THEORETICAL MODELING OF SMALL-SCALE DOMAIN
SWITCHING AND FRACTURE OF FERROELECTRIC MATERIALS

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to the required standard

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Abstract

The intrinsic electromechanical properties and quick response to external excitations make ferroelectrics an ideal material for fabrication of sensors, actuators and adaptive (smart) structures. Ferroelectrics have been increasingly employed beyond the linear regime as characterized by linear piezoelectricity. Electric fields and forces required to achieve large actuation result in mechanical and electrical degradation. Understanding of coupled electromechanical behavior and fracture mechanics of ferroelectrics is very important to the reliability and efficient design of devices made out of them. Some problems related to fracture mechanics of ferroelectrics are investigated theoretically in this thesis.

A unique feature of ferroelectrics is their ability to rotate the direction of spontaneous polarization (i.e. domain switching) by 180° or non-180°, when subjected to a large electric field or stress. Domain switching is the major source of material non-linearity and has a significant influence on crack-tip electroelastic field. By examining the change of free energy before and after switching of an elliptic crystallite in a poled ferroelectric, a domain switching criterion which predicts the critical loading to trigger polarization switching is proposed for ferroelectric materials. This new criterion considers the interaction of the applied field with the switching strains and polarization and the change of electroelastic properties of the switched domain.

A theoretical model similar to transformation toughening of zirconia-containing ceramics is proposed to investigate the effects of small-scale domain switching at a crack tip on crack tip field intensity factors. The new domain-switching criterion is used to predict the switching zone around a crack tip. A fundamental solution for a crack interacting with stress-free transformation strains and electric field-free polarization is obtained by using the Leknitskii’s formalism. A Reuss-type approximation is proposed to model polycrystalline ferroelectrics. The influence of electromechanical loading and polar direction on apparent fracture toughness is numerically investigated for insulating and conducting cracks and qualitatively compared with available experiments.
The theoretical models are extended to analyze the electroelastic field at the tip of a closed insulating (or conducting) crack or an embedded electrode. The effect of domain switching on the near-tip field is examined. The tensile stress ahead of a closed crack tip may lead to crack growth, while the intensified stress at an electrode-ceramic interface may lead to segmentation cracks and electrode delamination as observed in experimental studies of multi-layer stack actuators.
Table of Contents

Abstract ........................................................................................................... ii
List of Tables ........................................................................................................ vi
List of Figures ......................................................................................................... vii
List of Symbols ...................................................................................................... xi
Acknowledgments ................................................................................................ xiv

1 Introduction ........................................................................................................ 1
  1.1 Active Materials .......................................................................................... 1
  1.2 Piezoelectricity ........................................................................................... 4
  1.3 Electrostriction ............................................................................................. 6
  1.4 Ferroelectricity ............................................................................................ 6
  1.5 Constitutive Behavior of Ferroelectric Ceramics ......................................... 9
  1.6 Fracture of Ferroelectric Materials ............................................................... 12
    1.6.1 Experimental Investigations ................................................................ 14
    1.6.2 Theoretical Investigations .................................................................... 17
      1.6.2.1 Linear piezoelectric crack model ...................................................... 17
      1.6.2.2 Fracture criterion ............................................................................ 21
      1.6.2.3 Domain switching and crack tip non-linear effects ...................... 21
  1.7 Scope of the Present Work .......................................................................... 23

2 A Theoretical Model For Domain Switching and Evolution ............................. 27
  2.1 Overview ..................................................................................................... 27
  2.2 Eshelby Tensor for Elliptic Inclusion ........................................................ 28
  2.3 Model for Polarization Switching ............................................................... 35
  2.4 Ferroelectric Domain Evolution ................................................................... 42
    2.4.1 180° Domain Nucleus ......................................................................... 45
List of Tables

Table 1.1 Material constants of poled piezoelectric ceramics ..................... 5
Table 3.1 Material constants of PZT-5H and PZT PIC-151 ............................ 81
Table 3.2 Total energy release rate of a conducting crack in PZT PIC-151 .......... 102
# List of Figures

| Figure 1.1 | Concept of a smart structure for vibration control | 1 |
| Figure 1.2 | Illustration of (a) direct and (b) converse piezoelectric effects | 2 |
| Figure 1.3 | Two types of piezoelectric bimorphs, (a) antiparallel polarization type and (b) parallel polarization type | 3 |
| Figure 1.4 | Multilayer piezoelectric ceramic actuator | 4 |
| Figure 1.5 | Electric polarization ($P$) versus electric field ($E$) curve for ferroelectric Materials | 7 |
| Figure 1.6 | Unit cell of lead zirconate titanate (PZT), (a) below and (b) above the Curie temperature | 7 |
| Figure 1.7 | Paraelectric and ferroelectric phases of barium titanate ($\text{BaTiO}_3$) with the direction denotes the spontaneous polarization, $P_s$ | 8 |
| Figure 1.8 | Poling of ferroelectric ceramics. $E_p$ denotes the poling electric field | 9 |
| Figure 1.9 | Variation of (a) electric polarization with electric field, (b) strain with electric field and (c) stress with strain | 10 |
| Figure 1.10 | Unit cell configuration for (a) $180^\circ$, and (b) $90^\circ$ ferroelectric domain switching | 11 |
| Figure 1.11 | Unit cell configuration for $90^\circ$ ferroelastic domain switching | 12 |
| Figure 1.12 | Crack configuration in a piezoelectric multilayer actuator [22] | 13 |
| Figure 1.13 | Effect of electric field on the crack length of, (a) PZT-8 [27] and (b) PZT-4 [28] | 15 |
| Figure 1.14 | Effect of electric field on the crack length of PZT EC61, (a) negative field and (b) positive field [29] | 15 |
| Figure 1.15 | Effect of electric field on fracture load of, (a) PZT-4 [31] and PZT-841 [32] | 16 |
| Figure 1.16 | SEM morphology of the etched surface of poled PLZT ceramics, (a) without and (b) with applied lateral electric field. (b) is showing $90^\circ$ |
domain switching near a crack tip [49] ........................................ 22

Figure 2.1 Piezoelectric elliptic inclusion subjected to eigenstrains $\varepsilon^*$ and eigen electric displacement $D^*$ ............................................................... 29

Figure 2.2 $180^\circ$ domain nucleus in $\text{BaTiO}_3$ single crystal ................. 45

Figure 2.3 Free energy contours $(G/2\pi\varepsilon^0 A)$ for a $180^\circ$ domain nucleus, (a) isotropic, uncoupled solution, (b) anisotropic, coupled solution ......................... 47

Figure 2.4 Evolution of a $180^\circ$ elliptic domain nucleus with time, (a) the semi-axis $a$, and (b) the semi-axis $b$ ............................................................... 48

Figure 2.5 $90^\circ$ domain nucleus in $\text{BaTiO}_3$ single crystal ....................... 50

Figure 2.6 Free energy contours $(G/2\pi\varepsilon^0 A)$ for a $90^\circ$ domain nucleus, (a) isotropic, uncoupled solution, (b) anisotropic, coupled solution ......................... 52

Figure 2.7 Evolution of a $90^\circ$ elliptic domain nucleus with time, (a) the semi-axis $a$, and (b) the semi-axis $b$ ............................................................... 53

Figure 2.8 Stress $\sigma_{22}$ ahead of the right major axial apex of an elliptic void, (a) without and (b) with the effects of remanent strains and remanent polarization ............................................................... 56

Figure 2.9 Electric field $E_2$ ahead of the right major axial apex of an elliptic void, (a) without and (b) with the effects of remanent strains and remanent polarization ............................................................... 57

Figure 2.10 Effect of the slenderness of an elliptic vacuum void on the energy release rate $J$, (a) without and (b) with the effects of remanent strains and remanent polarization ........................................................................ 62

Figure 2.11 Effect of the dielectric property of an elliptic void on the energy release rate $J$, (a) without and (b) with the effects of remanent strains and remanent polarization ........................................................................ 63

Figure 3.1 An insulating (or a conducting) crack in a piezoelectric solid subjected to remote electromechanical loading ........................................... 65

Figure 3.2 Small-scale domain switching zone around the tip of an insulating (or a conducting) crack ................................................................. 66
Figure 3.3 90° and 180° domain switching ........................................... 69
Figure 3.4 A semi-infinite crack interacting with a circular spot that has undergone stress-free transformation strains $\varepsilon_i^*$ and electric field-free polarization $D_i^*$ .......................................................... 71
Figure 3.5 Variations of $\alpha_i$ and $\alpha_l$ with the poling angle $\phi$ for insulating and conducting cracks ................................................................. 83
Figure 3.6 Switching zones induced by an electric field, (b) crack-tip stress intensity factor due to an electric field for different initial poling directions ...... 86
Figure 3.7 Switching zones induced by an applied stress field ($\phi = 0^\circ$ and $90^\circ$), (b) crack-tip stress intensity factor due to applied for different initial poling directions ................................................................. 88
Figure 3.8 Switching zones induced by combined loading for case I, (b) switching zones due to combined loading for case II ........................................... 90,
Figure 3.9 Crack-tip stress intensity factors under combined loading for different initial poling direction $\phi$ ................................................................. 92
Figure 3.10 Crack-tip stress intensity factors under combined loading for different electric loading levels ................................................................. 92
Figure 3.11 Switching zones induced by an electric field, (b) crack-tip stress intensity factor due to an electric field for different poling directions $\phi$ ............ 95
Figure 3.12 Switching zones induced by an applied stress field, (b) crack-tip stress intensity factor due to an applied stress field for different poling directions $\phi$ ................................................................. 96
Figure 3.13 Switching zones induced by combined loading for different electric loading levels, (a) $\alpha = 0.5$, (b) $\alpha = 1.0$ ................................................. 98
Figure 3.14 Crack-tip stress intensity factor under combined loading for different poling directions $\phi$ ................................................................. 99
Figure 3.15 Crack-tip stress intensity factors under combined loading for different electric loading levels ................................................................. 100
Figure 3.16 Variation of the applied stress intensity factor with the electric field
intensity factor for PZT PIC-151 [34] ................................................. 101

Figure 3.17 Switching zones around the tip of a closed insulating (conducting) crack under a pure electric field loading ......................................................... 103

Figure 3.18 Model I stress intensity factor at the tip of a closed insulating crack due to an electric field ............................................................. 104

Figure 3.19 Model I stress intensity factor at the tip of a closed conducting crack due to an electric field ............................................................. 105

Figure 4.1 Simplified model for an embedded electrode tip in a multilayer actuator .......................................................................................... 108

Figure 4.2 Electrode interacting with a circular spot with eigenstrains and eigen Polarization ........................................................................... 111

Figure 4.3 Localized switching zone around an embedded electrode tip ............ 115

Figure 4.4 Variation of normal stress $\sigma_{11}$ with polar angle $\theta$ ..................... 116

Figure 4.5 Variation of normal stress $\sigma_{22}$ with polar angle $\theta$ ..................... 117

Figure 4.6 Variation of shear stress $\sigma_{12}$ with polar angle $\theta$ ..................... 118

Figure 4.7 Variation of hoop stress $\sigma_{\theta\theta}$ with polar angle $\theta$ .................... 119

Figure 4.8 Variation of electric field $E_1$ with polar angle $\theta$ ....................... 120

Figure 4.9 Variation of electric field $E_2$ with polar angle $\theta$ ....................... 120
List of Symbols

\(a\)  \(a\) Major semi-axis of an ellipse or crack half length
\(b\)  \(b\) Minor semi-axis of an ellipse
\(C\)  \(C\) Elastic stiffnesses
\(D\)  \(D\) Electric displacement vector
\(D^*\)  \(D^*\) Eigen electric displacement vector
\(E_c\)  \(E_c\) Coercive electric field
\(E_i^\infty\)  \(E_i^\infty\) Remote electric field
\(e\)  \(e\) Piezoelectric constants
\(E\)  \(E\) Electric field vector
\(g\)  \(g\) Piezoelectric constants
\(G_c\)  \(G_c\) Critical energy barrier for domain switching
\(G_{tip}\)  \(G_{tip}\) Crack-tip total energy release rate
\(H\)  \(H\) Viscosity matrix
\(J\)  \(J\) Energy release rate of an elliptic flaw without the effects of remanent strains and remanent polarization
\(J'\)  \(J'\) Energy release rate of an elliptic flaw with the effects of remanent strains and remanent polarization
\(k\)  \(k\) Dielectric constants
\(k_c\)  \(k_c\) Dielectric permittivity of an elliptic flaw (or a crack)
\(K_t\)  \(K_t\) Remote mode I stress intensity factor
\(K_{IC}\)  \(K_{IC}\) Intrinsic fracture toughness
\(K_{tip}\)  \(K_{tip}\) Local mode I stress intensity factor
\(K_{II}\)  \(K_{II}\) Remote mode II stress intensity factor
\(K_{tip}\)  \(K_{tip}\) Local mode II stress intensity factor
\(K_D\)  \(K_D\) Remote electric displacement intensity factor
\(K_{tip}\)  \(K_{tip}\) Local electric displacement intensity factor
Remote electric field intensity factor $K_E$

Local electric field intensity factor $K_E^{mp}$

Characteristic length for domain evolution $l_0$

Electroelastic moduli $L$

Domain wall mobility $M$

Magnitude of spontaneous polarization $P_s$

Remanent polarization vector $P^r$

Spontaneous polarization vector $P^s$

Piezoelectric Eshelby tensor $Q$

Elastic compliances $S$

Characteristic time for domain evolution $t_0$

Displacement in the $i$-th direction $u_i$

Total potential energy of a ferroelectric body $U$

Potential energy of a ferroelectric body in the absence of an inclusion $U_0$

Potential energy due to a ferroelectric inclusion $U_I$

Young's modulus $Y$

Generalized strain vector $Z$

Generalized remanent strain vector $Z^r$

Generalized spontaneous strain vector $Z^s$

Generalized eigenstrain vector $Z^*$

Ratio of the minor semi-axis to the major semi-axis $\alpha$

Ratio of electric loading to mechanical loading $\alpha_E$

Dielectric constants $\beta$

Strain tensor $\varepsilon_{ij}$

Eigenstrain vector $\varepsilon^*$

Remanent strain vector $\varepsilon^r$

Spontaneous strain vector $\varepsilon^s$
\( \phi \)  Poling angle
\( \varphi_n \)  Complex potential functions for a 2-D piezoelectric medium
\( \gamma_r \)  Switching strain corresponding to 90° domain switching
\( \mu \)  Shear modulus
\( \nu \)  Poisson’s ratio
\( \sigma_{ij} \)  Stress tensor
\( \sigma_m \)  Remote stresses
\( \psi \)  Electric potential
\( \Delta K_I \)  Switching induced mode I stress intensity factor
\( \Delta K_{II} \)  Switching induced mode II stress intensity factor
\( \Delta K_D \)  Switching induced electric displacement intensity factor
\( \Delta K_E \)  Switching induced electric field intensity factor
\( \Delta P \)  Switching polarization
\( \Delta u \)  Crack opening displacement
\( \Delta \epsilon \)  Switching strains
\( \Delta \psi \)  Jump of electric potential across a crack
\( \Phi \)  Potential function vector
\( \Lambda \)  Domain wall energy density
\( \Sigma^0 \)  Remote electromechanical loading
\( \Sigma^1 \)  Stress and electric fields inside an elliptic inclusion
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Chapter 1

INTRODUCTION

1.1 Active Materials

The study of active materials (e.g. piezoelectrics, shape memory alloys, electrorheological fluids, etc.) and smart structures has attracted considerable attention since the early nineties [1]. The key components of a smart structure are a surface mounted and/or embedded system of sensors and actuators, and a control system. The actuators used in smart structures are normally made of active materials and are based on the coupled electromechanical and/or thermomechanical properties of active materials. Smart structures are used for active control of vibration, noise and shape. Recent applications include aircraft cabin noise control, shape control of helicopter blades, vibration control of space trusses and robotic arms, etc. Active materials such as piezoelectrics and shape memory alloys are also used to build the key elements of microelectromechanical systems (MEMS). Fig. 1.1 shows a ‘smart’ beam with two surface mounted piezoelectric sensors/actuators and a controller that is used for active control of vibrations. The sensor measures the beam vibration and sends a signal to the controller which through a feedback control algorithm drives the actuator to control the vibrations of the beam.

![Figure 1.1. Concept of a smart structure for vibration control](image)
An essential characteristic of an active material is the coupling between mechanical, electromagnetic and/or thermal fields. The constitutive relation of an active material has non-zero off-diagonal submatrices corresponding to such coupling. The strength of the coupling between different fields depends on the magnitude of the elements of off-diagonal sub-matrices in the constitutive relationship. For example, in the case of a piezoelectric material, the application of pressure results in an electric field. This effect is known as the direct piezoelectric effect (Fig. 1.2(a)) and is the basis for the development of piezoelectric sensors. On the contrary, a piezoelectric solid deforms when subjected to an applied electric field, which is the converse (indirect) piezoelectric effect (Fig. 1.2(b)). The converse piezoelectric effect is used in the design of actuators.

![Figure 1.2. Illustration of (a) direct and (b) converse piezoelectric effects.](image)

Other active materials include shape memory alloys (thermo-mechanical coupling), magnetostrictive materials (magneto-mechanical coupling) and electro-rheological fluids (change of viscosity due to electric field) [1]. These materials can also be used to design sensors and actuators and be integrated with feedback control systems to build smart structures [2]. The use of active materials such as piezoelectrics as sensors has a long history and the technical issues related to such applications have been thoroughly investigated in the past. However, the use of active materials such as piezoelectrics as actuators for smart structures is of more recent origin and requires further research. A major challenge is the development of reliable active materials with sufficiently large coupling coefficients to produce larger strokes (forces) under moderate
electric and/or magnetic fields. Fatigue, fracture and hysteresis are important issues in the selection of active materials for actuators in smart structures.

This study focuses on a few problems related to fracture of piezoelectric materials that are important to the design of reliable actuators. Substantial efforts have recently been made in the analysis and fabrication of piezoelectric actuators for various applications [3]. Piezoelectric actuators can be broadly classified into two categories; flexural actuators, such as unimorph and bimorph actuators, and extensional actuators such as multilayer stack actuators. In order to circumvent the shortcoming of small actuation strains (~ 0.1%) of piezoelectric materials, different amplification mechanisms are used to realize a large actuation under a moderate electric field. Fig. 1.3 shows two types of piezoelectric bimorph actuators. A bimorph generates actuation (bending) because one of the piezoelectric layers is subjected to an extension and the other to a contraction. There is no internal electrode in the anti-parallel polarization type shown in Fig. 1.3(a).

![Figure 1.3. Two types of piezoelectric bimorphs, (a) antiparallel polarization type and (b) parallel polarization type.](image)

Figure 1.3 shows a typical co-fired multilayer stack actuator, which is made up of thin ceramic layers alternating with embedded thin film electrodes. The thickness of a ceramic layer in a stacked actuator is in the order of 100 μm and the thickness of an electrode is about 10 μm. In the stacked configuration, the actuator is taking advantage of the fact that the piezoelectric coefficient is highest in the poling direction. Since the actuation strain is small in piezoelectrics ($10^{-4}$~$10^{-2}$ under an applied electric field of
about 1MV/m), tens to several hundreds of ceramic layers are stacked together to generate an appreciably larger stroke. The stack configuration can reduce the driving voltage to about 100-200 V and produce a reasonable stroke. As the stroke requirement of actuators is continuing to increase to satisfy the emerging applications in advanced technology areas, the reliability of piezoelectric actuators has become a major concern due to their brittle behaviour, low fracture toughness (~1 MPa√m) and high hysteresis.

![Diagram of multilayer piezoelectric ceramic actuator](image)

**Figure 1.4. Multilayer piezoelectric ceramic actuator.**

### 1.2 Piezoelectricity

Piezoelectricity is used to characterize the linear relationship between the electrical and mechanical response of a select group of materials [4]. It was discovered in 1880 by Jacques and Pierre Curie during their study of the effect of pressure on naturally occurring crystals such as quartz, zincblende and tourmaline [5]. Piezoelectricity was later found in polycrystalline ceramics. A necessary condition for the existence of piezoelectricity is that the unit cell of a material is non-centrosymmetric. Of all the 32 crystal point groups, 21 classes are non-centrosymmetric and 20 of these are piezoelectric. Note that one class lacking a center of symmetry is not piezoelectric due to other combined symmetry elements.
The linear constitutive relations of a piezoelectric material can be expressed in the following form by choosing the elastic strains and the electric field as the independent variables.

\[
\begin{align*}
\sigma &= C^E \gamma - e^T E \\
D &= e \gamma + k^T E
\end{align*}
\tag{1.1}
\]

where \( \sigma, \gamma, D \) and \( E \) are the stress, strain, electric displacement and electric field vectors respectively and \( C^E, e \) and \( k^T \) denote the elastic stiffness, piezoelectric constants and dielectric permittivities, respectively.

