult. Note that \( f_i, f_{II}, \) and \( f_{III} \) must all be greater than zero and the sum \( f_i + f_{II} + f_{III} = 1 \) since the trace of the remanent strain tensor is zero for volume conserving remanent strain states. Also note that the ratios of \( \varepsilon_R^{e_i}/\varepsilon_o \) can range from \(-1\) to \(2. \) The conditions that the coordinate volume fractions must be greater than zero correspond to lock-up states which will be discussed further in the next sections. Notice that there is an anisotropy in the remanent strains that can occur in tension versus compression. For example, when \( f_i = 1 \) and \( f_{II} = f_{III} = 0 \) the maximum principal strain is equal to \( 2\varepsilon_o, \) and in compression when \( f_i = 0 \) and \( f_{II} = f_{III} = 0.5 \) the minimum principal strain is equal to \(-\varepsilon_o. \)

This anisotropy is a true physical response and can be found in experiments (Fett et al., 1998) and self-consistent calculations (Huber et al., 1999), see Figure 2. Figure 2 is a plot of the stress-strain behavior for an unpoled, tetragonal ferroelectric calculated by the self-consistent model of Huber et al. (1999).

For a general state of remanent strain we would like to describe the elastic compliance as a function of the coordinate volume fractions. This task is likely to be best accomplished by some form of self-consistent or composite averaging theory. However, we do know that when \( f_i, f_{II}, f_{III} = (1, 0, 0) \) the elastic compliance must be given by \( \hat{S}_{ijkl} \) with the \( x_i \) direction as the axis of transverse symmetry and when \( f_i, f_{II}, f_{III} = (1/3, 1/3, 1/3) \) the elastic compliance must take its isotropic form, \( L_{ijkl}. \) Also, during axisymmetric straining along the \( x_i \) direction when \( f_i, f_{II}, f_{III} = (f_i, (1-f_i)/2, (1-f_i)/2) \) the compliance should retain transverse symmetry about the \( x_i \) axis. Therefore, we propose the following functional fit as a possibility for describing \( \hat{S}_{ijkl}. \)

\[ S_{ijkl} = (3L_{ijkl} - \hat{S}_{ijkl} - \hat{S}_{ijkl}^{II} + (2\hat{S}_{ijkl}^{II} + \hat{S}_{ijkl}^{III} - 3L_{ijkl}) f_i \]

\[ + (\hat{S}_{ijkl}^{II} + 2\hat{S}_{ijkl}^{III} - 3L_{ijkl}) f_{II} \]

if \( f_i, f_{II} > f_{III} \)

(2.5a)

\[ S_{ijkl} = (3L_{ijkl} - \hat{S}_{ijkl} - \hat{S}_{ijkl}^{III} + (2\hat{S}_{ijkl}^{III} + \hat{S}_{ijkl}^{II} - 3L_{ijkl}) f_i \]

\[ + (\hat{S}_{ijkl}^{III} + 2\hat{S}_{ijkl}^{II} - 3L_{ijkl}) f_{II} \]

if \( f_i, f_{II} < f_{III} \)

(2.5b)

\[ S_{ijkl} = (3L_{ijkl} - \hat{S}_{ijkl} - \hat{S}_{ijkl}^{II} + (2\hat{S}_{ijkl}^{II} + \hat{S}_{ijkl}^{III} - 3L_{ijkl}) f_i \]

\[ + (\hat{S}_{ijkl}^{II} + 2\hat{S}_{ijkl}^{III} - 3L_{ijkl}) f_{II} \]

if \( f_i, f_{III} > f_{II} \)

(2.5c)
where the elastic compliance tensors with the Roman numeral superscripts correspond to the transversely isotropic tensors introduced in Equation (2.3) with the axis of symmetry aligned in the principal strain direction corresponding to the superscripted Roman numeral. For a general remanent strain state the compliance tensor will be orthotropic with this description. Note that this function is not biased toward any of the coordinate volume fractions. This form is not a smooth function in volume fraction space but it is the simplest function that meets the criteria discussed in the previous paragraph. Again, physically based models could be implemented to describe the elastic compliance as a function of the coordinate volume fractions but that is not the purpose of this paper. Our primary goal is to described the evolution of remanent strain both before and during lock-up.