The above equations can be derived using the first and the second laws of thermodynamics and the Helmholtz free energy expression, see Lines and Glass [6] for a complete derivation. Note that if the piezoelectric constants vanish \( (e = 0) \), then eqn. (1.1) is reduced to two separate constitutive equations with one corresponding to a linear elastic solid and the other for a linear dielectric. The number of nonzero independent material constants in eqn. (1.1) is determined by the symmetry class of a material [7]. For example, quartz belongs to the trigonal trapezohedral class (class 32) and it has 13 independent material constants. Widely used piezoelectric materials such as poled piezoelectric ceramics have hexagonal pyramidal symmetry (class 6mm) and they have 10 independent material constants (Table 1.1).

Table 1.1 Material constants of piezoelectric ceramics poled along the \( x_3 \)-axis

<table>
<thead>
<tr>
<th>Elastıc constants</th>
<th>Piezoelectric constants</th>
<th>Dielectric constants</th>
</tr>
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<tbody>
<tr>
<td>( \begin{pmatrix} c_{11} &amp; c_{12} &amp; c_{13} &amp; 0 &amp; 0 &amp; 0 \ c_{12} &amp; c_{11} &amp; c_{13} &amp; 0 &amp; 0 &amp; 0 \ c_{13} &amp; c_{13} &amp; c_{33} &amp; 0 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 0 &amp; c_{44} &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 0 &amp; 0 &amp; e_{44} &amp; 0 \ 0 &amp; 0 &amp; 0 &amp; 0 &amp; 0 &amp; c_{66} \end{pmatrix} )</td>
<td>( \begin{pmatrix} 0 &amp; 0 &amp; e_{13} \ 0 &amp; 0 &amp; e_{13} \ 0 &amp; 0 &amp; e_{33} \ 0 &amp; e_{15} &amp; 0 \ e_{15} &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 0 \end{pmatrix} )</td>
<td>( \begin{pmatrix} k_{11} &amp; 0 &amp; 0 \ 0 &amp; k_{11} &amp; 0 \ 0 &amp; 0 &amp; k_{33} \end{pmatrix} )</td>
</tr>
<tr>
<td>( c_{66} = (c_{11} - c_{12})/2 )</td>
<td></td>
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1.3 Electrostriction

In the previous section, a linear electromechanical coupling effect known as piezoelectricity was introduced. However, there is another type of electromechanical coupling effect called electrostriction where the electric field induced strain is proportional to the square of the electric field [3]. Therefore, the electrostrictive strain is independent of the polarity (sign) of the electric field. Though electrostriction exists in all dielectric materials, most of them are not classified as electrostrictive materials, because they generate very small electrostrictive strains ($10^{-7} \sim 10^{-5} \%$ at 1 MV/m) [8]. On the other hand, some materials such as lead magnesium niobate (PMN) and lead zinc niobate (PZN) exhibit significant electrostrictive effects and can generate strains as large as those of piezoelectric ceramics such as lead zirconate titanate (PZT) and lead lanthanum zirconate titanate (PLZT) [3]. Electrostrictive materials can also be used to design actuators for various applications. These materials show little hysteresis in their dielectric response.

1.4 Ferroelectricity

An important subgroup of piezoelectric materials is ferroelectrics, which typically display dielectric hysteresis in the electric polarization vs. the electric field response as shown in Fig. 1.5 [9]. This class of materials has a spontaneous electric polarization, i.e. self-generated polarization in the absence of an electric field which can be reversed in direction by applying an electric field. This phenomenon is called ferroelectricity and was discovered in 1921 in single-crystal materials (Rochelle salt) and subsequently in polycrystalline ceramics such as barium titanate (BaTiO$_3$), PZT, PLZT and others [10]. A few important properties of a ferroelectric material can be defined by using Fig. 1.5. Remanent polarization ($P_r$) is defined as the residual polarization when the electric field returns to zero and the coercive electric field ($E_c$) is defined as the electric field at which the electric polarization reduces to zero. Important information can be obtained from the hysteresis curve. For example, high remanent polarization ($P_r$) implies high internal
polarizability, high strain and high electromechanical coupling whereas a high coercive field \( (E_c) \) relates to a small grain size.

Figure 1.5. Electric polarization \( (P) \) versus electric field \( (E) \) curve for ferroelectric materials.

Ferroelectric ceramics account for about one half of electroceramics used in industry [11]. They are used in capacitors, particularly multilayer capacitors (MLC), because of the high dielectric constants. Ferroelectric random access memory (FRAM) devices are another widely used application. Ferroelectric materials are also used as sensors and actuators. Commonly used ferroelectric materials are polycrystalline oxide ceramics of barium titanate and lead zirconate titanate which have a perovskite-type \( (ABO_3) \) unit cell as shown in Fig.1.6.

Figure 1.6 Unit cell of lead zirconate titanate (PZT), (a) below and (b) above the Curie temperature.
Above a critical temperature known as the Curie temperature, a ferroelectric material is in the paraelectric phase and has a cubic unit cell structure. Below the Curie temperature, barium titanate and lead zirconate titanate are in the ferroelectric phase. Barium titanate can have a tetragonal, orthorhombic, or rhombohedral structure as the temperature decreases (Fig. 1.7). PZT has either a tetragonal or rhombohedral structure in the ferroelectric phase depending on its composition. It has become the preferred material for transducer applications due to its higher Curie temperature and higher electromechanical coupling coefficients. Dopants are commonly used to modify the mechanical and dielectric properties of PZT ceramics. Those doped with acceptors such as Fe$^{3+}$ replacing Ti$^{4+}$ or Zr$^{4+}$ are called hard PZTs, while soft PZTs are doped with elements such as Nb$^{5+}$ replacing Zr$^{4+}$ or La$^{3+}$ replacing Pb$^{2+}$. Hard PZTs have lower dielectric constants, dielectric losses, coupling factors, and mechanical compliance and a higher coercive electric field when compared to soft PZTs.

![Diagram of cubic, tetragonal, orthorhombic, and rhombohedral phases of barium titanate (BaTiO$_3$) with the direction denoting the spontaneous polarization, $P_s$.](image)

Figure 1.7. Paraelectric and ferroelectric phases of barium titanate (BaTiO$_3$) with the direction denotes the spontaneous polarization, $P_s$.

Polycrystalline ferroelectric ceramics are composed of small grains with each grain being a ferroelectric single crystal (Fig. 1.8). They are produced by sintering of fine powders of oxide metals followed by a cooling process. When cooling through the Curie temperature, the unit cells of a ferroelectric ceramic do not spontaneously polarize in the same direction, and domains, which are regions within grains of the ceramic that have the same spontaneous polarization, are formed to minimize the free energy of the system (Fig. 1.8). The polar directions of neighboring domains differ from each other by either 180° or 90°. The interface between two domains that have opposite spontaneous
polarization is called a 180° domain wall, while a 90° domain wall refers to the interface between two adjacent domains with their spontaneous polarization perpendicular to each other. Since domains are randomly orientated when cooling through the Curie temperature, the net (average) polarization is zero and the material shows no electromechanical coupling. In order to produce electromechanical coupling effect in a ferroelectric ceramic, a strong DC electric field (~3E_c) is applied to align the spontaneous polarization of domains closely along the direction of the applied electric field (Fig. 1.8). This process is called poling which results in nonzero macroscopic residual strains and electric polarization, namely the remanent strains and remanent polarization. After poling, a ferroelectric ceramic becomes a useful piezoelectric.

1.5 Constitutive Behavior of Ferroelectric Ceramics

Under small stress and electric fields, ferroelectric ceramics can be characterized by a linear piezoelectric constitutive law (eqn. 1.1). However, under large electric and stress fields, they show strong nonlinearity and hysteresis which cannot be described by linear piezoelectricity. Fig. 1.9 shows the typical relationships between electric polarization and electric field (Fig. 1.9(a)), strain and electric field (Fig. 1.9(b)) and stress and strain (Fig. 1.9(c)) of ferroelectric materials.

Several experimental studies have been conducted to examine the constitutive behavior of ferroelectric materials under electric and/or mechanical loading. Lynch [12] studied the mechanical and electrical response of PLZT 8/65/35 under a constant uniaxial
force and a varying electric field parallel to the poling axis. He observed that the coercive electric field changed with the applied compressive stress and both the remanent strain and remanent polarization decreased with increasing compressive stress (leading to depolarization). Schaufele and Hardtl [13] studied the behavior of neodymium-doped soft PZT and iron-doped hard PZT with variable zirconium concentrations under a varying compressive stress and a constant electric field parallel to the poling direction. They found that the coercive stress is linearly dependent on the applied electric field. More recently, Chen and Lynch [14] investigated the behavior of PLZT 8/65/35 under biaxial mechanical and electrical loading. They observed that a compressive stress applied perpendicular to the poling direction (also the electrical loading direction) has an effect on the stress-strain curve and the electric displacement-electric field curve, but no effect on the coercive electric field.

The macroscopic nonlinear behavior of ferroelectric ceramics can be attributed to the changes of microstructure due to external electrical and mechanical loading [15]. The unit cell of PZT below the Curie temperature is polar and there is a relative displacement between the central Ti$^{4+}$ (Zr$^{4+}$) ion and the surrounding Pb$^{2+}$ and O$^{2-}$ ions (Fig. 1.6 (a)). This relative displacement results in a net electric dipole moment. The dipole moment per unit volume is identified as the spontaneous polarization. Under small stress and electric fields, the electric polarization of a unit cell undergoes a reversible change. An applied
stress results in a relative displacement between the positive and negative ion and an applied electric field changes the relative displacement between the positive and negative ions and results in an elastic deformation of a unit cell. These macroscopic manifestations are referred to as the direct and the converse piezoelectric effects.

![Diagram](image)

Figure 1.10. Unit cell configuration for (a) 180°, and (b) 90° ferroelectric domain switching.

Under stress and electric fields higher than some critical values, the response of a unit cell and hence domains in a ferroelectric are different. An electric field greater than the coercive field ($E_c$) produces a 180° or 90° rotation of the spontaneous polarization of a ferroelectric domain as shown in Fig. 1.10. This phenomenon is known as ferroelectric domain (polarization) switching. 180° domain switching results in a complete reversal of the spontaneous polarization, but no changes in the shape and dimensions and therefore no strain. However, 90° switching induces a strain because of the rotation of the spontaneous polarization. A higher stress can rotate the polar direction of the domain by 90° only as shown in Fig. 1.11. This is called 90° ferroelastic domain switching. The four types of ferroelastic domain switching shown in Fig. 1.11 are energetically equivalent. It has been demonstrated that ferroelectric and ferroelastic domain switching are the major
sources of material nonlinearities in ferroelectric ceramics [15]. Considerable efforts have recently been made to simulate the macroscopic material behavior of ferroelectric materials by using various micromechanics based domain switching models [15-19].

Figure 1.11. Unit cell configuration for 90° ferroelastic domain switching

1.6 Fracture of Ferroelectric Materials

As mentioned previously, the development of electromechanical actuators based on the converse piezoelectric effect has major challenges due to the brittle behaviour, low fracture toughness and hysteresis effects of poled ceramics. Furuta and Uchino [20] observed crack initiation and subsequent propagation at an embedded electrode of a piezoelectric multilayer actuator under cyclic electric loading. Abrurtani et al. [21] investigated the failure mechanisms of electrostrictor and piezoelectric ceramic multilayer actuators under an alternating electric field. They observed that cracks initiated at the edge of an internal electrode in a piezoelectric actuator and obliquely propagated to the neighboring electrodes (Y-shaped crack pattern). Delamination cracks were found at ceramic and electrode interfaces. Schneider et al. [22] investigated crack configurations in piezoelectric multilayer actuators under a high cyclic electric field (2.5 kV/mm) and observed segmentation cracks (cracks perpendicular to the electrode) during 1-10 cycles, electrode tip cracks during 50-500 cycles, matrix cracks during 500-2000 cycles,
electrode delamination during 500-2000 cycles and finally the dielectric breakdown (Fig. 1.12).

Figure 1.12. Crack configuration in a piezoelectric multilayer actuator [22].

Though much progress has been made in experimental and theoretical investigations related to fracture of piezo/ferroelectric materials, some important issues remain unsolved. For example, the role of electrical loading on fracture is not well understood and there are conflicting experimental findings on the effect of an applied electric field on crack propagation (enhancing vs. retarding). Another important issue is the electric boundary condition on the crack surfaces, which has a significant influence on fracture behavior. The electric boundary condition on the crack surfaces can be permeable, impermeable or conducting to an electric field, depending on the medium inside the crack. Another issue is the validity of theoretical models based on linear fracture mechanics and classical piezoelectric descriptions for ferroelectric materials. This may not be adequate because the stress and electrical fields are highly concentrated around a crack tip and the material behaves nonlinearly under a large electric and/or stress field. A review of previously reported key experimental and theoretical investigations related to fracture of piezo/ferroelectric materials is presented in the following section in order to define the scope of the present study.
1.6.1 Experimental investigations

Several experimental studies have been carried out to measure the fracture toughness of ferroelectric materials under pure mechanical loading. Fracture toughness of ferroelectric ceramics such as BaTiO$_3$ and PZT ranges from 0.8 to 1.7 MPa$\sqrt{m}$ [23] and generally depends on temperature, grain size and composition of the ceramic. Fracture toughness of these materials exhibits anisotropic behavior, with a higher value in the poling direction and a lower value in the directions perpendicular to the poling axis [24, 25, and 26]. Pisarenko et al. [24] reported that the ratio of fracture toughness along the poling direction to that perpendicular to it was in the range of 1.15-2.36 for four different ceramics.

Tobin and Pak [27] conducted indentation tests on PZT-8 under a load of 4.9 N combined with an electric field of intensity $-4.7$ to $4.7$ kV/cm. They found that crack length is longer under a positive field (same as the poling direction) and shorter under a negative field (opposite to the poling direction), for a crack perpendicular to the poling direction (Fig. 1.13(a)). In addition, the polarity of the applied electric field did not have a significant effect on the propagation of a crack parallel to the poling direction. Sun and Park [28] performed indentation tests on PZT-4 under loads of 4.45 N and 22.24 N, respectively (Fig. 1.13(b)). Their findings agree with that of Tobin and Pak [27] for a load of 4.45 N, i.e. a positive field tends to enhance crack propagation, while a negative one retards propagation. However, both positive and negative fields enhanced crack propagation under a load of 22.24 N. Wang and Singh [29] conducted indentation tests on PZT EC-65 under loads varying from 4.9 to 11.76 N and found that a negative field of $-5$ kV/cm produced longer cracks in directions parallel and perpendicular to the poling direction (Fig.1.14). Their findings did not agree with those of Tobin and Pak [27] and Sun and Park [28]. More recently, Lynch [30] performed indentation fracture tests on PLZT 8/65/35 using a load of 39.2 N and reported that a positive electric field enhances crack propagation in the direction perpendicular to the poling axis.
Figure 1.13. Effect of electric field on the crack length of, (a) PZT-8 [27] and (b) PZT-4 [28].

Figure 1.14. Effect of electric field on the crack length of PZT EC61, (a) negative field and (b) positive field [29].

Other techniques such as compact tension and three or four-point bending tests have also been used to investigate fracture of ferroelectric ceramics. Park and Sun [31] conducted compact tension fracture tests on PZT-4 with a notch perpendicular to the poling direction. They reported that the fracture load showed approximate linear dependence on the applied electric field in the range of $-5 \text{ kV/cm}$ to $5 \text{ kV/cm}$ and a
positive field reduced the fracture load (Fig. 1.15(a)). Fu and Zhang [32] conducted compact tension tests on PZT-841 and observed that both positive and negative applied electric fields reduced the apparent fracture toughness (Fig. 1.15(b)). However, the effect of a negative electric field is more pronounced than a positive field. Fu and Zhang [32] also measured the apparent fracture toughness of PZT-841 using indentation tests with a load of 49.0 N and an electric field ranging from −4 to 4 kV/cm. Their indentation tests and compact tension tests showed similar effects of an electric field on the apparent fracture toughness.

![Graph](image)

Figure 1.15. Effect of electric field on fracture load of, (a) PZT-4 [31] and PZT-841 [32].

Limited experimental studies are available on conducting cracks. Heyer et al. [33] conducted four-point bending tests on PZT PIC-151 bars with conducting cracks parallel to the poling direction and reported that the apparent fracture toughness ($K_{IC}$) of a conducting crack increased as the electric field intensity factor ($K_E$) varied from $-90$ kV/√m to $30$ kV/√m. Fu et al. [34] investigated conducting cracks parallel to the poling direction in PZT-4 under pure mechanical loading and pure electric loading. It was
observed that dielectric breakdown was often accompanied by fracture under pure electric field loading. They found that the critical energy release rate for a conducting crack under pure electric loading was about 25 times that of a mechanically loaded crack. It has been reported that the mechanism of crack propagation in piezoelectrics under mechanical field is different from that due to an electric field. Mechanically induced cracking appears to be transgranular, whereas electrically induced cracking appears to be intergranular.

1.6.2 Theoretical investigations

In order to explain the experimentally observed fracture behavior of ferroelectric materials and to facilitate the design of actuators, several theoretical studies have been reported in the literature. Similar to the inconsistencies in experimental findings, predictions based on some theoretical models are also questionable. A review of key theoretical studies on fracture of electroelastic materials is given in the following section.

1.6.2.1 Linear piezoelectric crack model

Based on linear piezoelectricity, a number of theoretical studies have been presented for fracture of piezoelectric materials. A major issue with the theoretical studies (also experimental) is the type of electric boundary condition on the crack surfaces. Parton [35] conducted the first study of a crack in a piezoelectric material by assuming the following continuity conditions for the normal electric displacement ($D_n$) and electric potential ($\psi$),

$$D_n^+ = D_n^-, \quad \psi^+ = \psi^-$$

(1.2)

where the ‘+’ and the ‘−’ signs refer to the upper and the lower crack surfaces, respectively. The above condition is known as the electrically permeable boundary condition. Sosa and Khutoryansky [36] studied the problem of a piezoelectric plane with an elliptic void and obtained the electroelastic field of a permeable crack by degeneration. Based on the permeable assumption (eqn. 1.2), both the stress intensity factors and the
crack tip energy release rate are independent of the applied electrical loading, which contradicts the experimental observations [27-32].

Deeg [37] studied dislocations, cracks and inclusions in piezoelectric media and assumed the crack surfaces to be electrically impermeable, i.e. the crack surfaces are charge-free and the electric field inside the crack is zero. The impermeable crack assumption can be expressed as,

$$D^+_n = D^-_n = 0$$  \hspace{1cm} (1.3)

Pak [38] gave a detailed argument for neglecting the electric field inside a crack based on the fact that the magnitude of the dielectric constant of a piezoelectric material is three orders higher than that of air (vacuum). The impermeable crack boundary condition was later adopted by Pak [39] and Sosa [40] to derive the two-dimensional electromechanical field near a crack tip. Suo et al. [41] established a fracture mechanics framework for ferroelectric materials based on linear piezoelectricity and a small scale domain switching condition. They presented analytical solutions for two-dimensional impermeable crack problems in homogeneous materials and bi-materials. In addition to the conventional elastic stress intensity factors, an electric displacement intensity factor ($K_{1IV}$) was introduced. They showed that $K_{1IV}$ was independent of applied mechanical loading for a Griffith crack and the energy release rate was a non-positive definite function of applied electromechanical loading. For example, a negative energy release rate is induced by a pure electric field, which implies that an electric field only cannot drive a crack to grow. Based on the impermeable assumption, both positive and negative electric fields tend to reduce the energy release rate and consequently retard crack propagation.

Hao and Shen [42] introduced the following semi-permeable crack face boundary condition.

$$D^+_n = D^-_n, \quad D^+_n \Delta u_n = -k_c \Delta \psi$$  \hspace{1cm} (1.4)
where $\Delta u_n$ is the crack opening displacement, $\Delta \psi$ is the jump of electric potential across a crack and $k_c$ is the dielectric constant inside a crack.

Eqn. 1.4 can be reduced to the permeable condition (eqn. 1.2) if $\Delta u_n = 0$, or to the impermeable condition (eqn. 1.3) if $k_c = 0$. Based on the semi-permeable condition, the electric displacement on the crack surfaces is a constant that depends on material properties and applied electromechanical loading. Therefore, the dielectric property of the medium inside a crack plays an important role in fracture of piezoelectric materials.

If the medium inside a crack is conductive, the crack face electric boundary condition can be expressed as,

$$E^+_t = E^-_t = 0$$

where $E_t$ denotes the tangential electric field component.

The study of conducting cracks is vital to the understanding of dielectric failure of multilayer actuators, where conducting cracks can grow to bridge neighboring electrodes.

There are a few studies on the applicability of various idealizations used in theoretical crack models. By investigating the problem of an elliptical flaw in an isotropic dielectric, McMeeking [43] demonstrated that the electroelastic field near a flaw boundary is determined by the ratio of the minor semi-axis to the major semi-axis and the ratio of the permittivity of the material and the flaw. He showed that the impermeable assumption is not valid for very slender flaws, though the permittivity of air or vacuum is much less than that of materials like PZT, but actually nonzero. Dunn [44] studied the effect of crack face boundary conditions on the energy release rate of piezoelectric solids and found that the crack face boundary conditions have a significant effect on the energy release rate. Zhang et al. [45] studied the behavior of cracks by investigating an elliptical cavity using the exact boundary conditions which are consistent with the principles of electrostatics. The crack opening profile is found to be very sensitive to the electric field.
inside a crack, and in turn, the crack opening profile affects the electric field. They proposed a self consistent approach to calculate the energy release rate and showed that, for a permeable crack, an applied electric field does not contribute to the energy release rate when the undeformed crack profile is used, while an electric field resists crack propagation when the deformed crack profile is used. Similar findings have been obtained by McMeeking [46], who used the finite element method to calculate the crack tip energy release rate for PZT-4 compact tension specimen using both the undeformed and deformed crack profiles.

In the case of actuators, fracture problems are more complicated when compared to situations involving a homogeneous piezoelectric medium. The interaction between embedded electrodes and the host ceramic is very complex and different fracture patterns have been discovered in experiments [20-22]. Several theoretical models have been proposed to explain the fracture mechanisms of multilayer actuators. Yang and Suo [47] showed that the electric field at an embedded electrode (conducting sheet) in an electrostrictive matrix is intense and nonuniform. They obtained the stress intensity factors at the tip of an insulating crack directly ahead of an electrode tip and found that cracking can be suppressed in multilayer actuators if the thickness of each ceramic layer is lower than a critical value. Their model was further elaborated by Hao et al. [48] who studied a crack emanating directly from an internal electrode tip in unpoled ferroelectric multilayer actuators. Note that the above studies were focused on the investigation of cracks in electrostrictive or unpoled ferroelectric materials. Only a few studies are available in the literature concerning the more practically interesting case of cracks in poled ferroelectric actuators. Ru [49] studied collinear electrode layers at the interface of two-piezoelectric half-planes subjected to electric charge at each electrode. The electrode layers are assumed to be very thin and more compliant than surrounding ceramic layers. Based on linear piezoelectricity, a singular electroelastic field was found near the tip of an electrode layer.
1.6.2.2 Fracture criterion

Another issue that requires further theoretical and experimental study is the type of fracture criterion to be used for piezoelectric materials. Two types of fracture criteria are reported in literature, with one based on the crack-tip stress intensity factors and the other based on the crack-tip energy release rates. In the case of isotropic materials, the crack paths predicted by stress intensity factor and energy release rate criteria are nearly identical. However, this is not the case for anisotropic materials such as piezoelectrics. Fracture analysis based on linear piezoelectricity predicts that the stress intensity factors based on either the impermeable or the permeable assumption are independent of an applied electric field for a Griffith crack. This prediction is inconsistent with experimental findings [27-32]. On the other hand, the linear piezoelectric crack model also predicts that both positive and negative electric fields reduce the total (mechanical and electrical) energy release rate and consequently retard crack propagation. This prediction also contradicts experimental observations.

In order to resolve the discrepancy between theoretical predictions and experimental observations, Park and Sun [31] proposed the mechanical strain energy release rate, instead of the total energy release rate, as a suitable fracture criterion. Predictions based on the mechanical strain energy release rate criterion coupled with the impermeable crack assumption agree qualitatively with the experiment observations of Park and Sun [31]. However, this criterion lacks a clear physical explanation. Moreover, this criterion predicts that a pure electric field cannot drive a crack to propagate, which contradicts the experimental findings [50, 51]. Material anisotropy has a significant effect on crack propagation and should be considered in the development of reliable fracture criteria for piezoelectric materials.

1.6.2.3 Domain switching and crack tip non-linear effects

All the above mentioned studies are based on linear piezoelectricity. The complex fracture behaviour noted in experimental studies and the discrepancies between the experimental results and theoretical predictions may be attributed to localized material
nonlinear effects. For example, crack-tip stress and electric fields are highly intensified and small-scale domain switching in the vicinity of a crack tip has been observed in experiments under electric as well as mechanical loading [52, 53, 54]. Fig. 1.16 shows the SEM morphology of the etched surface for a poled PLZT ceramic without and with a laterally applied electric field [52] and 90° ferroelectric domain switching is observed near the crack tip due to an applied electric field. The switched domains near a crack tip induce incompatible strains and electric polarization under the constraint of the unswitched material, and thereby change the near-tip electric and stress field. Such domain switching induced changes to crack tip field intensity factors may help explain some features of the material behaviour observed in experiments.

![SEM morphology of the etched surface](image)

Figure 1.16. SEM morphology of the etched surface of poled PLZT ceramics, (a) without and (b) with applied lateral electric field. (b) is showing 90° domain switching near a crack tip [52].

The development of continuum models for ferroelectric and ferroelastic switching remains a challenging task because of the evolving microstructure and polycrystalline nature of the materials. However, some progress has been made in recent years [15-19]. In their seminal study, McMeeking and Hwang [55] obtained the potential energy change in a piezoelectric material due to instantaneous introduction of a spherical inclusion and proposed an energy criterion to simulate switching of a crystallite in a ferroelectric polycrystalline material. The matrix and inclusion were treated as isotropic materials and the electromechanical coupling (piezoelectric effect) in the matrix was not included. If
the piezoelectric effect of the inclusion is also neglected, potential energy of the inclusion can be further reduced to the summation of energy of an isotropic elastic inclusion and an isotropic dielectric inclusion. Hwang et al [18] extended the work of McMeeking and Hwang [55] to model domain switching of polycrystalline materials. Huber et al [19] recently presented a micromechanics model based on self-consistent calculation of polycrystals with rate-independent, non-hardening crystal plasticity.

By analogous to phase-transformation induced toughening of ceramics [56, 57], Zhu and Yang [58] proposed a small-scale domain switching model based on Hwang et al switching criterion [15] to examine the effect of crack tip domain switching on the apparent fracture toughness of ferroelectrics. In the switching-toughening model of Zhu and Yang [58], a transformation wake shields the crack tip. Consequently, the local stress intensity factor is different from the applied stress intensity factor. It is assumed that the local intensity factor controls crack propagation. The model was used to provide a mechanistic explanation for electric field induced cracking and electric fatigue [59, 60]. In these studies, ferroelectric materials are modeled as isotropic elastic dielectrics and the influence of electromechanical coupling and material anisotropy are neglected.

1.7 Scope of the Present Work

Based on the above literature review, several key issues related to fracture behaviour of ferroelectric materials remain unsolved and need further investigation. These include:

- an appropriate theoretical model including the crack face electric boundary conditions for fracture analysis;
- an experimentally verified fracture criterion for general electromechanical loading;
- theoretical development of a domain switching criterion that takes into consideration full piezoelectric coupling and anisotropy;
• the effects of small-scale domain switching on crack tip field intensity factors for both single crystal and polycrystalline materials;

• the effects of macroscopic non-linear material behaviour including non-instantaneous domain switching;

• the mechanics of delamination, branch and bridging cracks in ceramic actuators;

• the behavior of conducting cracks and dielectric breakdown mechanisms in multilayer ceramic actuators.

The study of all the above issues is beyond the scope of this thesis. Instead, the present study focuses on the development of a theoretical basis for instantaneous domain switching and its influence on crack tip field intensity factors. This direction is chosen with the goal of possibly explaining the role of electric loading on fracture by using a consistent theoretical treatment of crack tip nonlinearities. In practical applications involving smart structures, ceramic actuators are subjected to repeated electric loading and the actuator failure normally occurs due to applied electric loading. Therefore, any attempt to improve the current understanding and prediction of material behaviour under electric loading would be of significant value to future engineering applications of ceramic actuators.

In Chapter 2, the basic building block for the present study, which is the generalized Eshelby tensor for an elliptical piezoelectric inclusion of different properties in a parent piezoelectric plane, is derived using analytical techniques. The Eshelby tensor is then applied to derive the free energy expression due to the introduction of an elliptic crystallite into a poled ferroelectric material. Based on the change of free energy before and after ferroelastic/ferroelectric switching of the crystallite, a modified domain switching criterion is proposed. The new switching criterion includes the contribution of spontaneous strains and spontaneous polarization as well as the elastic strains and electric displacements to the reduction of potential energy. The effect of a change of material...
properties before and after switching of the inclusion is also included in the new criterion. Hence, a complete domain switching criterion that takes into consideration important material characteristics of ferroelectric materials is presented in the thesis.

The free energy expression of an elliptic inclusion is applied to simulate the evolution of 180° and 90° domain nuclei in ferroelectric crystals. In addition, the energy release rate associated with the self-similar propagation of an elliptical flaw (or a crack) in a material with non-zero remanent strains and remanent polarization is computed by using the free energy expression. The energy release rate for electrically impermeable, permeable and conducting cracks can be obtained by degenerating the ellipse to a crack. The dielectric property and the geometry of a flaw are shown to play important roles in the electroelastic field and the energy release rate during crack propagation.

In Chapter 3, the new domain switching criterion is applied to investigate the effect of near-tip domain switching on the behavior of electrically insulating and conducting cracks. The changes of field intensity factors (toughness variation) are evaluated by a scheme similar to that used in the study of phase-transformation induced toughening of ceramics. To this end, a new fundamental solution for a semi-infinite crack (insulating or conducting) interacting with stress-free transformation strains (eigenstrains) and electric field-free polarization (eigen polarization) is derived. The new fundamental solution is used to formulate the apparent fracture toughness change induced by domain switching in uniformly poled single crystal materials. Toughness variation of polycrystalline ferroelectrics is estimated by a Reuss-type approximation. The role of electric loading on the propagation of insulating and conducting cracks is examined and qualitatively compared with available experimental data in the literature. The possibility of crack closure is also considered in the theoretical modeling. The conditions for electric field induced closure of insulating and conducting cracks are established. Mixed boundary-value problems corresponding to closed cracks are solved. The crack closure model may provide useful information on a theoretical basis for crack growth under a cyclic electric field.
In Chapter 4, the electroelastic field at the tip of an embedded electrode in a layered stack actuator (Fig. 1.4) is examined by using an idealized electrode-ceramic configuration. At an embedded electrode tip, the electric field is non-uniform and highly concentrated, causing incompatible strains and thereby stresses which result in crack initiation. Experiments demonstrated that a crack nucleates at an embedded electrode tip and interfacial debonding occurs between an electrode and the ceramic layers leading to the failure of actuators [20-22]. Although in practical applications, the bulk ceramic is loaded in the linear regime, the intensified electric and stress field near an electrode tip can lead to localized domain switching and consequently change the fracture behaviour of an actuator. An idealized model of an electrode embedded at the interface of two-piezoelectric half planes with opposite polarization is analyzed to examine the electroelastic field at the tip of an electrode in a stack actuator. Important features of the electrode tip field are identified and qualitatively compared with previously reported experimental findings. The conclusions of the present study and the recommendations for future work are presented in Chapter 5.
Chapter 2

A THEORETICAL MODEL FOR DOMAIN SWITCHING AND EVOLUTION

2.1 Overview

The basic building block for the analysis presented in this chapter and the remainder of the thesis is the solution for two-dimensional piezoelectric Eshelby tensor, which relates the constraint strains and electric polarization in an elliptic inclusion to specified uniform eigenstrains and eigenelectric displacement in the inclusion. Previous solutions for piezoelectric Eshelby inclusion problems [61-65] were derived for inclusions with specified eigenstrains and an eigenelectric field instead of eigenstrains and eigenelectric displacement. The latter choice is physically more meaningful in modeling domain (polarization) switching as these quantities can be directly related to switching induced spontaneous strains and spontaneous polarization.

The Eshelby tensor presented here is formulated by using the extended Lekhnitskii's formalism, and the free energy expression due to the introduction of an elliptic crystallite into a poled ferroelectric matrix is also obtained. By examining the change of potential energy before and after polarization switching of the crystallite, a domain switching criterion which considers both the interaction of applied electromechanical loading with switching strains and switching polarization and the changes in the electroelastic properties of the switched crystallite is obtained.

Two basic problems related to ferroelectric materials are analyzed by using the piezoelectric Eshelby tensor. First, the free energy expression of an elliptic piezoelectric inclusion is applied to simulate the evolution of 180° and 90° domain nuclei in ferroelectric crystals by extending the uncoupled theoretical model of Loge and Suo [66]. Next, the free energy expression is employed to investigate the energy release rate of self-similar propagation of an elliptic flaw (or a crack). Remanent strains and remanent
polarization induced in ferroelectric ceramics due to poling are shown to have an important effect on the energy release rate. This is consistent with the findings of Landis and McMeeking, who demonstrated that the energy release rate for a non-polar piezoelectric is not equal to that for a similar piezoelectric with remanent polarization but otherwise identical linear properties [67].

2.2 Eshelby Tensor for Elliptic Inclusion

Consider a piezoelectric medium with a Cartesian coordinate system \((x_1, x_2, x_3)\) defined as shown in Fig 2.1. In the absence of body forces and free electric charges, the governing equations for plane strain deformations \((e_{33} = e_{31} = e_{32} = 0, E_3 = 0)\) of a medium with its poling axis parallel to the \(x_2\)-axis can be expressed as [40]

\[
\varepsilon = S \sigma + g^T D, \quad E = -g \sigma + \beta D \tag{2.1}
\]

\[
\sigma_{ij} = 0, \quad D_{ii} = 0 \quad (i, j = 1, 2) \tag{2.2}
\]

where two-dimensional strain vector \(\varepsilon = (\varepsilon_{11} \varepsilon_{22} 2\varepsilon_{12})^T\), stress vector \(\sigma = (\sigma_{11} \sigma_{22} \sigma_{12})^T\), electric displacement vector \(D = (D_1 D_2)^T\), electric field vector \(E = (E_1 E_2)^T\), and \(S, g\) and \(\beta\) denote the reduced elastic, piezoelectric and dielectric constants in two dimensions, respectively.

Note that the out-of-plane stress \(\sigma_{33}\) and electric displacement \(D_3\) are non-zero and depend on the in-plane stress and electric field components. The eqn (2.1) also hold for the plane stress case \((\sigma_{31} = \sigma_{32} = \sigma_{33} = 0, and D_3 = 0)\) with appropriately modified \(S, g\) and \(\beta\) matrices. For ferroelectric materials, the eqn. (2.1) implies that the reference configuration corresponds to the poled state with non-zero remanent strains and remanent polarization, which is indeed a deformed state.

The general solution for the two-dimensional electroelastic field can be obtained by solving the eqns. 2.1 and 2.2 by using complex potential functions. There are two
formalisms available in the literature for the solution of the governing equations, namely
the Stroh's formalism based on the extension of displacement potentials for elastic
materials [41, 68, 69] and the Lekhnitskii's formalism based on the extension of stress
potentials in elasticity [40, 70, 71]. By using the Lekhnitskii's formalism, the following
general solutions can be obtained.

$$<u_1, u_2, \psi> = 2 \Re \sum_{n=1}^{3} <p_n, q_n, s_n > \phi_n(z_n)$$

(2.3)

$$<\epsilon_{11}, \epsilon_{22}, 2\epsilon_{12}> = 2 \Re \sum_{n=1}^{3} <p_n, \mu_nq_n, q_n + \mu_np_n > \phi'_n(z_n)$$

(2.4)

$$<\sigma_{11}, \sigma_{22}, \sigma_{12}> = 2 \Re \sum_{n=1}^{3} <\mu_n^2, 1, -\mu_n > \phi'_n(z_n)$$

(2.5)

$$<E_1, E_2, D_1, D_2> = -2 \Re \sum_{n=1}^{3} <s_n, t_n, -\mu_n \delta_n, \delta_n > \phi'_n(z_n)$$

(2.6)
where \( u_i \) and \( \psi \) denote the elastic displacement in the \( i \)-th direction and the electric potential respectively; \( \text{Re} \) denotes the real part of a complex quantity; \( z_n = x_n + \mu_n x_2 \) and \( \mu_n \) denote the three complex roots with positive imaginary parts of the characteristic equation (A1) in the appendix A; \( \varphi_n(z_n) \) are three complex potential functions to be determined from appropriate boundary conditions; \( \varphi'_n(z_n) \) denote the derivatives of \( \varphi_n(z_n) \) with respect to \( z_n \); and the complex constants \( p_n, q_n, s_n, t_n \) and \( \delta_n \) appearing in eqns. 2.3-2.6 are related to the electroelastic properties of the material (Appendix A).

Now consider an elliptic piezoelectric inclusion \( \Omega \) with semi-axes \( a \) and \( b \) in an infinite piezoelectric plane \( V \) as shown in Fig 2.1. The inclusion is subjected to uniform eigenstrains \( \varepsilon^* = (\varepsilon_{11}^*, \varepsilon_{22}^*, 2\varepsilon_{12}^*)^T \) and uniform eigenelectric displacement \( D^* = (D_1^*, D_2^*)^T \). Eigenstrain means a stress-free strain such as a thermal strain or a phase transformation strain, and an eigen electric displacement refers to an electric field free electric displacement such as the spontaneous polarization change induced by domain switching. The objective here is to derive the piezoelectric Eshelby tensor \( Q \) which relates the constrained strains \( \varepsilon_\Omega \) and constrained electric displacement \( D_\Omega \) inside the inclusion to \( \varepsilon^* \) and \( D^* \).

In the presence of eigenfield \( \varepsilon^* \) and \( D^* \), the constitutive relations for the inclusion can be expressed by modifying the eqn. 2.1 as,

\[
\varepsilon - \varepsilon^* = S\sigma + g^T(D - D^*), \quad E = -g\sigma + \beta(D - D^*)
\]

(2.7)

or

\[
\sigma = C(\varepsilon - \varepsilon^*) - e^T E, \quad D - D^* = e(\varepsilon - \varepsilon^*) + K E
\]

(2.8)

where \( C, e \) and \( K \) can be obtained by directly inverting the constitutive relations given by eqn. 2.1 and \( C = (S + g^T q^{-1} g)^{-1} \), \( e = \beta^{-1} g C \), \( K = \beta^{-1} + \beta^{-1} g C g^T \beta^{-1} \).
Following Eshelby’s treatment of an elastic inclusion [72], a three-step decomposition is adopted to obtain the solution for Eshelby tensor. The piezoelectric inclusion is (i) removed from the matrix and allowed to undergo a transformation with strains $\varepsilon^*$ and electric displacement $\mathbf{D}^*$, (ii) restored to its original elliptic shape by applying appropriate surface tractions and a surface charge, and (iii) put back into the matrix, and surface tractions and a surface charge are applied to the inclusion to cancel those introduced in step (ii). Through these operations, the constrained displacements and electric potential produced by $\varepsilon^*$ and $\mathbf{D}^*$ are equivalent to those produced in an identical body without eigenstrains and eigenelectric displacement, but subjected to effective surface tractions $\tau_i^e$ ($i=1,2$) and a surface charge $\rho^e$ acting on the surface of the inclusion, where

$$
\tau_i^e = \sigma_{ij}^e n_j, \quad \rho^e = D_i^e n_i 
$$

(2.9)

$$
\sigma^e = C \varepsilon^*, \quad \mathbf{D}^e = \mathbf{D}^* - \varepsilon \varepsilon^* 
$$

(2.10)

and $n_i$ ($i=1,2$) are the components of the unit outward normal at a point on the surface $\Gamma$ of $\Omega$.

The resulting constrained displacements and electric potential can be obtained by integrating a point source solution over the surface of the elliptic inclusion. The coupled field at a point $\mathbf{x}$ induced by point forces $f_i$ and a point charge $\rho$ acting at a point $\mathbf{x}^*$ on $\Gamma$ is given by eqns. 2.3-2.6 with,

$$
\varphi_n(z_n) = A_n \ln(z_n - z_n^*), \quad n=1, 2, 3
$$

(2.11)

where $z_n^* = x_1^* + \mu_n x_2^*$.