3. FERROELASTIC SWITCHING

As described in the introduction, upon cooling from above the Curie temperature a ferroelectric ceramic is on average isotropic. Furthermore, application of stress to an unpoled ferroelectric sample will not create any polarization in the sample. Therefore, in the absence of applied electric fields, the rate form of the constitutive behavior for an unpoled ferroelectric is

\[ \dot{\varepsilon}_{ij} = S_{ijkl} \dot{\sigma}_{kl} + \dot{S}_{ijkl} \sigma_{kl} + \dot{\varepsilon}_{ij}^R \]  \hspace{1cm} (3.1)

Note that the second term on the right hand side of Equation (3.1) will be zero if we assume that the elastic properties of the material remain isotropic during switching.

We now proceed to describe the remanent strain rates as a function of the current stress state. Note that ferroelastic switching is a volume conserving process and therefore, if we neglect changes in stored energy due to changes in elastic properties, hydrostatic stress does not contribute to the driving force for ferroelastic transformation. As for metal plasticity, the switching surface for ferroelastic materials can be described in terms of the invariants of the deviatoric stress (Hill, 1950). Furthermore, we will assume, as in $J_2$ flow plasticity, that the switching condition can be adequately described using only the second invariant of the deviatoric stress, $J_2$. We postulate that switching will occur when

\[ \sigma_\tau^2 = \frac{3}{2} s_{ij} s_{ij} = \sigma_o^2 \]  \hspace{1cm} (3.2)

where $\sigma_\tau$ is the tensile equivalent effective stress, $s_{ij}$ is the deviatoric stress given by

\[ s_{ij} = \sigma_{ij} - \frac{1}{3} \sigma_{kk} \delta_{ij} \]  \hspace{1cm} (3.3)

and $\sigma_o$ is the tensile switching (yield) stress which is a material property. If the effective stress is less than $\sigma_o$ then the material responds elastically with the remanent strain rates equal to zero. When the switching condition in Equation (3.2) is met we follow the prescription of $J_2$ flow plasticity and assume that the remanent strain rates are normal to the switching surface prescribed in Equation (3.2) such that

\[ \dot{\varepsilon}_{ij}^R = \lambda \frac{\partial \sigma_{ij}^2}{\partial \sigma_{ij}} = 3\lambda s_{ij} \]  \hspace{1cm} (3.4)

where $\lambda$ is a multiplier of undetermined magnitude selected kinematically within a given analysis.

Assuming that the material remains elastically isotropic during switching, i.e., $\dot{S}_{ijkl} = \dot{S}_{ijkl} = \dot{S}_{ijkl} = L_{ijkl}$, the rate form of this constitutive law can be written as

\[ \dot{s}_{ij} = 2\mu \dot{\varepsilon}_{ij} - 3\mu \frac{s_{ij} s_{kl}}{\sigma_o^2} \dot{\varepsilon}_{kl} \]  \hspace{1cm} (3.5)

For the deviatoric stress rates, where $\dot{e}_{ij} = \dot{e}_{ij} - (1/3)\delta_{ik}\dot{\delta}_{ij}$ is the total deviatoric strain and again $\mu$ is the shear modulus (see Hill, 1950 for details). The hydrostatic stress rate is then

\[ \dot{\sigma}_{kk} = \frac{2\mu(1+\nu)}{1-2\nu} \dot{\varepsilon}_{kk} \]  \hspace{1cm} (3.6)

A significant difference between ferroelastic switching and metal plasticity is that ferroelastic switching is essentially a twinning process which limits the amount of remanent strain that can accumulate. Unlike dislocations which are generated by sources and can cause ever increasing amounts of plastic slip, domain walls can only move through the crystal lattice once creating a finite amount of deformation. Once the domain walls have exhausted their switching potential the lattice “locks up” and further deformation occurs elastically.