The complex constants $A_n$ are determined from the following set of equations based on the conditions of force and charge equilibrium and single-valued displacements and electric potential.
\[
\text{Im} \sum_{n=1}^{3} \mu_n A_n = \frac{f_1}{4\pi}, \quad \text{Im} \sum_{n=1}^{3} -A_n = \frac{f_2}{4\pi}, \quad \text{Im} \sum_{n=1}^{3} -\delta_n A_n = \frac{\rho}{4\pi}
\] (2.12)

\[
\text{Im} \sum_{n=1}^{3} p_n A_n = 0, \quad \text{Im} \sum_{n=1}^{3} q_n A_n = 0, \quad \text{Im} \sum_{n=1}^{3} s_n A_n = 0
\] (2.13)

After solving the above linear equations for \( A_n \) and using the eqn. 2.9, the solution for \( A_n \) can be expressed as,

\[
A_n = A_{n1} f_1 + A_{n2} f_2 + A_{n3} \rho = F_{n1} n_1^* + F_{n2} n_2^*
\] (2.14)

where \( n_i^* \) are the components of the unit outward normal at \( x^* \) and \( F_{ni} = A_{n1} \sigma_{li}^p + A_{n2} \sigma_{l2}^p + A_{n3} D_{li}^p \) \((i=1, 2)\).

Thereafter the complex potential functions corresponding to the constrained electroelastic field due to the introduction of an elliptic inclusion can be expressed as,

\[
\varphi_n'(z_n) = \oint_{\Gamma} \frac{(F_{n1} n_1^* + F_{n2} n_2^*) ds}{z_n - z_n^*}
\] (2.15)

For a point \( z^* (= x_1^* + ix_2^*) \) on \( \Gamma \), \( n_1^* ds = dx_2^* \) and \( n_2^* ds = -dx_1^* \), and the equation 2.15 is reduced to

\[
\varphi_n'(z_n) = B_n \oint_{\Gamma} \frac{dz^*}{z_n - z_n^*} + C_n \oint_{\Gamma} \frac{d\bar{z}^*}{z_n - z_n^*} = B_n I_n + C_n J_n
\] (2.16)

where \( B_n = -\frac{1}{2} (F_{n2} - iF_{n1}) \), \( C_n = -\frac{1}{2} (F_{n2} + iF_{n1}) \), \( \bar{z}^* \) is the complex conjugate of \( z^* \) and the contour integrals \( I_n \) and \( J_n \) can be evaluated by using the Cauchy's theorem [73].

Inside the piezoelectric inclusion \((x \in \Omega)\), \( I_n \) and \( J_n \) are constant, and

\[
I_n = -\frac{2\pi i (a+b)}{a - ib \mu_n}, \quad J_n = -\frac{2\pi i (a-b)}{a - ib \mu_n}
\] (2.17)
For a point in the matrix \( X \in V \), \( I_n \) and \( J_n \) are given by

\[
I_n = \frac{\pi i[(a + b) - (a - b) / T_n] (X + T_n \bar{X}) - [(X + T_n \bar{X})^2 - 4T_n]^{1/2}}{(a - ib \mu_n) [(X + T_n \bar{X})^2 - 4T_n]^{1/2}}
\]

(2.18)

\[
J_n = \frac{\pi i[(a - b) - (a + b) / T_n] (X + T_n \bar{X}) - [(X + T_n \bar{X})^2 - 4T_n]^{1/2}}{(a - ib \mu_n) [(X + T_n \bar{X})^2 - 4T_n]^{1/2}}
\]

(2.19)

where \( T_n = (a + ib \mu_n) / (a - ib \mu_n) \) and \( X = (z + \bar{z}) / 2a + (z - \bar{z}) / 2b \).

The constrained strains \( \varepsilon_\Omega \) and electric field \( E_\Omega \) inside the inclusion can be expressed in terms of \( \sigma^p \) and \( D^p \) as

\[
\begin{pmatrix}
\varepsilon_\Omega \\
E_\Omega
\end{pmatrix} =
\begin{bmatrix}
P & R \\
M & N
\end{bmatrix}
\begin{pmatrix}
\sigma^p \\
D^p
\end{pmatrix}
\]

(2.20)

where the elements of matrices \( P, R, M \) and \( N \) are determined by eqns. 2.4, 2.6, 2.16 and 2.17.

Note that the strains and the electric field within the inclusion are constant. Similar conclusions can be applied to ellipsoidal elastic inclusions [72]. By considering the symmetry properties of 2-D electroelastic Green's functions (see eqns. 2.11 and 2.14), the following properties of \( P, R, M \) and \( N \) can be established [62].

\[
P^T = P, \quad M^T = R, \quad N^T = N
\]

(2.21)

The piezoelectric Eshelby tensor \( Q \) which relates \( \varepsilon_\Omega \) and \( D_\Omega \) to \( \varepsilon^* \) and \( D^* \) is finally derived by using eqns. 2.8, 2.10 and 2.20 as,

\[
\begin{pmatrix}
\varepsilon_\Omega \\
D_\Omega
\end{pmatrix} = Q
\begin{pmatrix}
\varepsilon^* \\
D^*
\end{pmatrix}
\]

(2.22)

where
The above solution corresponds to specified eigenstrains and eigenelectric displacement in an inclusion and is more readily applicable to domain switching modeling than the previous solutions corresponding to specified eigenstrains and an eigenelectric field [63], [65] as $\varepsilon^*$ and $D^*$ can be directly related to switching induced spontaneous strains and spontaneous polarization. The piezoelectric Eshelby tensor has found applications in the prediction of electroelastic properties of piezoelectric composites [74] and in nonlinear constitutive modeling of ferroelectric materials [16], [18], [19]. Its counterpart, elastic Eshelby tensor, has been widely used to predict the elastic properties of composite materials and to model the mechanical response of materials undergoing phase-transformation, such as shape memory alloys and transformation toughening of ceramics [75, 76].

The electroelastic field at $X \in V$ within the matrix can be expressed as,

$$\begin{bmatrix} \varepsilon(X) \\ D(X) \end{bmatrix} = Q(X) \begin{bmatrix} \varepsilon^* \\ D^* \end{bmatrix}$$

(2.24)

where the constraint tensor $Q(X)$ can be determined by using the eqns. 2.4, 2.6, 2.16, 2.18 and 2.19.

The symmetry property of the piezoelectric Eshelby tensor $Q$ is investigated in the following section. For convenience, the constitutive relations in the $e$-form [eqn. 2.8] are converted into the following $h$-form,

$$\begin{bmatrix} \sigma \\ E \end{bmatrix} = \begin{bmatrix} C^* & -h^T \\ -h & \beta^* \end{bmatrix} \begin{bmatrix} \varepsilon \\ D \end{bmatrix} - \begin{bmatrix} \varepsilon^* \\ D^* \end{bmatrix} = L \begin{bmatrix} \varepsilon \\ D \end{bmatrix} - \begin{bmatrix} \varepsilon^* \\ D^* \end{bmatrix}$$

(2.25)
where \( C' = C + e^T K^{-1} e, \ h = K^{-1} e, \ \beta' = K^{-1}. \)

It can be shown that the piezoelectric Eshelby tensor \( Q \) has the following symmetric property,

\[
(LQ)^T = LQ
\]  
(2.26)

Though a similar result is available in the literature for elastic inclusion problems [75], the corresponding result for a piezoelectric Eshelby inclusion is new.

By using eqn. 2.23, it is easy to verify that

\[
(LQ)_{11} = CPC - CR e + e^T K^{-1} e - e^T MC + e^T Ne
\]

\[
(LQ)_{12} = CM^T - e^T N - e^T K^{-1}, \ (LQ)_{21} = MC - Ne - K^{-1} e
\]

\[
(LQ)_{22} = N + K^{-1}
\]  
(2.27)

It is noted from eqn. 2.27 that the symmetry of \( C \) and \( K \) together with eqn. 2.21 leads to

\[
(LQ)^T = (LQ)_{11}, \ (LQ)^T_{12} = (LQ)_{21}, \ (LQ)^T_{22} = (LQ)_{22}
\]  
(2.28)

Therefore the symmetry [eqn. 2.26] of \( LQ \) is proved. It can be shown that the symmetry of the tensor remains valid for piezoelectric inclusions with arbitrary shape, provided that the eigenfields \( \epsilon^* \) and \( D^* \) are uniform within the inclusion, and the constrained fields in eqn. 2.22 are replaced by their respective average values [62].

2.3 Model for Polarization Switching

In this section, the piezoelectric Eshelby tensor derived in the preceding section is applied to formulate a polarization switching criterion for a crystallite by taking into
account full electromechanical coupling, material anisotropy and changes in material properties of the switched crystallite.

Consider an infinite piezoelectric medium \( V \) with electroelastic moduli \( \mathbf{L} \) [see eqn.2.25], remanent strains \( \mathbf{\varepsilon}^r \) and remanent polarization \( \mathbf{P}^r \). The medium contains an elliptic inhomogeneity \( \Omega \) which has electroelastic moduli \( \mathbf{L}^* \), spontaneous strains \( \mathbf{e}^s \) and spontaneous polarization \( \mathbf{P}^s \), which are in general different from \( \mathbf{L}, \mathbf{\varepsilon}^r \) and \( \mathbf{P}^r \) respectively. When the material is subjected to a remote stress \( \sigma_0 \) and electric field \( E_0 \), the electroelastic field induced due to the presence of the inhomogeneity can be determined by the equivalent inclusion method [63], [72]. The stress and electric field inside the inhomogeneity can be expressed as,

\[
\mathbf{\Sigma} = \mathbf{L}^* (\mathbf{Z}^* - \mathbf{Z}^s + \mathbf{Z}^r) \tag{2.29}
\]

where generalized stress vector \( \mathbf{\Sigma} = (\sigma \mathbf{E})^\top \) and generalized strain vector \( \mathbf{Z} = (\mathbf{e} \mathbf{D})^\top \).

The uniform stress and electric field in the absence of inhomogeneity is denoted by \( \mathbf{\Sigma}^0 \) and is equal to \( \mathbf{L}(\mathbf{Z}^0 - \mathbf{Z}^r) \). Let \( \tilde{\mathbf{\Sigma}} \) and \( \tilde{\mathbf{Z}} \) denote the disturbed generalized stress and strain vectors in the inhomogeneity, then,

\[
\mathbf{\Sigma}^0 + \tilde{\mathbf{\Sigma}} = \mathbf{L}^* (\mathbf{Z}^0 - \mathbf{Z}^s + \tilde{\mathbf{Z}}) \tag{2.30}
\]

It can be shown that the disturbed fields \( \tilde{\mathbf{\Sigma}} \) and \( \tilde{\mathbf{Z}} \) are constant inside the inhomogeneity. Based on this fact, the equivalent inclusion method is introduced [63], [72]. The coupled electroelastic field in the actual inhomogeneity can be obtained by considering an inclusion (by definition, with the same electroelastic moduli \( \mathbf{L} \) as the matrix) of the same shape and orientation with otherwise fictitious eigenstrains and eigenelectric displacement \( \mathbf{Z}^* \). Therefore the stress and the electric field inside the fictitious inclusion can be expressed as.
\[ \Sigma^0 + \tilde{\Sigma} = L(Z^0 - Z^s + \tilde{Z} - Z^r) = L(Z^0 - Z^r + \tilde{Z} - Z^{**}) \]  

(2.31)

where \( Z^{**} = Z^r + Z^s - Z^r \) stands for a modified eigenfield accounting for the difference between the generalized spontaneous and remanent strain vectors in the matrix and the inhomogeneity.

Based on results derived in the preceding section, the constrained strains and electric displacement inside the equivalent inclusion can be expressed in terms of the eigenfield \( Z^{**} \) as,

\[ \tilde{Z} = QZ^{**} \]  

(2.32)

where \( Q \) is the piezoelectric Eshelby tensor [eqn. 2.23].

Equating the stress and electric field [eqn. 2.30] of the actual inhomogeneity and those [eqn. 2.31] of the equivalent inclusion leads to,

\[ Z^{**} = B^{-1}[(L - L^r)(Z^0 - Z^r) + L^s(Z^s - Z^r)] \]  

(2.33)

where \( B = L - (L - L^r)Q \).

The electroelastic field in the elliptic inhomogeneity is consequently determined by eqn. 2.31.

With the electroelastic field of the inclusion determined, the potential energy of the piezoelectric inclusion-matrix system can be obtained. The total potential energy \( U \) of the matrix \( V \) and inhomogeneity \( \Omega \) can be expressed by the summation of the potential energy in the absence of an inhomogeneity \( (U^0) \) and that due to the introduction of an inhomogeneity \( (U^t) \) [55],

\[ U = U^0 + U^t \]  

(2.34)

where
\[ U^0 = \frac{1}{2} \int_{\Omega} \left[ \sigma_{ij}^0 (\varepsilon_{ij}^0 - \varepsilon_{ij}^p) + E_i^0 (D_i^0 - P_i^p) \right] dV - \int_s \sigma_{ij}^0 n_j u_i^0 ds + \int_s \phi^0 D_i^0 n_i ds \]  
(2.35)

\[ U^I = \frac{1}{2} \int_{\Omega} \left[ \sigma_{ij}^0 (\varepsilon_{ij}^0 - \varepsilon_{ij}^p) + E_i^0 (\bar{D}_i - P_i^p) \right] dV - \int_s \sigma_{ij}^0 n_j \bar{u}_i ds + \int_s \phi^0 \bar{D}_i n_i ds \]

\[ + \frac{1}{2} \int_{\Omega} \left[ \bar{\sigma}_{ij} (\varepsilon_{ij}^0 - \varepsilon_{ij}^p) + \bar{E}_i (D_i^0 - P_i^p + \bar{D}_i - P_i^p) \right] dV \]  
(2.36)

with

\[ \varepsilon_{ij}^p = \varepsilon_{ij}^0 - \varepsilon_{ij}^p \quad \text{in} \quad \Omega; \quad \text{and} \quad = 0 \quad \text{in} \quad V \]  
(2.37)

\[ P_i^p = P_i^0 - P_i^p \quad \text{in} \quad \Omega; \quad \text{and} \quad = 0 \quad \text{in} \quad V \]  
(2.38)

and quantities with superscripts '0' and 'p' denote uniform electroelastic field in the absence of an inhomogeneity and the disturbed field due to the presence of an inhomogeneity, respectively, and \( s \) denotes the boundary of the system. McMeeking and Hwang [55] derived the expression of \( U^I \) by decomposing the original inhomogeneity problem into two subproblems: one has nonzero \( \varepsilon_{ij}^p \) and \( P_i^p \) in the inhomogeneity without applied loading, and the other with zero \( \varepsilon_{ij}^p \) and \( P_i^p \) but subjected to applied loading \( \Sigma^0 \).

In this study, the expression of \( U^I \) is derived by generalizing the approach of Mura [76] for elastic inhomogeneity problems.

Applying the divergence theorem [76] to the fifth and the sixth terms of eqn. 2.36,

\[ \frac{1}{2} \int_{\Omega} \bar{\sigma}_{ij} (\varepsilon_{ij}^0 - \varepsilon_{ij}^p + \varepsilon_{ij}^p - \varepsilon_{ij}^0) dV = - \frac{1}{2} \int_{\Omega} \bar{\sigma}_{ij} \varepsilon_{ij}^p d\Omega \]  
(2.39)

\[ \frac{1}{2} \int_{\Omega} \bar{E}_i (D_i^0 - P_i^p + \bar{D}_i - P_i^p) dV = - \frac{1}{2} \int_{\Omega} \bar{E}_i P_i^p d\Omega \]  
(2.40)

Since \( \bar{\sigma}_{ij} n_j = 0 \) and \( \bar{\phi} = 0 \) on the boundary \( s \), \( \bar{\sigma}_{ij,i} = 0 \) and \( \bar{D}_{i,i} = 0 \) in \( V + \Omega \),

\[ \int_{\Omega} \bar{\sigma}_0 dV = 0 \quad \text{and} \quad \int_{\Omega} \bar{E}_i dV = 0. \]
By introducing the equivalent inclusion with eigenstrains $\varepsilon_0^*$ and eigenelectric displacement $D_i^*$, it is easy to verify that, the first and the second terms in eqn. 2.36,

$$\frac{1}{2} \int_{V+\Omega} [\sigma_{ij}^0 (\varepsilon_{ij}^0 - \varepsilon_{ij}^p) + E_i^0 (D_i^0 - P_i^p)]dV$$

$$= \frac{1}{2} \int_{V+\Omega} [\sigma_{ij}^0 (\varepsilon_{ij}^0 - \varepsilon_{ij}^p) + E_i^0 (D_i^0 - P_i^p) + \sigma_{ij}^0 \varepsilon_{ij}^* + E_i^0 D_i^*]dV$$

$$= \frac{1}{2} \int_{\Omega} (\sigma_{ij}^0 \varepsilon_{ij}^* + E_i^0 D_i^*)d\Omega$$ (2.41)

Applying the divergence theorem to the third and the fourth terms of eqn. 2.36 and in view of eqn. 2.41,

$$\int_S \sigma_{ij}^0 n_j \tilde{u}_i ds - \int_S \phi^0 \tilde{D}_i n_i ds = \int_{V+\Omega} (\sigma_{ij}^0 \varepsilon_{ij}^* + E_i^0 \tilde{D}_i) dV$$

$$= \int_{\Omega} [\sigma_{ij}^0 (\varepsilon_{ij}^* + \varepsilon_{ij}^p) + E_i^0 (D_i^* + P_i^p)] d\Omega$$ (2.42)

Finally, the contribution of the inhomogeneity to the potential energy is obtained as,

$$U' = -\frac{1}{2} \int_{\Omega} [\sigma_{ij}^0 (\varepsilon_{ij}^* + \varepsilon_{ij}^p) + E_i^0 (D_i^* + P_i^p)] d\Omega - \frac{1}{2} \int_{\Omega} [(\sigma_{ij}^0 + \tilde{\sigma}_{ij}) \varepsilon_{ij}^p + (E_i^0 + \tilde{E}_i) P_i^p] d\Omega$$

$$= -\frac{mub}{2} [(\Sigma^0)^T \mathbf{Z}^{**} + (\Sigma^1)^T \mathbf{Z}^p]$$ (2.43)

where $\Sigma^1$ denotes the stress and electric fields inside the inhomogeneity.

The first term in eqn. 2.43 denotes the interaction between the external field $\Sigma^0$ with the modified eigenfield $\mathbf{Z}^{**}$, while the second term expresses the interaction of the internal field $\Sigma^1$ with the transformation strains and polarization $\mathbf{Z}^p (= \mathbf{Z}^* - \mathbf{Z}^r)$. 

39
The complete solution for potential energy release during polarization switching of an elliptic inhomogeneity is now derived using the results obtained in the preceding sections. When an elliptic inhomogeneity (crystallite) with electroelastic moduli $L_1$ and spontaneous field $Z_1^s$ is switched to another state with electroelastic moduli $L_2$ and spontaneous field $Z_2^s$ in a poled ferroelectric material which has moduli $L$ and remanent field $Z_r$, the potential energy reduction $\Delta U$ due to switching from state 1 to 2 is given by,

$$\Delta U = U_1 - U_2 = (U^0 + U_1^p) - (U^0 + U_2^p)$$  (2.44)

Using the potential energy expression (2.43) together with the symmetry of the electroelastic moduli $L$, $L_1$, $L_2$ and the piezoelectric Eshelby tensor [eqn. 2.26], it can be shown that (see Appendix A),

$$\Delta U = \frac{\pi ab}{2} [(\Sigma_1^1 + \Sigma_2^1)^T (Z_2^p - Z_1^p) + (\Sigma_1^1)^T (L_2^{-1} - L_1^{-1}) \Sigma_2^1]$$  (2.45)

Note that the above result derived using the Eshelby inclusion model is new and is identical to the local energy release due to polarization switching which was obtained very recently by Kessler and Balke [77]. Therefore, the present study established the equivalence between the approach used by Kessler and Balke and the Eshelby inclusion model.