Consider the internal state variables given in Equations (2.4a)–(c). We assume that lock-up occurs when one of the coordinate volume fractions is equal to zero. Hence, two different lock-up states can be attained, i.e., one or two of the coordinate volume fractions can be equal to zero. For the remainder of this discussion all indices for strains and stresses will be referred to the principal strain directions $1 = I$, $2 = II$ and $3 = III$. First consider the case where $f_1 = 1$ and $f_{II} = f_{III} = 0$. This situation corresponds to the case where a tensile bar has been loaded in the $I$ direction and the remanent strain is in the state $\epsilon_{ij}^R = \epsilon_{ij} \delta_{ij} - \delta_{ij}$. In this state, further application of tensile load in the $I$ direction causes the bar to deform elastically. The lock-up conditions given by $f_1 = 0$ and $f_{II} = f_{III} = 0$ imply that Equation (3.2) is no longer valid if the remanent strain rates derived from Equations (3.2) and (3.4) will cause $f_1$ or $f_{III}$ to be less than zero. In this state of tensile lock-up, continued change in remanent strain can only occur if the principal directions of the remanent strain rotate. This feature can be captured by defining the switching surface as
\[ \sigma_{y}^2 = 3(\sigma_{12}^2 + \sigma_{13}^2) = \sigma_{e}^2 \quad \text{when} \quad f_{III} = f_{III} = 0 \] (3.7)

Utilizing the normality condition yields the remanent strain rates as

\[ \varepsilon_{11}^R = \varepsilon_{22}^R = \varepsilon_{33}^R = \varepsilon_{23}^R = 0 \] (3.8a)

\[ \varepsilon_{12}^R = \varepsilon_{21}^R = 3\lambda\sigma_{12} \] (3.8b)

\[ \varepsilon_{13}^R = \varepsilon_{31}^R = 3\lambda\sigma_{13} \] (3.8c)

Note that Equations (3.7)–(3.8) are only valid if use of Equations (3.2) and (3.4) would imply that \( f_{II} \) or \( f_{III} \) would become less than zero. Otherwise Equations (3.2) and (3.4) are used. Also note that Equations (3.7)–(3.8) can be easily generalized to the cases where \( f_1 = f_{II} = 0 \) or \( f_1 = f_{III} = 0 \).

Again assuming that the material remains elastically isotropic during switching, the rate form of the constitutive law for this lock-up state can be written as

\[ \dot{\sigma}_{11} = 2\mu \dot{\varepsilon}_{11} + \frac{2\mu(1+\nu)}{(1-2\nu)} \varepsilon_{kk} \] (3.9a)

\[ \dot{\sigma}_{22} = 2\mu \dot{\varepsilon}_{22} + \frac{2\mu(1+\nu)}{(1-2\nu)} \varepsilon_{kk} \] (3.9b)

\[ \dot{\sigma}_{33} = 2\mu \dot{\varepsilon}_{33} + \frac{2\mu(1+\nu)}{(1-2\nu)} \varepsilon_{kk} \] (3.9c)

\[ \dot{\sigma}_{23} = 2\mu \dot{\varepsilon}_{23} \] (3.9d)

\[ \dot{\sigma}_{12} = 2\mu \dot{\varepsilon}_{12} + \frac{6\mu}{\sigma_o^2} \sigma_{12} (\sigma_{12} \dot{\varepsilon}_{12} + \sigma_{13} \dot{\varepsilon}_{13}) \] (3.9e)

\[ \dot{\sigma}_{13} = 2\mu \dot{\varepsilon}_{13} + \frac{6\mu}{\sigma_o^2} \sigma_{13} (\sigma_{12} \dot{\varepsilon}_{12} + \sigma_{13} \dot{\varepsilon}_{13}) \] (3.9f)

Figure 3 is a plot of the shear stress versus remanent shear strain behavior of the material after it has attained a state of tensile lock-up for three levels of applied axial stress in the initial lock-up direction. Notice that the principal strain direction rotates from parallel to the x direction to 45° degrees to this axis. Also note that there is a considerable amount of remanent deformation occurring at a relatively constant shear stress before a secondary lock-up state is attained.

Now consider the lock-up state where only one of the coordinate volume concentrations is equal to zero, i.e., \( f_{III} = 0 \) and \( f_1, f_{II} \neq 0 \). In this situation we must prevent \( f_{III} \) from becoming less than zero. We can accomplish this by defining the switching surface as

\[ \sigma_{e}^{n2} = \frac{3}{4}(\sigma_{11} - \sigma_{22})^2 + 3(\sigma_{12}^2 + \sigma_{23}^2 + \sigma_{31}^2) = \sigma_{0}^{2} \] (3.10)

when \( f_{III} = 0 \)

Then the remanent strain rates are

\[ \dot{\varepsilon}_{11}^R = \frac{3}{2} \lambda (\sigma_{11} - \sigma_{22}) \] (3.11a)

\[ \dot{\varepsilon}_{22}^R = \frac{3}{2} \lambda (\sigma_{22} - \sigma_{11}) \] (3.11b)

\[ \dot{\varepsilon}_{33}^R = 0 \] (3.11c)

\[ \dot{\varepsilon}_{12}^R = \dot{\varepsilon}_{21}^R = 3\lambda \sigma_{12} \] (3.11d)

\[ \dot{\varepsilon}_{13}^R = \dot{\varepsilon}_{31}^R = 3\lambda \sigma_{13} \] (3.11e)

\[ \dot{\varepsilon}_{23}^R = \dot{\varepsilon}_{32}^R = 3\lambda \sigma_{23} \] (3.11f)

Assuming that the material remains elastically isotropic during switching, the rate form of the constitutive law for this lock-up state can be written as

\[ \dot{\sigma}_{11} = \dot{\sigma}_{11}^R + \frac{3\mu(1+\nu)}{(1-2\nu)} \varepsilon_{kk} - \frac{1}{2} \dot{\sigma}_{33} \] (3.12a)

\[ \dot{\sigma}_{22} = \dot{\sigma}_{22}^R + \frac{3\mu(1+\nu)}{(1-2\nu)} \varepsilon_{kk} - \frac{1}{2} \dot{\sigma}_{33} \] (3.12b)

\[ \dot{\sigma}_{33} = 2\mu \dot{\varepsilon}_{33} + \frac{2\mu(1+\nu)}{(1-2\nu)} \varepsilon_{kk} \] (3.12c)

\[ \dot{\sigma}_{23} = \dot{\sigma}_{32}^R \] (3.12d)

\[ \dot{\sigma}_{13} = \dot{\sigma}_{31}^R \] (3.12e)

\[ \dot{\sigma}_{12} = \dot{\sigma}_{21}^R \] (3.12f)
where
\[ \dot{s}_{ij} = 2\mu \dot{e}_{ij}^* - 3\mu \frac{\sigma_{ij}^{\text{eff}}}{\sigma_0^2} \dot{e}_{ij}^* \]  
(3.13)

with
\[ s_{ij}^{\text{eff}} = \frac{1}{2}(\sigma_{ij} - \sigma_{kl} \delta_{ij}) \quad e_{ij}^{\text{eff}} = \frac{1}{2}(e_{ij} - e_{kl} \delta_{ij}) \]  
(3.14a)
\[ s_{ij}^{\text{eff}} = \frac{1}{2}(\sigma_{ij} - \sigma_{kl} \delta_{ij}) \quad e_{ij}^{\text{eff}} = \frac{1}{2}(e_{ij} - e_{kl} \delta_{ij}) \]  
(3.14b)
\[ s_{ij}^{\text{eff}} = 0 \quad e_{ij}^{\text{eff}} = 0 \]  
(3.14c)
\[ s_{ij}^{\text{eff}} = \sigma_{ij} \quad e_{ij}^{\text{eff}} = e_{ij} \]  
(3.14d)
\[ s_{ij}^{\text{eff}} = \sigma_{ij} \quad e_{ij}^{\text{eff}} = e_{ij} \]  
(3.14e)
\[ s_{ij}^{\text{eff}} = \sigma_{ij} \quad e_{ij}^{\text{eff}} = e_{ij} \]  
(3.14f)