For a ferroelectric crystallite to switch, the driving force associated with the reduction in the total potential energy should overcome the conjugate friction force corresponding to energy dissipation with domain wall nucleation and propagation. By treating the switching of a ferroelectric crystallite as an instantaneous process and assuming there exists a critical energy barrier for domain switching as introduced by Hwang et al. [15], a crystallite is predicted to switch [based on eqn. 2.45] when

$$\frac{1}{2} [(\Sigma_1^1 + \Sigma_2^1)^T (Z_2^p - Z_1^p) + (\Sigma_1^1)^T (L_2^{-1} - L_1^{-1}) \Sigma_2^1] \geq G_c$$  (2.46)
where the left-hand side is the specific potential energy release during domain switching while the right-hand side denotes the critical energy barrier associated with polarization switching.

Note that the critical energy barrier may be different for 90° and 180° degree switching. For given electromechanical loading, the actual switching direction selects that with largest energy release, if more than one switching direction simultaneously satisfies the switching criterion (2.46).

The first term in the left-hand side of eqn. (2.46) expresses the work done by the average stress and electric fields before and after switching to the changes in spontaneous strains and spontaneous polarization. The second term characterizes the contribution of the changes in electroelastic moduli to the energy release and can play an important role in domain switching modeling. Though the anisotropy in elastic and dielectric properties may be small, the change in piezoelectric constants may not be neglected since they are directionally dependent. Moreover, the second term in eqn. (2.46) has to be considered when the electroelastic field is quite high such as in the prediction of nonlinear process zone (switching zone) around a crack tip.

By neglecting the differences between the local electroelastic field and the applied external field, the above switching criterion is further simplified as

\[
(\Sigma^0)^T(Z^p_2 - Z^p_1) + \frac{1}{2}(\Sigma^0)^T(L_2^{-1} - L_1^{-1})\Sigma^0 \geq G_c
\]  \hspace{1cm} (2.47)

For weakly anisotropic ferroelectric materials \((L_1 = L_2)\) under moderate electromechanical loading far from their coercive fields, the switching criterion eqn. 2.47 can be further reduced to that of Hwang et al. [15]

\[
(\Sigma^0)^T(Z^p_2 - Z^p_1) \geq G_c
\]  \hspace{1cm} (2.48)
2.4 Ferroelectric Domain Evolution

Without going to the details of the nonequilibrium thermodynamic process of polarization switching, a criterion that predicts the critical load to uniformly switch a crystallite in a ferroelectric is obtained in the preceding section. Polarization switching is realized through nucleation and subsequent movement of domain walls. The load to uniformly switch a ferroelectric is much larger than that needed to trigger a domain wall movement [66]. Direct observation of domain wall movement in single crystals during the application of electrical and mechanical fields has been reported. For example, Munoz-Saldana et al.[78] studied stress induced domain wall movement in BaTiO$_3$ single crystals by scanning force microscopy (SFM). However, direct observation of movement of domain walls in polycrystals is nontrivial due to grain-grain interaction and material complexities. In this section, domain evolution in a single crystal material is simulated by using the Eshelby tensor solution derived in the previous section.

Loge and Suo [66] established a theoretical framework based on variational principles to simulate ferroelectric domain evolution. They described the energetics and kinetics for domain evolution and presented numerical results for 180° and 90° domain nuclei evolution in single crystal BaTiO$_3$ in the absence of electromechanical coupling and material anisotropy. In this study, a new free energy expression based on the linear description of a ferroelectric near its spontaneous state is instead used to simulate domain evolution.

Consider the evolution of an elliptic cylindrical nucleus with electroelastic moduli $L'$, spontaneous strains $\varepsilon'$ and spontaneous polarization $P'$ in a large parent domain with electroelastic moduli $L$ [see eqn. 2.25 for definition], spontaneous strains $\varepsilon$ and spontaneous polarization $P$ subjected to external electromechanical loading $\Sigma^o$. The geometry of the evolving nucleus can be described by two generalized coordinates, i.e. the semi-axes $a$ and $b$. In view of the results in Section 2.3 [eqn. 2.43], the Gibbs free
energy due to the introduction of the nucleus into the parent ferroelectric domain can be expressed as,

$$G(a, b) = \Lambda s - \frac{\pi ab}{2}[(\Sigma^0)^T \mathbf{Z}^{**} + (\Sigma^1)^T \mathbf{Z}^p]$$  \hfill (2.49)$$

where the first and the second terms denote the domain wall energy and the potential energy due to introduction of the elliptic nucleus, respectively, $\Lambda$ is the domain wall energy density (assumed to be isotropic in this study) and $s$ the circumference of the elliptic nucleus.

By assuming the thermodynamic pressure is proportional to the velocity of domain wall movement and minimizing a functional consisting of the free energy rate and a dissipation potential, the following ordinary differential equations which govern the evolution of an elliptic nucleus can be obtained [66],

$$\begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} \begin{bmatrix} \frac{d\theta}{dt} \\ \frac{df_a}{dt} \\ \frac{df_b}{dt} \end{bmatrix} = \begin{bmatrix} f_a \\ f_b \end{bmatrix}$$  \hfill (2.50)$$

where $\mathbf{H}$ is a viscosity matrix, $f_a$ and $f_b$ are thermodynamic driving forces and

$$H_{11} = \int_0^{2\pi} \frac{b^2 \cos^4 \theta}{M \sqrt{a^2 \sin^2 \theta + b^2 \cos^2 \theta}} d\theta$$  \hfill (2.51)$$

$$H_{22} = \int_0^{2\pi} \frac{a^2 \sin^4 \theta}{M \sqrt{a^2 \sin^2 \theta + b^2 \cos^2 \theta}} d\theta$$  \hfill (2.52)$$

$$H_{12} = H_{21} = \int_0^{2\pi} \frac{ab \sin^2 \theta \cos^2 \theta}{M \sqrt{a^2 \sin^2 \theta + b^2 \cos^2 \theta}} d\theta$$  \hfill (2.53)$$

with $M$ denoting the domain wall mobility. Given initial semi-axes of an elliptic nucleus, its evolution history can be traced by numerically integrating the differential equations given by (2.50).
The generalized forces associated with the evolution of an elliptic nucleus is calculated by

\[
f_a = -\frac{\partial G}{\partial a} = -\Lambda \frac{\partial s}{\partial a} + \frac{\pi b}{2} [(\Sigma^0)^T Z^{**} + (\Sigma^1)^T Z^p] + \frac{\pi ab}{2} [(\Sigma^0)^T \frac{\partial Z^{**}}{\partial a} + (\Sigma^1)^T \frac{\partial Z^p}{\partial a}] \tag{2.54}
\]

\[
f_b = -\frac{\partial G}{\partial b} = -\Lambda \frac{\partial s}{\partial b} + \frac{\pi a}{2} [(\Sigma^0)^T Z^{**} + (\Sigma^1)^T Z^p] + \frac{\pi ab}{2} [(\Sigma^0)^T \frac{\partial Z^{**}}{\partial b} + (\Sigma^1)^T \frac{\partial Z^p}{\partial b}] \tag{2.55}
\]

where

\[
\frac{\partial s}{\partial a} = \int_0^{2\pi} \frac{a \sin^2 \theta}{\sqrt{a^2 \sin^2 \theta + b^2 \cos^2 \theta}} d\theta \tag{2.56}
\]

\[
\frac{\partial s}{\partial b} = \int_0^{2\pi} \frac{b \cos^2 \theta}{\sqrt{a^2 \sin^2 \theta + b^2 \cos^2 \theta}} d\theta \tag{2.57}
\]

\[
\frac{\partial Z^{**}}{\partial a_i} = B^{-1}(L - L') \frac{\partial Q}{\partial a_i} Z^{**} \quad (a_i = a, b) \tag{2.58}
\]

\[
\frac{\partial \Sigma^1}{\partial a_i} = [L(Q - I)B^{-1}(L - L') + L] \frac{\partial Q}{\partial a_i} Z^{**} \quad (a_i = a, b) \tag{2.59}
\]

and \(I\) denotes a 5 by 5 identity matrix.

Numerical solutions based on eqn. 2.50 for 180° and 90° domain nuclei evolution in BaTiO₃ single crystals are presented to show the major features of 2-D domain evolution. The electroelastic material constants of BaTiO₃ single crystal poled in the \(x_3\)-direction are given by [5]

\[
c_{11} = 27.5, \quad c_{12} = 15.16, \quad c_{13} = 17.89, \quad c_{22} = 16.48, \quad c_{44} = 5.43 \quad (10^{10} \text{ N/m}^2)
\]

\[
e_{21} = -2.69, \quad e_{22} = 3.65, \quad e_{16} = 21.3 \quad \text{(C/m}^2\text{)}
\]

\[
k_{11} = 17.4, \quad k_{22} = 0.96 \quad (10^{-9} \text{ F/m})
\]

and spontaneous strain, \(\varepsilon_s = 0.01\) and spontaneous polarization, \(P_s = 0.26 \text{ C/m}^2\).
2.4.1 180° domain nucleus

![Diagram of 180° domain nucleus in BaTiO₃ single crystal.]

Figure 2.2. 180° domain nucleus in BaTiO₃ single crystal.

When a ferroelectric crystal is subjected to a large electric field opposite to its polar direction, the electric field tends to rotate the polar direction by 180°. This leads to 180° domain nucleus (Fig. 2.2). By neglecting electromechanical coupling, the Gibbs free energy due to the introduction of a 180° nucleus into the parent domain can be determined solely by electrostatics, see Loge and Suo [66] and Landauer [79] for details.

Figures 2.3(a) and 2.3(b) show the contours of constant levels of Gibbs free energy without and with the piezoelectric coupling, respectively. The results in Fig. 2.3(a) correspond to an isotropic permittivity, $k = 1.0 \times 10^{-8}$ F/m. In order to examine the effects of electromechanical coupling and material anisotropy, the electric field loading for both cases is set to identical value, i.e. $E_2^\infty = -0.5$ MV/m, which is about five times the coercive electric field of the material [80]. Domain wall energy density and domain
wall mobility for 180° domain nucleus are estimated to be $\Lambda = 0.01 \text{ J/m}^2$ and $M = 4.8 \times 10^{-4} \text{ m}^3/\text{s N}$, respectively [66]. A characteristic length $l_0 = \Lambda k/\mu^2$ is used to normalize the semi-axes $a$ and $b$. When a needle-shaped domain ($a = 0$ or $b = 0$) elongates, the potential energy terms [see eqn. (2.49)] vanish and the domain wall energy increases the total free energy. Along a path with large aspect ratio $b/a$, the free energy increases with increasing nucleus size for a smaller nucleus, reaches a peak at the saddle point and then decreases with increasing nucleus size for a larger nucleus. The free energy contour has a saddle point at $(a, b) \approx (33l_0, 3400l_0)$ in Fig. 2.3(a), while it sees a saddle point $(a, b) \approx (33l_0, 7300l_0)$ in Fig. 2.3(b). Due to electromechanical coupling and highly anisotropic dielectric properties of BaTiO$_3$ single crystal, the 180° nucleus tends to evolve in a path with even higher aspect ratio when compared to a case that neglects both electromechanical coupling and material anisotropy.

The free energy contours shown in Figure 2.3 can provide qualitative answers to the fate of a 180° domain nucleus in a material. Since the free energy decreases as the domain wall evolves, a small nucleus far from the saddle point of the energy surface tends to shrink and the nucleus is free to expand beyond the saddle point [79]. Figures 2.4(a) and 2.4(b) show the time history of the semi-axes $a$ and $b$ during evolution respectively. As an illustrative example, the initial semi-axes are set to $a = 200l_0$ and $b = 8000l_0$ (beyond the saddle point) in the following simulation. The electric field loading level is identical to that of Fig. 2.3. A characteristic time $t_0 = l_0^2/MA$ is used to normalize the evolution time. To decrease the free energy, the semi-axis ($a$) perpendicular to the polar direction of the nucleus decreases first and then increases with time. When the material is modeled as an isotropic dielectric, the semi-axis ($b$) parallel to the polar direction elongates approximately proportional to the time. When the material is modeled as an anisotropic dielectric or a piezoelectric, the evolution history is more complicated. Note that the magnitudes of $a$ and $b$ corresponding to the coupled solution are lower and higher than their corresponding isotropic uncoupled solutions,
Figure 2.3. Free energy contours \((G/2\pi\gamma\Lambda)\) for a 180° domain nucleus, (a) isotropic, uncoupled solution, (b) anisotropic, coupled solution.
Figure 2.4. Evolution of a 180° elliptic domain nucleus with time, (a) the semi-axis $a$, and (b) the semi-axis $b$. 
respectively. This implies that a 180° nucleus tends to evolve in a path with a higher aspect ratio when both electromechanical coupling and material anisotropy are considered. The effect of dielectric anisotropy on 180° domain evolution is also highlighted. Additional simulations of nuclei with other initial dimensions showed evolution behavior very similar to those presented in Fig. 2.4.

The effect of a compressive stress along the polar direction on domain evolution is also investigated. To this end, the growth of a 180° nucleus under the same electric loading ($E_2^- = -0.5\text{MV/m}$) combined with a compressive stress $\sigma_{22}^-$ up to -10 MPa is simulated. The numerical solutions are nearly identical to those of Fig. 2.4. It implies that a compressive stress applied along the polar direction has little effect on 180° domain evolution. This is somewhat consistent with the finding of Burcsu [80], who found that the coercive electric field of BaTiO$_3$ single crystal was relatively insensitive to applied stress.

2.4.2 90° domain nucleus

A ferroelectric crystal tends to rotate its polar direction by 90° when it is subjected to a compressive stress applied parallel to the polar direction. Alternatively, a tensile stress or an electric field perpendicular to the polar axis can also induce a 90° polar rotation (Fig. 2.5). It is known that 90° nucleus grows at 45° away from the polar axis of the parent domain [81]. In the following simulation, the polar axes of the nucleus and the parent domain are directed along the $x_1$- and $x_2$-axis, respectively. For BaTiO$_3$ single crystals, the electric and stress loading shown in Fig. 2.5 results in a compressive normal stress $\sigma_{33}^- = -0.36\sigma_{11}^-$ and a 90° domain nucleus in the $x_1x_2$-plane. Numerical results for 90° domain evolution are given in the following.
Figures 2.6(a) and 2.6(b) show the contours of the Gibbs free energy without and with the anisotropic and piezoelectric effects respectively. The nucleus-parent domain system is subjected to pure mechanical loading $\sigma_{22}^{\infty} = -\sigma_{11}^{\infty} = -15 \text{ MPa}$, which is about half the uniaxial coercive stress for 90° domain switching [78]. The isotropic uncoupled solutions [Fig. 2.6(a)] correspond to permittivity $k = 10^{-8} \text{ F/m}$, shear modulus, $\mu = 50 \text{ GPa}$ and Poisson’s ratio, $\nu = 1/3$. The domain wall energy density for 90° domain nucleus is estimated to be $\Lambda = 0.002 \text{ J/m}^2$ [66]. A characteristic length $l_0 = \Lambda / \mu \gamma_s^2$ (switching strain $\gamma_s = 0.015$) is used to normalize the semi-axes $a$ and $b$. The qualitative behavior of the Gibbs free energy contour for 90° domain nucleus is similar to that of 180° domain nucleus shown in Fig. 2.4. The free energy contour has a
saddle point at \((a, b) \approx (32l_0, 5700l_0)\) when the material is modeled as an isotropic elastic dielectric [Fig. 2.6(a)], while it sees a saddle point \((a, b) = (32l_0, 5100l_0)\) if the crystal is treated as a piezoelectric [Fig. 2.6(b)]. Note that the solutions shown in Fig. 2.6(a) and Fig. 2.6(b) are very similar. This can be explained by the fact that the crystal is under pure mechanical loading and the elastic moduli of BaTiO₃ are weakly anistropic in contrast to its dielectric properties.

Though the qualitative behavior of the evolution of a 90° domain nucleus is similar to that of a 180° domain nucleus, some numerical results for 90° domain evolution are presented in the following. Figure 2.7 shows the time history of the semi-axes \(a\) and \(b\) during the evolution respectively. As an example, the initial semi-axes are set to \(a = 500l_0\) and \(b = 5000l_0\) respectively. Both the isotropic uncoupled and the anisotropic coupled solutions are presented. A characteristic time \(t_0 = l_0^2 / M\Lambda\) is used to normalize the evolution time. The semi-axis \(a\) decreases first and then increases almost linearly with the evolution time. The semi-axis \(b\) increases sharply during the initial adjustment period and thereafter increases linearly with time. The forward wall motion (along the \(x_2\)-direction) is much faster than the side wall motion (along the \(x_1\)-direction). An electric field \((E_i^\text{m})\) applied perpendicular to the polar direction of the parent domain is shown to assist 90° domain growth in both directions, because \(E_i^\text{m}\) decreases the Gibbs free energy and tends to make the nucleus circular. The effects of material anisotropy and electromechanical coupling on a 90° domain nucleus are less distinct than a 180° domain nucleus.
Figure 2.6. Free energy contours ($G / 2\pi l_0 \Lambda$) for a 90° domain nucleus, (a) isotropic, uncoupled solution, (b) anisotropic, coupled solution.
Figure 2.7. Evolution of a 90° elliptic domain nucleus with time, (a) the semi-axis $a$, and (b) the semi-axis $b$. 

---

(a) Normalized semi-axis, $a/t_0$

(b) Normalized semi-axis, $b/t_0$
2.5 Energy Release Rate for Elliptic Flaw

Previous studies on cracks in ferroelectric materials are based on linear piezoelectric constitutive relations in the absence of remanent strains and remanent polarization. As noted by Landis and McMeeking [67], remanent strains and remanent polarization can play an important role in the energy release rate calculation for cracks in ferroelectric materials. In this section, the electroelastic field and the energy release rate of an elliptic void are re-examined by including the effects of remanent strains and remanent polarization.

Consider an elliptic flaw of semi-axes $a$ and $b$ in a poled ferroelectric ceramic with electroelastic moduli $L$, remanent strains $e^r$ and remanent polarization $P^r$ subjected to far field stress field $\sigma^{ff}_ij$ and electric field $E^{ff}_i$. The resulting electroelastic field due to the presence of the elliptic flaw can be simulated by the equivalent inclusion method described in Sec. 2.2. The elliptic flaw can be modeled as a piezoelectric inhomogeneity with vanishing elastic and piezoelectric constants and non-vanishing dielectric constants. Isotropic permittivity $k_c$ is assumed for the flaw in this study. The solutions for impermeable and conducting cracks can be recovered by setting the permittivity $k_c = 0$ and $\infty$, respectively. The electroelastic field outside the flaw is obtained by, (i) determining the equivalent eigenfield $Z'^m$ [eqn. 2.33] and (ii) using the constraint tensor $Q(X)$ of eqn. 2.24 to evaluate the electroelastic field. Numerical solutions are presented in the following for a flaw in PZT-4 poled in the $x_3$ direction. The material constants of PZT-4 are given by [31]

\[
\begin{align*}
c_{11} &= 13.9, \quad c_{12} = 7.43, \quad c_{13} = 7.78, \quad c_{33} = 11.3, \quad c_{44} = 2.56 \quad (10^{10} \text{ N/m}^2) \\
e_{21} &= -6.98, \quad e_{22} = 13.84, \quad e_{16} = 13.44 \quad (\text{C/m}^2) \\
k_{11} &= 6.00, \quad k_{22} = 5.47 \quad (10^{-9} \text{ F/m})
\end{align*}
\]
Fig. 2.8(a) and Fig. 2.8(b) show the variation of normal stress $\sigma_{22}$ in front of the right major apex of an elliptic flaw (vacuum inside with $k_c = 8.85 \times 10^{-12}$ F/m) with the aspect ratio $\alpha = b/a$ for zero and non-zero remanent strains and remanent polarization, respectively. Remanent strains $\varepsilon^r = (-0.001, 0.002, 0)^T$ and remanent polarization $\mathbf{P}^r = (0.0, 0.30)^T$ are assumed in the numerical study [82]. A crack of 2mm subjected to $\sigma_{22}^* = 20$ MPa has a stress intensity factor that is close to the fracture toughness of PZT-4. As shown in Fig. 2.8, the normal stress is highly concentrated near the apex of the flaw. This concentration intensifies as the aspect ratio $\alpha$ decreases and $\sigma_{22}$ becomes singular as $\alpha$ approaches zero, which corresponds to the case of a center slit crack. The effect of remanent strains and remanent polarization on the normal stress at the major apex is trivial. Additional numerical results have been obtained for impermeable ($k_c = 0$), conducting ($k_c = \infty$) and permeable flaws with dielectric constant other than that of a vacuum. These results confirm that remanent strains and polarization have a negligible influence on $\sigma_{22}$ at the major apex, regardless of the permittivity of the elliptic flaw.

Figures 2.9(a) and 2.9(b) show the distribution of electric field $E_2$ in front of the right major apex with $\alpha$. The electric field is concentrated near the major apex and its magnitude decreases as $\alpha$ decreases. When $\alpha$ approaches zero, the elliptic flaw is reduced to a permeable crack and $E_2$ remains finite (non-singular), which is different from the behaviour of $\sigma_{22}$. Remanent strains and remanent polarization have a significant influence on $E_2$ ahead of the major apex. The effect of remanent polarization is equivalent to that of a very strong electric field loading of a flaw (vacuum inside). Additional numerical results have been carried out for impermeable ($k_c = 0$) and conducting ($k_c = \infty$) flaws. For an impermeable flaw, $E_2$ becomes singular as $\alpha$ approaches zero. The electric field corresponding to a non-zero remanent field is much higher than that corresponding to a zero field. For a conducting flaw, $E_2$ remains finite.
Figure 2.8. Stress $\sigma_{22}$ ahead of the right major axial apex of an elliptic void, (a) without and (b) with the effects of remanent strains and remanent polarization.
\( \sigma_{zz} = 20 \text{ (MPa)} \)
\( E_z^* = 0.1 \text{ (MV/m)} \)
\( a = 1.0 \text{ mm} \)

Figure 2.9. Electric field \( E_2 \) ahead of the right major axial apex of an elliptic void, (a) without and (b) with the effects of remanent strains and remanent polarization.
even for the degenerated case of a conducting crack and the remanent field has a negligible effect on both the stress and electric fields.

Now consider the energy release rate of an elliptic flaw in a poled ceramic. During the growth of a flaw, the ratio of the minor semi-axis to the major semi-axis ($\alpha = b/a$) is assumed to be constant, which implies self-similar propagation. Therefore, the total potential energy of the system is,

$$U = U^0 - \frac{ma^2}{2}[\alpha (\Sigma^0)^T Z^{**} + \alpha (\Sigma^1)^T Z^p]$$

(2.60)

where $U^0$ is the potential energy of medium without a flaw when subjected to the same remote loading.

Since the piezoelectric Eshelby tensor for an elliptical inclusion is uniquely determined by the aspect ratio $b/a$ (see eqn. 2.17 for details), the terms inside the bracket of the right-hand side of eqn. 2.60 remain unchanged during flaw propagation. Following the calculation of the energy release rate of an elliptic flaw in an isotropic elastic dielectric [83], the energy release rate ($J$) for self-similar propagation of a flaw in a ferroelectric can be expressed by,

$$J = -\frac{1}{2} \frac{\partial U}{\partial a} = \frac{ma}{2}[\alpha (\Sigma^0)^T Z^{**} + \alpha (\Sigma^1)^T Z^p]$$

(2.61)

or,

$$J = \frac{ma}{2} \alpha (\Sigma^0)^T A^{-1} (L - L^*)L^{-1} \Sigma^0 + \frac{ma}{2} \alpha (Z^p)^T [I + (L^*)^T (A^{-1})^T + L(Q - I)A^{-1}$$

$$\quad (L - L^*)L^{-1}]\Sigma^0 + \frac{ma}{2} \alpha (Z^p)^T L(Q - I)A^{-1}L^*Z^p$$

(2.62)

where $I$ denotes a $5 \times 5$ identity matrix.
The above result that takes into consideration the effects of remanent strains and remanent polarization is new. The quadratic term in eqn. 2.62 is actually the classical result based on linear piezoelectricity without the effect of the remanent field, the linear term in the equation is due to the interaction of applied loading with remanent strains and remanent polarization, and the third term is exclusively dependent on remanent field. The effect of the remanent field on the energy release rate is clearly and explicitly identified in the present derivation.

Let $J$ and $J'$ denote the energy release rates for a slit crack without and with the effect of remanent strains and remanent polarization respectively. For a permeable crack ($k_e = \text{finite but nonzero}$) in PZT-4,

$$J = a[2.7671(\sigma_{12}^m)^2 + 3.6292(\sigma_{22}^m)^2]\times10^{-11}$$

$$J' = J + a[1.8996\sigma_{11}^m + 0.1441\sigma_{22}^m - 1.0685\times10^2 E_2^m]\times10^{-7} - a\times159.7420$$

and the energy release rate is independent of the remote electric field parallel to the crack face. Note that the above solution for $J$ is identical to that of Zhang et al. [45].

The solutions for $J$ and $J'$ for an insulating crack are,

$$J = a[-4.3698\times10^3(\sigma_{11}^m)^2 + 2.7671\times10^3(\sigma_{12}^m)^2 + 3.6267\times10^3(\sigma_{22}^m)^2 + 0.4916\sigma_{11}^m E_2^m + 3.7299\times10^2 \sigma_{22}^m E_2^m - 13.8254\times10^{-2}(E_2^m)^2]\times10^{-9}$$

$$J' = J + a[1.4699\times10^{-2} \sigma_{11}^m + 1.1152\times10^{-3} \sigma_{22}^m - 0.8268 E_2^m] - a\times1.2360\times10^7$$

and $J$ is identical to the solution of Zhang et al. [45] except for a sign error in the first term of their results. A remote electric field applied parallel to the crack face has no influence on $J$ and $J'$. The results with and without the consideration of a remanent field are substantially different. The physical explanation is that remanent strains and remanent polarization can cause residual strain energy and depolarization energy, which could significantly contribute to the energy release of an impermeable flaw.
The energy release rates for a conducting crack with and without the effects of remanent strains and remanent polarization are

\[ J = J' = a[17.966(E_1^e)^2 + 3.4025 \times 10^{-2}(\sigma_{12}^w)^2 + 3.6292 \times 10^{-2}(\sigma_{22}^w)^2 + 67.578\sigma_{12}^w E_1^e] \times 10^{-9} \quad (2.67) \]

The last term is neglected in the results of Zhang et al. [45]. An electric field perpendicular to the crack surface does not contribute to the energy release rate, because it cannot disturb the electroelastic field. Eqn. 2.66 implies that an electric field applied parallel to a conducting crack can drive the crack to propagate. The energy release rates (eqns. 2.63–2.67) show that the dielectric property of a center slit crack significantly affects its propagation behavior.

To further investigate the effects of a remanent field on the energy release rate, elliptic flaws with different aspect ratios and different dielectric properties are studied. Fig. 2.10 shows the variation of energy release rate for an elliptic vacuum flaw \( k_c = 8.85 \times 10^{-12} \text{F/m} \) with the magnitude of electrical field \( E_2 \) for different aspect ratios. The mechanical loading is represented by \( \sigma_{22}^\infty = 20 \text{MPa} \). In the absence of a remanent field, both a positive and a negative electric field tend to reduce the energy release rate and thus retard flaw growth. However, a positive field tends to decrease the energy release rate, while a negative field tends to increase it, when the effect of a remanent field is considered. In both cases, the effect of an applied electric field on the energy release rate diminishes as the aspect ratio decreases. The solution for a very slender elliptic flaw \( (\alpha = 10^{-5}) \) approaches the limiting case of a permeable crack (Eqns. 2.63 and 2.64), while the solution for an impermeable crack (Eqns. 2.65 and 2.66) is closer to that of a blunt elliptic flaw \( (\alpha = 10^{-2}) \). Similar findings were obtained by Dunn [44] for the Mode III case corresponding to out-of-plane shear and in-plane electrical loading. Fig. 2.10(b) shows that the magnitude of the energy release rate in the presence of a remanent field depends significantly on the geometry \( (\alpha = b/a) \) of the flaw.
Fig. 2.11 shows the variation of the energy release rate with $E_2$ for elliptic flaws with different dielectric constants ($k_c$) but identical aspect ratio ($\alpha = 10^{-3}$). In Fig. 2.11, the solutions are shown for $k_c$ normalized with respect the dielectric permittivity of a vacuum ($k_0 = 8.85 \times 10^{-12}$ F/m). The solutions corresponding to $k_c / k_0 = 10^{-3}$ are closer to the limiting case of an impermeable crack, while the solutions for $k_c / k_0 = 10^3$ are closer to that of a conducting crack. As the dielectric constant of the flaw increases, the effect of the applied electric field on the energy release rate diminishes. In the limiting case of a conducting flaw, $E_2$ has indeed no effect on the energy release. It is noted from Fig. 2.10 and Fig. 2.11 that a remanent field may have significant effects on the energy release of an elliptic flaw, especially in the case of an impermeable flaw. However, for a conducting flaw, a remanent field shows no effect on the electroelastic field and consequently the energy release rate.

The geometry, dielectric property and presence of remanent field significantly affect the electroelastic field and energy release rate of an elliptic flaw in a ferroelectric. A remanent field shows a minor effect on the stress profile. However, its effects on the electric field and the energy release rate are quite pronounced and seem to be overestimated as far as the magnitude of the energy release rate is concerned. This may result from two assumptions made previously, i.e. a linear description for the material behavior of ferroelectrics and self-similar propagation of an elliptic flaw. Highly concentrated electric and stress fields near the boundary of a flaw could practically lead to domain switching which dissipates energy during flaw growth. To accurately calculate the energy release rate during flaw growth, finite element models for ferroelectrics with nonlinear constitutive relations accounting for polarization switching are required. Moreover, the assumption of self-similar propagation of flaws and cracks may not be valid as poled ferroelectric ceramics are in general anisotropic and crack branching has been observed in experiments [20, 22, 51].
Figure 2.10. Effect of the slenderness of an elliptic vacuum void on the energy release rate $J$, (a) without and (b) with the effects of remanent strains and remanent polarization.
Figure 2.11. Effect of the dielectric property of an elliptic void on the energy release rate $J$, (a) without and (b) with the effects of remanent strains and remanent polarization.
Chapter 3

THEORETICAL MODELING OF DOMAIN SWITCHING EFFECTS ON FRACTURE

3.1 Overview

An important non-linearity in fracture of ferroelectric materials is associated with the polarization switching zone induced at the tip of a crack. Fracture toughness variation (change of stress intensity factors) due to such localized switching near the tip of an insulating or a conducting crack is investigated in this chapter with the objective of explaining some of the experimentally observed behavior. First, the shape of switching zone around a crack tip is predicted by using the domain switching criterion presented in the previous chapter. Thereafter, fracture toughness variation of conducting and insulating crack is evaluated by using a scheme similar to that used in the study of transformation toughening of ceramics [58-60]. In order to extend the transformation toughening model to the present class of problems, the solutions for electroelastic field intensity factors of a semi-infinite insulating or conducting crack induced by stress-free transformation strains and electric field-free polarization have to be derived. These solutions are used to compute the modified field intensity factors at the crack tip. Numerical solutions for switching-induced stress intensity factors (toughness variation) are presented for electrical, mechanical and combined loading. The role of an electric field on the propagation of insulating and conducting cracks under combined loading is investigated and compared qualitatively with experimental results.

Under some loading and poling configurations, crack closure takes place in ferroelectric materials. The contact of crack surfaces under electric loading has been observed in experiments [50, 51] and in the finite element modeling of insulating cracks [84, 85]. Ru [86] was the first to theoretically investigate electric field-induced crack closure. In this study, the loading conditions for crack closure are derived and the case of
a closed crack is formulated by using the extended Lekhnitskii’s formalism. Explicit expressions are derived for crack closure conditions for both insulating and conducting cracks under arbitrary poling directions. Moreover, polarization switching near a closed insulating or conducting crack tip is investigated and its effect on the near-tip field is examined.

3.2 Domain Switching Zone Near A Crack Tip

Consider an insulating (or a conducting) center crack of length $2a$ in a ferroelectric material poled at an angle $\phi$ with the $x_1$ axis (Fig. 3.1). The material is subjected to remote stress $\sigma_{ij}^\infty$ and remote electric field $E_i^\infty$. If the crack is open under the electromechanical loading, both the normal and the tangential tractions vanish at the crack. Moreover, the electric boundary conditions on the crack surfaces are given by eqns. 1.3 and 1.5 for insulating and conducting cracks, respectively.

Figure 3.1. An insulating (or a conducting) crack in a poled ferroelectric subjected to remote electromechanical loading.
The intensified electromechanical field near a crack-tip is of major research interest in fracture mechanics. For an insulating crack, the near-tip field can be approximated by the general solution given by eqns. 2.3-2.6 coupled with the following potential functions [71], which correspond to the coordinate system with its origin at the crack tip (Fig. 3.2):

\[
\phi_n'(z_n) = (A_{n1}K_I + A_{n2}K_{II} + A_{n3}K_D) \frac{1}{2\sqrt{2\pi z_n}} \quad (n = 1, 2, 3)
\]  

(3.1)

where

\[
\begin{bmatrix}
A_{11} & A_{12} & A_{13} \\
A_{21} & A_{22} & A_{23} \\
A_{31} & A_{32} & A_{33}
\end{bmatrix} = \begin{bmatrix}
1 & 1 & 1 \\
-\mu_1 & -\mu_2 & -\mu_3 \\
-\delta_1 & -\delta_2 & -\delta_3
\end{bmatrix}^{-1}
\]  

(3.2)

and \(K_I\), \(K_{II}\) and \(K_D\) denote the stress intensity factors for Mode I and Mode II, and the electric displacement intensity factor; \(K_I = \sqrt{\pi a \sigma_{22}^\infty}\), \(K_{II} = \sqrt{\pi a \sigma_{12}^\infty}\) and \(K_D = \sqrt{\pi a D_2^\infty}\) for a center crack with half-length \(a\) under remote stress field \(\sigma_{22}^\infty\), \(\sigma_{12}^\infty\) and remote electric displacement loading \(D_2^\infty\).

Applied loading: \(K_I, K_{II}, K_D (K_E)\)

---

Figure 3.2. Small-scale domain switching zone around the tip of an insulating (or a conducting) crack.
Note that an electric displacement loading parallel to the crack \( D_1^w \) has no effect on the crack-tip field. If remote electrical loading is an electric field \( E_2^w \) instead of an electric displacement \( D_2^w \), \( K_D \) can be related to \( K_I, K_{II} \) and an electric field intensity factor \( K_E = \sqrt{\pi a E_2^w} \) as,

\[
K_D = \frac{1}{\beta_{11}\beta_{22} - \beta_{12}^2} \left[ \beta_{11} K_E + (\beta_{11} g_{22} - \beta_{12} g_{12}) K_I + (\beta_{11} g_{23} - \beta_{12} g_{13}) K_{II} \right]
\]

(3.3)

where \( \beta_{ij} \) and \( g_{ij} \) denote the elements of the matrices \( \beta \) and \( g \) of eqn. 2.1.

The electroelastic field of a conducting crack is given by eqn. 3.1 with the electric displacement intensity factor \( K_D \) replaced by an electric field intensity factor \( K_E \) [87]. For a conducting center crack, the expressions for the Mode I and Mode II stress intensity factors are the same as those of an insulating crack. However, contrary to the case of an insulating crack, a remote electric field perpendicular to a conducting crack \( E_2^w \) has no effect on the singular crack tip field, whereas an electric field parallel to it \( E_1^w \) induces an electric field intensity factor \( K_E = \sqrt{\pi a E_1^w} \). Note that for the case of a conducting crack, \( \delta_i \) in eqn. 3.2 are replaced by \( s_i \) \((i=1, 2, 3)\) instead (eqn. 2.3).

Under certain loading and poling configuration, an insulating or a conducting crack can be closed. In such cases, the near-tip potential functions given by eqn. 3.1 need to be modified. This limits the applicability of the present model. The analysis of closed cracks is presented in a latter part of this chapter.

The direction of spontaneous polarization of a region near a crack tip can be rotated by either 90° or 180° due to the intensified electroelastic field at the crack tip. By neglecting the difference in the electroelastic field before and after near-tip domain switching, the switching criterion (2.46) can be reduced to the following simplified version.
where the first term denotes the interaction of applied field with switching induced strains and electric polarization, and the second term denotes the contribution due to changes of material properties before and after switching.

In the previous studies of near-tip domain switching, the second term was neglected since these studies modeled ferroelectric materials as isotropic elastic dielectrics (no electromechanical coupling) [58-60]. This assumption leads to the energy based switching criterion of Hwang et al. [15]. In this study, eqn. 3.4 is instead used to obtain a more accurate description of the switching zone based on the electroelastic field \( \Sigma^0 = (\sigma_{11}, \sigma_{22}, \sigma_{12} E_1, E_2) \) obtained from the near-tip potential functions (eqn.3.1).

In the case of plane problems, there are three possible switching directions, i.e. 180°, 90° clockwise or 90° counterclockwise. Consider a ferroelectric domain with its spontaneous polarization forming an angle \( \omega \) with the \( x_1 \) axis (Fig. 3.3). The changes in spontaneous strain \( \Delta \epsilon_{ij} \) and polarization \( \Delta P_i \) for 90° domain switching can be expressed as:

\[
\Delta \epsilon = \gamma_s \begin{pmatrix} -\cos 2\omega & -\sin 2\omega \\ -\sin 2\omega & \cos 2\omega \end{pmatrix}
\]

\[
\Delta P = \sqrt{2} P_s \begin{pmatrix} \cos (\omega \pm \frac{3\pi}{4}) \\ \sin (\omega \pm \frac{3\pi}{4}) \end{pmatrix}
\]

where \( \gamma_s \) denotes the switching strain associated with 90° domain switching, \( P_s \) the magnitude of spontaneous polarization, and \( \frac{3\pi}{4} \) and \( -\frac{3\pi}{4} \) in eqn (3.6) correspond to clockwise and counterclockwise 90° domain switching, respectively.

For 180° domain switching, \( \Delta \epsilon_{ij} = 0 \) and
\[ \Delta P = -2P_s \begin{pmatrix} \cos \omega \\ \sin \omega \end{pmatrix} \] 

(3.7)

In order to use the domain switching criterion (3.4), switching induced transformation strains and electric polarization are assembled as,

\[ \mathbf{Z}_2^p - \mathbf{Z}_1^p = (\Delta \varepsilon_{11} \Delta \varepsilon_{22} 2\Delta \varepsilon_{12} \Delta P_1 \Delta P_2)^T \] 

(3.8)

Figure 3.3. 90° and 180° domain switching.

The geometry of the small switching zone around a crack tip (Fig. 3.2) can be determined by substituting the near tip field expressed by eqns. 2.3-2.6 and 3.1, and the changes in spontaneous strain and polarization (eqn. 3.8) into the energy based criterion (3.4). In this study, 90° and 180° domain switching are assumed to have the same energy barrier \( G_c = 2P_s E_c \) [15], where \( P_s \) is the magnitude of spontaneous polarization and \( E_c \) the coercive electric field for 180° switching. If two or more directions meet the switching criterion simultaneously, the actual switching occurs in the direction with highest free energy reduction. For a uniformly poled ferroelectric single crystal (mono-domain system), the spontaneous polarization of each domain aligns with the poling axis \((\omega = \phi)\). For a poled ferroelectric ceramic (poly-domain system), the orientation \((\omega)\) of
the ferroelectric domain changes, and it is necessary to know the orientation distribution of the domains to calculate the switching zone. The boundary of a domain switching zone corresponding to a given $\phi$ and $\omega$ can be determined by computing the switching zone radius $r(\theta)$ for different values of $\theta$.

### 3.3 Crack-Transformation Spot Interaction

Consider a plane piezoelectric medium (Fig. 3.2) with a semi-infinite insulating (or conducting) crack at $x_2 = 0, 0 \leq x_1$. A region $\Omega$ near the crack tip experiences stress-free transformation strains $\varepsilon_{ij}^*$ (i, j=1, 2) and electric field-free polarizations $D_i^*$ (i=1, 2). Due to the transformation strains and polarization, elevated stress and electric fields are induced at the crack tip. Field intensity factors induced at the crack tip due to $\varepsilon_{ij}^*$ and $D_i^*$ can be derived by generalizing Hutchinson’s treatment of a crack interacting with a circular transformation spot [88], or by using the weight function approach of Rice [89]. The former approach is used in the following derivation.

In the presence of transformation strains and polarization, the constitutive relations for region $\Omega$ are,

$$\varepsilon - \varepsilon^* = \mathbf{S}\sigma + \mathbf{g}^T(D - D^*)$$  \hspace{1cm} (3.9)

$$\mathbf{E} = -\mathbf{g}\sigma + \mathbf{p}(D - D^*)$$ \hspace{1cm} (3.10)

where $\varepsilon^* = (\varepsilon_{11}^*, \varepsilon_{22}^*, 2\varepsilon_{12}^*)^T$ and $D^* = (D_1^*, D_2^*)^T$.