Again, Equations (3.10)–(3.11) are only valid if use of Equations (3.2) and (3.4) would imply that \( f_{\text{II}} \leq 0 \). Otherwise Equations (3.2) and (3.4) are used. Also, Equations (3.10)–(3.11) can be generalized to the cases where \( f_1 \) or \( f_{\text{II}} \) equals zero.

Note once again that Equations (3.7)–(3.14) are referred to an orthogonal coordinate system aligned with the principal strain directions and that during remanent straining these directions may change. In order to refer to a fixed coordinate system one must utilize the appropriate tensor rotations on all stress and strain quantities during each increment of loading. Also recall that Equations (3.2)–(3.6) are always used first to predict the remanent strain increments but if a lock-up condition is violated then the appropriate lock-up form for the remanent strain rates must be used.

It may seem that Equations (3.7)–(3.14) were selected in an ad hoc manner to enforce the lock-up conditions. However, Equations (3.7)–(3.14) are derived from the assumption that remanent straining produces a characteristic amount of dissipation. Using Equations (3.2) and (3.4), and again neglecting changes in stored energy due to changes in elastic properties, the dissipation rate, \( \dot{w}_D \), can be written as
\[ \dot{w}_D = \sigma_j^{\text{eff}} \dot{e}_j^{\text{eff}} = 2\lambda \sigma_0^2 \dot{e}_j^{\text{eff}} \]  
(3.15)

where \( \dot{\varepsilon}_{ji}^{R} = \sqrt{\frac{2}{3}}e_{ji}^{R} \) is the tensile equivalent effective remanent strain rate. Then, by determining the allowable remanent strain rates associated with the two lock-up states described previously, it can be shown that Equations (3.7)–(3.8) and (3.10)–(3.11) each satisfy Equation (3.15) as well. In other words, if two material samples are subjected to different stress histories such that one sample locks up and the other does not, but both samples experience identical remanent strain histories, then the energies dissipated in each sample will be equal. Note that choices for the switching surfaces different from Equations (3.7) or (3.10) in the corresponding lock-up states would not produce this behavior.

A feature of ferroelastic switching that we have neglected in this constitutive law is the hardening that occurs as remanent deformation accumulates. One might propose to use an isotropic hardening law as is used for metal plasticity. However, the self-consistent calculations of Huber et al. (1999) (Figure 2) suggest that kinematic rather than isotropic hardening is required to best describe the hardening process. In fact, the mechanism which supports an isotropic hardening law, dislocation accumulation and interaction, does not occur in ferroelastic materials. The kinematic hardening effects are most likely due to constraint interactions between grains which are favorably oriented to switch under a given macroscopic applied stress state and those that are not. This interpretation is supported by the calculations of Huber et al. (1999), since in that work no hardening mechanism was implemented at the grain level but grain to grain constraint interactions were accounted for in an average/self-consistent fashion.

The significant feature that has been captured by this constitutive law is that when the material has achieved a lock-up state it is not prohibited from changing its remanent strain state completely, but rather only certain directions of deformation are forbidden. Therefore, even though the material is locked-up it retains some ability to deform remanently and this deformation can be described by some yield surface in stress space and a flow rule for the subsequent remanent strain rates. The yield surfaces and associated flow rules that we have chosen to describe the deformation in the two lock-up states are consistent with the assumption that remanent deformation proceeds at a characteristic rate of dissipation and at a characteristic level of effective stress which are not affected by the lock-up conditions. As such, the constitutive law is simple, yet contains the basic elements of appropriate ferroelastic behavior.