Now consider a semi-infinite insulating (or conducting) crack interacting with a circular region of area $dA = (\pi b^2)$ that has undergone a stress-free transformation strain $\varepsilon^*$ and electric field-free polarization $D^*$ (Fig. 3.4). The interaction problem can now be considered as the superposition of two sub-problems: (a) a circular region undergoing transformation strain $\varepsilon^*$ and polarization $D^*$ in an infinite plane, resulting in stresses $\sigma_{12}(x_1)$ and $\sigma_{22}(x_1)$, and electric displacement $\hat{D}_2(x_1)$ (insulating crack), or electric...
field \( \hat{E}_i(x_i) \) (conducting crack) on the crack face \( x_2 = 0, x_1 < 0 \); (b) the faces of a crack at \( x_2 = 0, x_1 < 0 \) subjected to loading \(-\dot{\sigma}_{12}(x_i), -\dot{\sigma}_{22}(x_i), \) and \(-\dot{D}_2(x_i)\) (insulating crack), or \(-\hat{E}_i(x_i)\) (conducting crack). By superposition, the traction-free boundary conditions and the electric boundary conditions of insulating crack (eqn. 1.3) or conducting crack (eqn. 1.5) are satisfied.

Figure 3.4. A semi-infinite crack interacting with a circular spot that has undergone stress-free transformation strains \( \varepsilon_y^* \) and electric field-free polarization \( \hat{D}_d^* \).

Subproblem (a) corresponds to the case of a circular inclusion in a plane piezoelectric medium. The solution for this subproblem can be directly obtained from the results of the elliptic inclusion problem studied in the previous chapter. The corresponding potential functions are given by

\[
\varphi_n' = G_n \left( \frac{z_n'}{\sqrt{z_n'^2 - b^2 (1 + \mu_n^2)}} - 1 \right) \quad (3.11)
\]

and

\[
G_n = \frac{2\pi i}{1 - i\mu_n} B_n - \frac{2\pi i}{1 + i\mu_n} C_n, \quad (n = 1, 2, 3) \quad (3.12)
\]

where \( B_n \) and \( C_n \) are given in the Chapter 2, \( z_n' = z_n - z_{n0} \) and \( z_{n0} = x_1c + \mu_n x_2c \) with \( (x_1c, x_2c) \) denoting the coordinates of the center of the spot.
The electroelastic field on the line $x_2 = 0, x_1 < 0$ can be expressed as,

$$
\langle \sigma_{12}(x_1), \sigma_{22}(x_1) \rangle = 2 \text{Re} \sum_{n=1}^{3} \langle -\mu_n, 1 \rangle G_n \left( \frac{x_1 - z_{n0}}{\sqrt{(x_1 - z_{n0})^2 - b^2(1 + \mu_n^2)}} \right) - 1) \tag{3.13}
$$

$$
\langle \hat{D}_2(x_1), \hat{E}_1(x_1) \rangle = 2 \text{Re} \sum_{n=1}^{3} \langle -\delta_n, -s_n \rangle G_n \left( \frac{x_1 - z_{n0}}{\sqrt{(x_1 - z_{n0})^2 - b^2(1 + \mu_n^2)}} \right) - 1) \tag{3.14}
$$

In the case of a differential area $dA = (\pi b^2)$, the eqns. 3.13 and 3.14 can be further simplified as,

$$
\langle \sigma_{12}(x_1), \sigma_{22}(x_1) \rangle = \text{Re} \sum_{n=1}^{3} \langle -\mu_n, 1 \rangle \frac{G_n (1 + \mu_n^2) dA}{\pi (x_1 - z_{n0})^2} \tag{3.15}
$$

$$
\langle \hat{D}_2(x_1), \hat{E}_1(x_1) \rangle = \text{Re} \sum_{n=1}^{3} \langle -\delta_n, -s_n \rangle \frac{G_n (1 + \mu_n^2) dA}{\pi (x_1 - z_{n0})^2} \tag{3.16}
$$

The solution to subproblem (a) is hence determined. When the faces of a semi-infinite insulating crack, which lies at $x_2 = 0, x_1 < 0$, are subjected to electromechanical loading $-\sigma_{12}(x_1), -\sigma_{22}(x_1), \text{and} -\hat{D}_2(x_1)$ (insulating crack), or $-\hat{E}_1(x_1)$ (conducting crack), the mode I and mode II stress intensity factors, and the electric displacement intensity factor (insulating crack), or electric field intensity factor are derived as [90]

$$
\langle dK_I, dK_{II}, dK_D \rangle = \sqrt{\frac{2}{\pi}} \int_{-\infty}^{0} \frac{1}{\sqrt{-x_1}} \langle \sigma_{22}, \sigma_{12}, \hat{D}_2 \rangle dx_1 \text{ (insulating crack)} \tag{3.17}
$$

$$
\langle dK_I, dK_{II}, dK_E \rangle = \sqrt{\frac{2}{\pi}} \int_{-\infty}^{0} \frac{1}{\sqrt{-x_1}} \langle \sigma_{22}, \sigma_{12}, \hat{E}_1 \rangle dx_1 \text{ (conducting crack)} \tag{3.18}
$$

The substitution of the eqns. 3.15 and 3.16 into 3.17 and 3.18 yields,

$$
\langle dK_I, dK_{II}, dK_D \rangle = \text{Re} \sum_{n=1}^{3} \sqrt{\frac{1}{2\pi}} \langle 1, -\mu_n, -\delta_n \rangle \frac{G_n (1 + \mu_n^2) dA}{z_{n0}^{3/2}} \text{ (insulating crack)} \tag{3.19}
$$

$$
\langle dK_I, dK_{II}, dK_E \rangle = \text{Re} \sum_{n=1}^{3} \sqrt{\frac{1}{2\pi}} \langle 1, -\mu_n, -s_n \rangle \frac{G_n (1 + \mu_n^2) dA}{z_{n0}^{3/2}} \text{ (conducting crack)} \tag{3.20}
$$
Using the eqns. 3.19 and 3.20 and replacing \( z_{\alpha 0} \) by \( z_n \), the following electroelastic field intensity factors induced by \( \epsilon^* \) and \( D^* \) acting over \( \Omega \) (Fig. 4.2) can be obtained.

\[
\langle K_1^*, K_{II}^* \rangle = \frac{1}{2\pi} \int_{\Omega} \text{Re} \sum_{n=1}^{3} \langle 1, -\mu_n \rangle \frac{G_n (1+\mu_n^2)}{z_n^{3/2}} d\Omega \tag{3.21}
\]

\[
K_D^* = \frac{1}{2\pi} \int_{\Omega} \text{Re} \sum_{n=1}^{3} -\delta_n G_n (1+\mu_n^2) \frac{d\Omega}{z_n^{3/2}} \text{ (insulating crack)} \tag{3.22}
\]

\[
K_E^* = \frac{1}{2\pi} \int_{\Omega} \text{Re} \sum_{n=1}^{3} -s_n G_n (1+\mu_n^2) \frac{d\Omega}{z_n^{3/2}} \text{ (conducting crack)} \tag{3.23}
\]

### 3.4 Toughness Variation Due to Domain Switching

The switched ferroelectric region near a crack tip induces incompatible strains and electric polarization under the constraint of the unswitched material, and consequently changes the crack-tip field. The remote electric and stress fields are characterized by the stress intensity factors \( K_1, K_{II} \) and electric displacement intensity factor \( K_D \) (insulating crack), or electric field intensity factor \( K_E \) (conducting crack). The relations between the electroelastic field intensity factors and the applied remote loading for insulating and conducting cracks are given in the previous section. However, the electroelastic field in the vicinity of a crack tip approaches a level characterized by local stress intensity factors \( K_{I1}, K_{II1} \) and local electric displacement intensity factor \( K_{D1} \), or local electric field intensity factor \( K_{E1} \) as a consequence of polarization switching near a crack tip. Let \( \Delta K_j \) \( [j=I, II, D (E)] \) denote the additional field intensities induced by polarization switching, then

\[
K_{I1}^{ip} = K_I + \Delta K_I, \quad j=I, II, D (E) \tag{3.24}
\]

The general solution for transformation strains and polarization induced stress and electric field intensity factors are given by (3.21)-(3.23). To investigate the effect of
domain switching on toughness variation, the transformation zone (switching zone) and
the distribution of transformation strains and polarization induced by near-tip switching
need to be determined.

Consider a continuum element and denote the orientation distribution function of
ferroelectric domains in the element by \( f(\omega) \). For unpoled piezoelectrics, \( f(\omega) \) is
uniform in all directions. After poling, \( f(\omega) \) is re-configured. Domains in the same
continuum element are assumed to be subjected to the same stress and electric fields
(Reuss-type approximation). Therefore, for an individual domain orientation, the energy
based domain-switching criterion (3.4) can be used to determine the fate of that domain.
The contribution of an individual domain (if switched) in that continuum element to the
field intensity factors is given by (3.21)- (3.23). Integration over all orientations in a
specific continuum element and then over all the continuum elements in the switching
zone gives rise to the total change of field intensities due to switching. Assuming that
\( f(\omega) \) is identical for all continuum elements within a switching zone, the field intensity
factors (\( \Delta K \)) induced by domain switching can be expressed as [58],

\[
\Delta K_j = \int_{-\pi}^{\pi} K_j^* (\omega) f(\omega) d\omega, \quad j = I, II, D(E)
\]  \hspace{1cm} (3.25)

where \( K_j^* (\omega) \) given by (3.21)- (3.23) denote the contribution of domains with their
spontaneous polarizations forming an angle \( \omega \) with the \( x_1 \) axis.

In this study, the directions of spontaneous polarization of all domains are
assumed to be within a cone of 90° for a poled ceramic. A simple orientation distribution
function \( f(\omega) \) is used for a ferroelectric ceramic with its poling direction characterized
by the angle \( \phi \) (Fig. 3.2).

\[
f(\omega) = \begin{cases} 
\frac{2}{\pi}, & \text{if } |\omega - \phi| \leq \frac{\pi}{4} \\
0, & \text{otherwise}
\end{cases}
\]  \hspace{1cm} (3.26)
To evaluate switching induced field intensity factors, the stress-free transformation strain $\varepsilon^*$ and electric field-free polarization $D^*$ in the switching zone $\Omega$ also need to be determined. Because the electromechanical properties of a domain are different before and after switching, the transformation strains $\varepsilon^*$ and polarization $D^*$ are in general different from the switching strains $\Delta \varepsilon$ and switching polarization $\Delta P$ appearing in (3.8). By assuming that the changes of material properties are small, the values of $\varepsilon^*$ and $D^*$ can be approximated by $\Delta \varepsilon$ and $\Delta P$, respectively. A more detailed analysis may resort to the equivalent inclusion method [63] to calculate $\varepsilon^*$ and $D^*$ from $\Delta \varepsilon$ and $\Delta P$. Note that explicit analytical solutions for $\Delta K_j$ are not attainable, numerical integration is thus used in the evaluation.

Using a stress intensity factor-based fracture criterion, a crack starts to propagate if the crack-tip stress intensity factor attains the intrinsic fracture toughness. In this study, attention is focused on a mode I crack. In such a case, a crack starts to grow if,

$$K_{ij}^{ip} = K_i + \Delta K_i = K_{ic}$$ \hspace{1cm} (3.27)

where $K_{ic}$ denotes the intrinsic fracture toughness of a ferroelectric material.

Since $\Delta K$ is an implicit function of applied mechanical and electrical loading $K_i, K_{ii}$ and $K_D$ or $K_E$, the critical stress intensity factor (the apparent fracture toughness, $K_i$) to trigger crack extension is different from the intrinsic fracture toughness $K_{ic}$. This leads to a domain switching-induced fracture toughness variation [58-60]. The present near-tip domain switching model predicts a dependence of fracture load on an applied electric field, which may be helpful to understand the experimentally observed effects of an applied electric field on apparent fracture toughness [27-33]. Note that, based on linear fracture mechanics, the crack tip stress intensity factors are independent of an applied electric field, which contradicts experimental observations. However, the present model may circumvent the discrepancies between experimental findings and theoretical predictions.
3.5 Crack Closure Model

Once a crack is closed, the singular crack-tip field characterized by eqn. 3.1 needs to be modified. The normal displacement and normal traction are continuous across the surfaces of a closed crack. In this section, the conditions for crack closure are first derived and the problems of closed insulating and conducting cracks are formulated using the extended Lekhnitskii's formalism. The effect of near-tip domain switching on a closed crack is also examined.

3.5.1 Crack closure conditions

Consider an insulating (or conducting) crack of width $2a$ on the $x_i$ axis of an infinite piezoelectric medium (Fig. 3.1) and subjected to remote stresses $\sigma_{ij}^{\infty}$ and remote electric field $E_i^{\infty}$. If the crack surfaces are open under remote electromechanical loading, the complex potential functions corresponding to this problem can be expressed as [71].

$$\phi_n(z_n) = a_n z_n - \frac{1}{2\sqrt{n\pi a}}(\Lambda_{n1}K_I + \Lambda_{n2}K_{II} + \Lambda_{n3}K_{IV})(z_n - \sqrt{z_n^2 - a^2}) \quad (n = 1, 2, 3) \quad (3.28)$$

where $a_n$ are three complex constants directly determined by the remote loading $\sigma_{ij}^{\infty}$ and $E_i^{\infty}$. Therefore, the jump of the displacement $u_2$ across the crack surfaces is given by

$$\Delta u_2 = -2[\text{Im} \sum_{n=1}^{3} q_n(\Lambda_{n1}K_I + \Lambda_{n2}K_{II} + \Lambda_{n3}K_{IV})\frac{\sqrt{a^2 - x_i^2}}{\sqrt{n\pi a}}] \quad (3.29)$$

where $K_{IV}$ denotes the electric displacement intensity factor ($K_D$) and the electric field intensity factor ($K_E$) for insulating and conducting cracks, respectively.

It follows that the condition for crack closure [$\Delta u_2 \leq 0$] is

$$\alpha_1K_I + \alpha_2K_{II} + \alpha_3K_{IV} \geq 0 \quad (3.30)$$
where \( \alpha_j = \text{Im} \sum_{n=1}^{3} q_n \Lambda_{nj} \) \((j = 1, 2, 3)\) are functions of material properties and poling angle \( \phi \).

Note that a crack remains open when a piezoelectric solid is subjected to remote tensile stress only, which implies \( \alpha_i \) is always negative regardless of \( \phi \).

### 3.5.2 Electroelastic field for closed cracks

Due to crack closure, the two surfaces of the crack are in contact, and the normal displacement and normal traction are continuous across the crack. Assume frictionless contact exists between the two crack surfaces. The mechanical and electrical boundary conditions corresponding to a closed crack are:

\[
\sigma_{22}^+ = \sigma_{22}^-, \quad \sigma_{12}^+ = \sigma_{12}^- = 0, \quad u_2^+ = u_2^- (-a \leq x_1 \leq a \text{ and } x_2 = 0) \quad (3.31)
\]

\[
D_2^+ = D_2^-, \quad E_{y1}^+ = E_{y1}^- = 0 \quad (\text{insulating crack}), \quad \text{or} \quad E_{y1}^+ = E_{y1}^- = 0 \quad (\text{conducting crack}) \quad (3.32)
\]

where the superscripts '+' and '-' indicate the quantities on upper and lower crack surfaces, respectively.

The remote loading and boundary conditions on the crack surfaces constitute a mixed boundary-value problem. The solution to this boundary-value problem can be obtained from the superposition of the following two subproblems: (i) an infinite piezoelectric medium without an insulating (or conducting) crack loaded by \( \sigma_{ij}^\infty \) and \( E_{ij}^\infty \), and (ii) the surfaces of an insulating (or conducting) crack \((x_2 = 0 \text{ and } -a \leq x_1 \leq a)\) are subjected to mechanical loading \( \sigma_{22} = -f_1(x) \), \( \sigma_{12} = -\sigma_{12}^\infty \) and electric loading \( D_2 = -D_2^\infty \) (insulating crack) or \( E_1 = -E_1^\infty \) (conducting crack). The unknown function \( f_1(x) \) in the subproblem (ii) is determined such that all the boundary conditions of the original problem are satisfied.

The general solutions to the subproblem (ii) are given by [91]
In view of the superposition of the subproblems (i) and (ii), all the boundary conditions of the original problem but the continuity condition of the normal displacement are satisfied. The continuity condition of the normal displacement in eqn. 3.31 is equivalent to

\[ u_{x,2}^* = u_{x,2}^* \quad (x_2 = 0 \text{ and } -a < x_1 < a) \]  

Substituting eqns. 2.3-2.6 and 3.33 into the above equation and using the Plemelj formulae [92], the following Cauchy integral equations with \( f_1 \) as an unknown can be obtained

\[ \int_0^a \frac{\sqrt{a^2-t^2}}{t-x_1} (\alpha_1 f_1(t) + \alpha_2 \sigma_{12}^\infty + \alpha_3 D_2^\infty) dt = 0 \quad \text{(insulating crack)} \]  
\[ \int_0^a \frac{\sqrt{a^2-t^2}}{t-x_1} (\alpha_1 f_1(t) + \alpha_2 \sigma_{12}^\infty + \alpha_3 E_1^\infty) dt = 0 \quad \text{(conducting crack)} \]

Applying the solutions for the inversion of Cauchy integral equations by Muskhelishvili [92], the solutions to (3.36) and (3.37) can be expressed as

\[ f_1(t) = -\frac{\alpha_2}{\alpha_1} \sigma_{12}^\infty - \frac{\alpha_3}{\alpha_1} D_2^\infty \quad \text{(insulating crack)} \]  
\[ f_1(t) = -\frac{\alpha_2}{\alpha_1} \sigma_{12}^\infty - \frac{\alpha_3}{\alpha_1} E_1^\infty \quad \text{(conducting crack)} \]

The present model predicts that an applied electric loading induces uniformly distributed normal tractions on the crack surfaces. Using the condition for crack closure
(3.30), it can be shown that the electric field-induced normal traction is negative, which ensures the validity of the present crack closure model. The electroelastic field intensity factors at the tip of a closed insulating (conducting) crack can be expressed as

\[
\langle K_I, K_{II}, K_D \rangle = \frac{1}{\sqrt{\pi a}} \int_{-a}^{a} \sqrt{\frac{a+t}{a-t}} \left( f_1, \sigma_{12}^\infty, D_2^\infty \right) dt \quad \text{(insulating crack)} \quad (3.40)
\]

\[
\langle K_I, K_{II}, K_E \rangle = \frac{1}{\sqrt{\pi a}} \int_{-a}^{a} \sqrt{\frac{a+t}{a-t}} \left( f_1, \sigma_{12}^\infty, E_1^\infty \right) dt \quad \text{(conducting crack)} \quad (3.41)
\]

Manipulation of the above equations together with the conditions for crack closure (3.30), results in,

\[
K_{II} = \sqrt{\pi a} \sigma_{12}^\infty, \quad K_D = \sqrt{\pi a} D_2^\infty \quad \text{(insulating crack)}
\]

or \( K_E = \sqrt{\pi a} E_1^\infty \) \( \text{(conducting crack)} \) (3.42)

\[
K_I = -\frac{\alpha_2}{\alpha_1} K_{II} - \frac{\alpha_3}{\alpha_1} K_{IV} \geq \sqrt{\pi a} \sigma_{22}^\infty \quad (3.43)
\]

Therefore the mode I stress intensity factor at the tip of a closed insulating (or conducting) crack is independent of the remote tensile loading \( \sigma_{22}^\infty \), but linearly dependent on the remote shear loading \( \sigma_{12}^\infty \) and the remote electric loading \( D_2^\infty \) (for an insulating crack) or \( E_1^\infty \) (for a conducting crack). On the contrary, the linear model based on an opened crack predicts that the stress intensity factors are independent of applied electric loading and an electric field-alone does not produce any stress intensity factor in the cases of insulating and conducting cracks. It is seen from eqn. 3.43 that the dominant-order of normal stress is tensile directly ahead of the tip of a closed crack under a pure electric field loading. This agrees with the numerical results of Kumar and Singh [84], [85] and the theoretical predictions of Ru [86]. Cao and Evan [50] and Lynch et al. [51] observed that as a crack grew, the crack surfaces opened and closed when the applied electric field alternated. The combination of the conventional traction-free model and the present crack closure model offers a possible explanation for the experimentally observed fatigue crack growth under a cyclic electric field. Once a crack is open under an electric
field, the crack will not grow since there is no stress intensity at the crack tip. However, after the electric field reverses its sign, the crack will be closed and induce positive stress intensity at the tip, which may again open the crack tip.