4. THE CRACK TIP IN A FERROELASTIC MATERIAL

Determination of the stresses and strains around a crack in a ferroelastic material is analogous to the solution for cracks in a plastic body with the added complicating feature of lock-up. The schematic in Figure 4 illustrates regions of constitutive behavior around a crack tip. In this section we will investigate the nature of the stress and strain fields in the region nearest to the crack tip, in the lock-up region.

In analyzing the crack tip we must first consider the process of deformation that the material ahead of the crack tip experiences. Initially, at very low loads the material will deform elastically. At some point the switching condition of Equation (3.2) will be met and the switching process will proceed. As further load is applied, one of the lock-up conditions will be met and ultimately the lock-up condition where
remnant strains only depend on $\theta$ then the associated stresses required to satisfy compatibility will also only depend on $\theta$ and will not be singular. As we will show for the Mode I case, the stresses and strains near the crack tip due to the applied loading are $O(r^{-1/2})$ while, as described above, the stresses due to the incompatible remanent strains are only $O(1)$. Therefore, it is appropriate to neglect the non-singular remanent contributions to the stress and strain when considering the asymptotic crack tip behavior. This argument is analogous to that used to derive the asymptotic stress and strain fields in a power-law hardening elastic-plastic material (Hutchinson, 1968).

Consider a crack with the $r$ and $\theta$ coordinate system centered on the crack tip and crack faces defined by $r \geq 0$ and $\theta = \pm \pi$. If we define the angle $\alpha$ to be the angle between the radial direction and the $m$ direction then

$$\alpha = \frac{1}{2} \arctan \left( \frac{2\sigma_{r\theta}}{\sigma_r - \sigma_{\theta\theta}} \right)$$

(4.2)

and care must be taken to choose the correct branch of the arc tangent function such that the $m$ direction is aligned with the maximum principal stress. Then the $m$ and $n$ directions are given by

$$m = \cos \alpha e_r + \sin \alpha e_\theta$$

(4.3a)

and

$$n = -\sin \alpha e_r + \cos \alpha e_\theta$$

(4.3b)

where $e_r$ and $e_\theta$ are unit vectors in the $r$ and $\theta$ directions respectively.

Use of the Airy stress function, $\Phi$, such that

$$\sigma_{rr} = \frac{1}{r} \frac{\partial \Phi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \Phi}{\partial \theta^2}$$

(4.4a)

$$\sigma_{r\theta} = \frac{\partial^2 \Phi}{\partial r \partial \theta}$$

(4.4b)

$$\sigma_{\theta\theta} = \frac{1}{r^2} \frac{\partial \Phi}{\partial \theta} - \frac{1}{r} \frac{\partial \Phi}{\partial r}$$

(4.4c)

allows us to satisfy mechanical equilibrium directly. If we assume that

$$\Phi = r^p \phi(\theta)$$

(4.5)

then this implies that $\sigma_{ij} = r^{p-2} \tilde{\sigma}_{ij}(\theta)$ and using Equation (4.1) we can write the strains as $\varepsilon_{ij} = r^{p-2} \tilde{\varepsilon}_{ij}(\theta)$ where the $\tilde{\cdot}$ signifies the theta dependence of the stress/strain components only. Then we can show that the infinitesimal
strain-displacement compatibility conditions result in the following ordinary differential equation in \( \theta \)

\[
\varepsilon_{rr}^{\prime} - 2(p-1)\varepsilon_{\theta\theta}^{\prime} + (p-1)(p-2)\varepsilon_{\theta\theta} - (p-2)\varepsilon_{rr} = 0 \quad (4.6)
\]

where the ' represents differentiation with respect to \( \theta \). Equations (4.1)–(4.5) can ultimately be used in Equation (4.6) to yield a governing ordinary differential equation for \( \Phi \).

The boundary conditions for a traction free crack are

\[
\sigma_{\theta\theta} = \sigma_{r\theta} = 0 \quad \text{for} \quad \theta = \pm \pi \quad (4.7)
\]

Due to the fact that the constitutive law, Equation (4.1), can be written as a complementary energy potential [see Ortiz, (1987)], which is a homogeneous function of degree two of the stress, and since it is assumed that a finite amount of elastic energy is stored at the crack tip, \( p \) will always be equal to 3/2, i.e., the stress and strain singularities go as \( r^{-1/2} \).

Surprisingly for the mode I loading scenario, where \( \sigma_{\theta\theta}(-\theta) = \sigma_{\theta\theta}(\theta) \), \( \sigma_{r\theta}(-\theta) = \sigma_{r\theta}(\theta) \) and \( \sigma_{r\theta}(-\theta) = -\sigma_{r\theta}(\theta) \), the isotropic mode I asymptotic solution for the stresses satisfies Equations (4.1)–(4.7). In other words

\[
\sigma_{rr} = \frac{K_1}{\sqrt{2\pi r}} \left( \frac{-\cos \frac{\theta}{2} + \cos \frac{\theta}{4}}{2} \right) \quad (4.8a)
\]

\[
\sigma_{\theta\theta} = \frac{K_1}{\sqrt{2\pi r}} \left( \frac{-\cos \frac{\theta}{2} + 3\cos \frac{\theta}{4}}{2} \right) \quad (4.8b)
\]

\[
\sigma_{r\theta} = \frac{K_1}{\sqrt{2\pi r}} \left( \frac{-\sin \frac{\theta}{2} + \sin \frac{\theta}{4}}{2} \right) \quad (4.8c)
\]

\[
\alpha = \begin{cases} 
\frac{\pi}{4} & \theta = 0 \\
\frac{\pi}{4} & -\pi \leq \theta < 0 \\
\frac{\pi}{4} & 0 < \theta \leq \pi 
\end{cases} \quad (4.9)
\]

Similar results were obtained by Hutchinson (1983) for materials undergoing linear creep-constrained grain boundary cavitation and by Ortiz (1987) for microcracking solid. The common feature in all of these models is that the anisotropic material compliance/viscosity is aligned with the principal stress direction.

Equation (4.1) and the strain displacement relations can be used to show that

\[
u_r = \frac{K_1 \sqrt{r}}{\sqrt{8\pi}} \cos \frac{\theta}{2} \quad (4.10a)
\]

\[
u_\theta = -\frac{K_1 \sqrt{r}}{\sqrt{8\pi}} \sin \frac{\theta}{2} \quad (4.10b)
\]

where

\[
B = 3S_{11} + 2S_{13} + 3S_{33} - (S_{11} - 2S_{13} + S_{33}) \cos \frac{\theta}{2} \quad (4.10c)
\]

with the + sign on the last term of Equation (4.10c) valid when \( -\pi \leq \theta < 0 \) and the - sign valid when \( 0 < \theta \leq \pi \). Then, a crack closure integral can be performed to determine the energy release rate, \( G \), as

\[
G = 33K_1^2 \quad (4.11)
\]

Note that the mode I case is special and that the isotropic mode II solution for the stresses does not satisfy Equations (4.1)–(4.7).

In this section we have determined the mode I asymptotic stress field near a crack tip in an unpoled ferroelectric material. In this case, though not written out explicitly, a governing differential equation for \( \Phi \), the Airy stress function, was obtained. The isotropic elasticity, mode I crack tip solution for the stresses satisfies the governing equation for \( \Phi \). However, this solution is only a piece of the ferroelastic fracture problem and further analysis using the constitutive law described in the first section of this paper is required to determine the relative sizes and shapes of the switching and lock-up zones depicted in Figure 4 and how they evolve as the crack grows.

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REFERENCES