3.5.3 Effect of domain switching

The near-tip domain switching model proposed for opened cracks in the sections 3.2, 3.3 and 3.4 can be easily extended to study closed cracks. By substituting the singular electric and stress fields characterized by eqn. 3.1 together with the field intensity factors given by eqns. 4.42 and 3.43 into the domain switching criterion (3.4), the switching zone near a closed crack tip can be determined. See sect. 3.2 for details.

Assume that the crack surfaces of a closed crack remain in contact after localized polarization switching occurs around the crack tip. The switching induced field intensity factors can be derived by using the approaches described in the sections 3.3 and 3.4. However, in deriving the fundamental solution for a closed crack interacting with transformation strains and polarization, the normal traction \( \sigma_{22}(x) \) applied to the crack at \( x_2 = 0, x_1 < 0 \) (Fig. 3.4) is replaced by

\[
\sigma_{22}(x_1) = -\frac{\alpha_2}{\alpha_1} \hat{\sigma}_{12}(x_1) - \frac{\alpha_3}{\alpha_1} \hat{D}_2(x_1) \quad \text{(insulating crack)}
\]

\[
\sigma_{22}(x_1) = -\frac{\alpha_2}{\alpha_1} \hat{\sigma}_{12}(x_1) - \frac{\alpha_3}{\alpha_1} \hat{E}_1(x_1) \quad \text{(conducting crack)}
\]

(3.44) (3.45)

to ensure the boundary conditions and continuity conditions for a closed crack are fully satisfied. The above argument can be inferred from (3.38) and (3.39). The solutions for switching induced field intensity factors \( K^* \) of a closed crack are obtained as,

\[
K_{II}^* = \sqrt{\frac{1}{2\pi}} \int_\Omega \text{Re} \sum_{n=1}^3 \frac{-\mu_n G_n (1 + \mu_n^2)}{z_n^{3/2}} d\Omega
\]

(3.46)

\[
K_{IV}^* = K_{IIV}^* = \sqrt{\frac{1}{2\pi}} \int_\Omega \text{Re} \sum_{n=1}^3 \frac{-\delta_n G_n (1 + \mu_n^2)}{z_n^{3/2}} d\Omega \quad \text{(insulating crack)}
\]

(3.47)
\[ K_{IV}^* = K_E^* = \sqrt{\frac{1}{2\pi}} \int_\Omega \text{Re} \sum_{n=1}^{N} -\frac{s_n G_n (1 + \mu_n^2)}{z_n^{3/2}} d\Omega \] (conducting crack) \hspace{1cm} (3.48)

\[ K_1^* = \frac{\alpha_2}{\alpha_1} K_{II}^* - \frac{\alpha_3}{\alpha_1} K_{IV}^* \] \hspace{1cm} (3.49)

The results for mode II stress intensity factor \( K_{II}^* \), electric displacement intensity factor \( K_D^* \) and electric field intensity factor \( K_E^* \) are identical to an open crack, whereas the mode I stress intensity factor \( K_1^* \) is linearly dependent on the mode II stress intensity factor \( K_{II}^* \) and the electric intensity factor \( K_{IV}^* \). The field intensity factors \( \Delta K \) induced by domain switching can be evaluated by (3.25) as in the case of open cracks.

### Table 3.1 Material constants of PZT-5H and PZT PIC-151

<table>
<thead>
<tr>
<th>Material</th>
<th>Elastic constants</th>
<th>Piezoelectric constants</th>
<th>Dielectric constants</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( S_{ij} )</td>
<td>( g_{ij} )</td>
<td>( \beta_{ij} )</td>
</tr>
<tr>
<td>PZT-5H</td>
<td>\begin{pmatrix} 8.440 &amp; -2.198 &amp; 0 \ -2.198 &amp; 6.871 &amp; 0 \ 0 &amp; 0 &amp; 18.369 \end{pmatrix}</td>
<td>\begin{pmatrix} 0 &amp; 0 &amp; 20.681 \ -8.160 &amp; 13.415 &amp; 0.0 \end{pmatrix}</td>
<td>\begin{pmatrix} 4.294 &amp; 0 \ 0 &amp; 4.880 \end{pmatrix}</td>
</tr>
<tr>
<td>PZT PIC-151</td>
<td>\begin{pmatrix} 9.361 &amp; -3.218 &amp; 0 \ -3.218 &amp; 8.784 &amp; 0 \ 0 &amp; 0 &amp; 28.853 \end{pmatrix}</td>
<td>\begin{pmatrix} 0 &amp; 0 &amp; 35.244 \ -18.363 &amp; 21.689 &amp; 0.0 \end{pmatrix}</td>
<td>\begin{pmatrix} 5.874 &amp; 0 \ 0 &amp; 6.581 \end{pmatrix}</td>
</tr>
</tbody>
</table>

\( \times 10^{-12} \) (m\(^2\)/N) \hspace{1cm} \times 10^{-3} \) (m\(^2\)/C) \hspace{1cm} \times 10^7 \) (V\(^2\)/N)
3.6 Numerical Results and Discussion

Attention is focused on the change in mode I stress intensity factor of a crack due to remote loading characterized by applied stress intensity factor $K$, and electric field intensity factor $K_E$. Note that a nonzero mode II stress intensity factor ($K^{II}_e$) may be introduced by domain switching caused by the applied loading. This may lead to crack deflection, and a multi-axial toughness criterion is needed to describe the fracture behavior. This topic is beyond the scope of the present study.

3.6.1 Crack closure conditions

Eqn. 3.30 is used to identify some cases of crack closure in ferroelectric materials under combined electrical and mechanical loading characterized by $K$, and $K_{IV}$. PZT-5H and PZT PIC-151 are used in the numerical study. The two-dimensional material constants appearing in eqn. 2.1 for PZT-5H and PZT PIC-151 poled in the $x_3$ direction are derived from their respective three-dimensional properties [39], [33]. These are given in Table 3.1. For PZT-5H and PZT PIC-151 poled in other directions, coordinate transformations are needed to obtain the corresponding material constants.

Figure 3.5 shows the variations of $\alpha_i$ and $\alpha_3$ with the poling direction $\phi$ for both insulating and conducting cracks. Note that $\alpha_3$ is magnified by $10^8$ for conducting cracks. The value of $\alpha_i$ is always negative regardless of the poling direction and the type of a crack (insulating or conducting). This implies that a crack is closed under a compressive stress perpendicular to the crack. Similar conclusion is well known for elastic materials. The value of $\alpha_3$ can be either positive or negative depending on the poling direction. It follows that an insulating or a conducting crack can be closed even with a tensile loading combined with an electrical loading. It is of interest to investigate pure electric field induced crack closure. An insulating crack disturbs an electric field applied perpendicular to it, while a conducting crack disturbs a field applied parallel to it. With the values of $\alpha_3$ shown in Fig. 3.5, it is found that an insulating crack is closed under an electric field
Figure 3.5. Variations of $\alpha_1$ and $\alpha_3$ with the poling angle $\phi$ for insulating and conducting cracks.
applied perpendicular to it and making an obtuse angle with the poling axis. For a conducting crack, crack closure occurs when the electric field is parallel to it and making an acute angle with the poling axis. The above conclusions agree with the numerical results of Kumar and Singh [84-85] and the theoretical solutions of Ru [86], who reported some special cases of crack closure, i.e. crack closure occurs for a conducting crack parallel to the poling axis under an electric field applied in the poling direction, and for an insulating crack perpendicular to the poling axis under an electric field applied opposite to the poling direction. The present results are more general.

3.6.2 Toughness variation of insulating crack

PZT-5H is used in the numerical study with $E_c = 0.9 \text{ MV/m}$ and $P_s = 0.38 \text{ C/m}^2$ based on experimental data [82]. The spontaneous polarization ($P_s$) is estimated from the remanent polarization ($P_r$) with $P_s = P_r / 0.83$ [15]. In the absence of experimental data, the switching strain ($\gamma_s$) for $90^\circ$ domain switching is assigned a representative value of 0.004. To investigate the effects of material anisotropy and electromechanical coupling, two different cases are considered: Case I, material anisotropy and electromechanical coupling of PZT-5H are included and the material properties are given by Table 3.1; Case II, the material is modeled as an isotropic elastic dielectric with Young’s modulus $E = 80 \text{ Gpa}$ and Poisson’s ratio $v = 1/3$ as in the previous study [60]. Note that the piezoelectric constants $g_{ij}$ are set to negligible values ($\sim 10^{-9} \text{ m}^2/\text{C}$) to obtain the solutions for Case II. Toughness variation of insulating cracks due to domain switching caused by an applied electric field, a stress field and combined loading is investigated.

Toughness variation under an electric field

A stationary crack under an applied electric field intensity factor $(K_E > 0)$ is considered. Since the crack is closed when the applied field forms an obtuse angle with the poling direction (see Section 3.6.1), only the case of a field making an acute angle ($0^\circ \leq \phi \leq 90^\circ$) with the polar axis is considered. Fig. 3.6(a) shows the shape of the
switching zones corresponding to the initial poling directions $\phi = 0^\circ$ (parallel to crack) and $\phi = 90^\circ$ (perpendicular to crack) of a mono-domain system ($\phi = \omega$). The coordinates in Fig. 3.6(a) are normalized by $r_0 = \left[ K_E / (2 \sqrt{\pi} E_c) \right]^2$. For a crack parallel to the poling direction, $90^\circ$ domain switching occurs ahead of the crack tip, while $180^\circ$ switching occurs behind it. For the case of a crack perpendicular to the poling direction, only $90^\circ$ domain switching occurs, at the rear of the crack tip. The size of the switching zone of a crack parallel to the poling direction is substantially larger than that of a crack perpendicular to it. This can be explained as follows: the states of domains with their polarizations aligning with the electric field vector are more energetically favorable than those with their polarizations perpendicular to the electric field vector. It is also noted from Fig. 3.6(a) that the effects of material anisotropy and electromechanical coupling on the geometry of the switching zone are relatively small for a crack under a pure electric field. The shape of the switching zone corresponding to $\phi = 90^\circ$ predicted by the present model for case II is identical to that of Zhu and Yang [60].

Fig. 3.6(b) shows the variation of the mode I stress intensity factor induced by domain switching of mono-domain and poly-domain systems with the initial poling direction $\phi$. Results are shown for cases I and II. First, the theoretical value of mode I stress intensity factor of a crack perpendicular to the poling direction ($\phi = 90^\circ$) of an isotropic mono-domain ferroelectric (also neglecting the piezoelectric coupling) under a pure electric field is used to verify the present model. As shown by Zhu and Yang [60],

$$K_I^{up} = \frac{Y_T}{16\pi(1-v^2)E_c} K_E \quad (\text{N} \cdot \text{Vm})$$

(3.50)

for this case. This is identical to $K_I^{up} / K_E = 7.958$ N/Vm obtained for case II based on the present model. Due to domain switching, an electric field induces positive mode I stress intensity at a crack tip. The tensile stress directly ahead of a crack tip may lead to electric field induced crack growth. The change of stress intensity factor of the mono-domain systems with the initial poling direction ($\phi$) is similar to that of poly-domain systems for
Figure 3.6. (a) Switching zones induced by an electric field, (b) crack-tip stress intensity factor due to an electric field for different initial poling directions.
the two cases under consideration. Toughness variation corresponding to a crack parallel to the poling direction \((\phi = 0^\circ)\) is larger than that of a crack perpendicular to poling axis \((\phi = 90^\circ)\). Crack-tip stress field is substantially higher when the material anisotropy and electromechanical coupling are considered (Case I), when compared with the uncoupled isotropic case (Case II). This implies that, in addition to switching induced strains, switching induced polarization also plays an important role in toughness variation of ferroelectric materials. The latter effect cannot be handled by the previous domain switching model where ferroelectrics were modeled as isotropic elastic dielectrics [58-60].

Toughness variation under an applied stress field

Consider a stationary crack under an applied stress field characterized by the mode I stress intensity factor \(K_r(>0)\). Domain switching zones are shown in Fig. 3.7(a) for a crack parallel to the poling direction \((\phi = 0^\circ)\) and that perpendicular to it \((\phi = 90^\circ)\) of mono-domain systems \((\phi = \omega)\). The switching zones for \(\phi = 90^\circ\) are scaled by a factor of 2. A length parameter \(r = [K_r/(\gamma_s/(P_E))]^2/8\pi\) is used to normalize the switching zone. As expected, only 90° domain switching occurs in both cases. This can be explained by the fact that the near-tip stress field is the dominant field under a pure mechanical loading, and a stress field induces 90° switching only. For \(\phi = 0^\circ\), switching occurs in front of the crack tip, while it happens at the rear of the tip for \(\phi = 90^\circ\). The switching zone based on the uncoupled model (cases II) is substantially larger than that corresponding to the coupled model (case I) for a crack parallel to the poling axis \((\phi = 0^\circ)\). For the case of a crack perpendicular to the poling direction \((\phi = 90^\circ)\), the switching zone is similar for both case I and case II. The size of the switching zone of a crack parallel to the poling direction \((\phi = 0^\circ)\) is substantially larger than that of a crack perpendicular to it \((\phi = 90^\circ)\). For the former case, the domains are easier to be switched, because the applied tensile stress is perpendicular to the spontaneous polarization of
Figure 3.7. (a) Switching zones induced by an applied stress field ($\phi = 0^\circ$ and $90^\circ$), (b) crack-tip stress intensity factor due to applied field for different initial poling directions.
domains. For the case of $\phi = 90^\circ$, domains are more difficult to be switched since the tensile stress is applied along the direction of spontaneous polarization.

Based on the uncoupled model (Case II), domain switching induces a negligible stress intensity factor (in the order of $10^{-5}$ of $K_I$). It can be shown that $\Delta K_I$ is equal to zero by using the switching model of Zhu and Yang [58]. The near-tip stress intensity corresponding to case I is shown in Fig. 3.7(b) for different initial poling directions. Switching induced stress intensity $\Delta K_I$ is less than 10% of the applied stress intensity $K_I$. The trend of toughness variation of the mono-domain system with $\phi$ is similar to that of the poly-domain system.

**Toughness variation under combined loading**

A stationary crack subjected to an applied remote stress intensity factor $K_I (> 0)$ and an electric field intensity factor $K_E$ is considered. Fig. 3.8(a) and Fig. 3.8(b) show the switching zones of a mono-domain system corresponding to case I (coupled model) and case II (uncoupled model) respectively, for three different initial poling directions $\phi = -90^\circ$, $0^\circ$ and $90^\circ$. A dimensionless parameter $\alpha_E = K_E P_s / K_I \gamma_s$ is used to measure the relative magnitude of the applied electric field and stress field. The solutions in Fig. 3.8 are corresponding to $\alpha_E = 1.0$. When the applied electric field aligns with the poling direction ($\phi = 90^\circ$), $90^\circ$ domain switching is found to occur behind a crack tip. When the applied field is opposite to the poling direction ($\phi = -90^\circ$), $180^\circ$ switching takes place ahead of a crack tip, while $90^\circ$ switching occurs behind the crack tip. For the case of an electric field perpendicular to the poling direction ($\phi = 0^\circ$), domain switching is mainly limited to the upper half-plane. Based on the comparison between Fig. 3.8(a) and 3.8(b), material anisotropy and electromechanical coupling are found to have an important effect on the geometry (size and shape) of the domain switching zone around a crack tip.
Figure 3.8. (a) Switching zones induced by combined loading for case I, (b) switching zones due to combined loading for case II.
Figs. 3.9 shows the variation of near-tip mode I stress intensity factor with the poling angle $\phi$ under an electric loading level of $\alpha_E = 1.0$. Both the mono-domain and the poly-domain solutions are presented for the coupled (case I) and the uncoupled (case II) cases. Based on the poly-domain solution (case I and case II), domain switching induces positive stress intensity ($\Delta K_I > 0$) at a crack tip. It follows that an applied electric field tends to decrease the apparent fracture toughness under combined loading. Based on the mono-domain solution for case II, an electric field may increase (if $\Delta K_I < 0$) or decrease (if $\Delta K_I > 0$) the apparent fracture toughness depending on the poling direction of the material. Switching induced stress intensity factor $\Delta K_I$ under an electric field applied opposite to the poling direction ($\phi = -90^\circ$) is much larger than that under a field aligned with the poling axis ($\phi = 90^\circ$). For the latter case, the uncoupled model (case II) predicts negligible toughness variation. The magnitude of toughness variation predicted by the coupled mode (case I) is several times that based on the uncoupled model (case II).

The effect of electrical loading level $\alpha_E$ on the switching induced stress intensity factor $\Delta K_I$ is investigated in Fig. 3.10 for a crack perpendicular to the initial poling direction ($\phi = 90^\circ$), which is the focus of previous theoretical and experimental investigations on fracture problems in piezoelectric materials. Based on the coupled model (case I), domain switching induces a positive stress intensity factor ($\Delta K_I > 0$) under both positive ($\alpha_E > 0$) and negative ($\alpha_E < 0$) electric fields. Therefore, an electric field decreases the apparent fracture toughness. The crack-tip field is more affected by a negative field than by a positive field. As the magnitude of $\alpha_E$ increases, the effect of an electric field on toughness variation intensifies. Based on the uncoupled model (case II), a positive electric field has negligible effect on fracture toughness variation, while a negative field tends to decrease the apparent fracture toughness. Switching induced stress intensity factor $\Delta K_I$ predicted by the coupled model (case I) is larger than that obtained by the uncoupled model (case II).
Figure 3.9. Crack-tip stress intensity factors under combined loading for different initial poling direction $\phi$.

Figure 3.10. Crack-tip stress intensity factors under combined loading for different electric loading levels.
Fig. 3.10 can be used to explain some experimental findings. Since either the stress intensity factor $K_I$ or the electric field intensity factor $K_E$ is not given in the reported experimental data [27-32], a qualitative comparison between experimental findings and theoretical predictions is made here. Tobin and Pak [27] and Park and Sun [31] reported that a positive electric field reduced fracture load, whereas a negative one increased it. On the contrary, Wang and Singh [29] reported that a positive electric field retarded crack growth, while a negative field enhanced it. Fu and Zhang [32] observed that both positive and negative applied electric fields reduced the apparent fracture toughness and the effect of a negative electric field was more pronounced than a positive field. The effect of an electric field on fracture toughness variation predicted by the present domain switching model based on insulating (impermeable) crack face boundary assumption qualitatively explains the experimental findings of Fu and Zhang [32]. Note that the crack face electric boundary conditions in the experimental studies [27-32] are unclear as these were not specially controlled. Therefore, a direct comparison between the experimental findings and theoretical predictions based on the impermeable crack assumption may not be appropriate.

3.6.3 Toughness variation of conducting crack

Using a four-point-bending device, Heyer et al. investigated the propagation of a conducting crack in PZT PIC-151 under combined electrical and mechanical loading [33]. In their experiments, NaCl solution, which served as an electrolyte, was used to fill the notch to produce a conducting crack. The fracture load was found to change with an applied electric field for a crack parallel to the poling direction. In order to compare with the experimental findings, PZT PIC-151 is used in the following numerical study with $E_c = 0.8$ MV/m [33]. The spontaneous polarization ($P_s$) is estimated to be $0.35$ C/m$^2$ and the switching strain $\gamma_s \approx 0.003$. Mode I stress intensity factor due to domain switching caused by an applied electric field, a stress field and combined loading is evaluated using the poly-domain approximation (3.25).
Toughness variation under an electric field

A stationary crack under an applied electric field characterized by the intensity factor $K_E (>0)$ is considered. Since the crack is closed when the applied field forms an acute angle with the poling axis (see section 3.6.1), only the case of an electric field making an obtuse angle ($90^\circ \leq \phi \leq 180^\circ$) with the polar direction is considered. Fig. 3.11(a) shows the switching zones corresponding to poling directions $\phi = 90^\circ$ and $180^\circ$ for a mono-domain system ($\phi = \omega$), where the spontaneous polarization of domains are uniformly aligned with the poling axis. For $\phi = 90^\circ$, the applied electric field is perpendicular to the poling axis and $90^\circ$ domain switching occurs ahead of the crack tip, while $180^\circ$ switching occurs behind it. A nonzero mode II stress intensity factor ($K_{II}^{rip}$) is induced due to an asymmetric switching zone. When the applied electric field is opposite to the poling axis ($\phi = 180^\circ$), $90^\circ$ domain switching occurs at the rear of the crack tip, while $180^\circ$ switching occurs at the front. The symmetric switching zone induces a zero mode II stress intensity factor at the crack tip. Fig. 3.11(b) shows the variation of near-tip model I stress intensity $K_I^{rip}$ with the poling angle $\phi$. For $90^\circ \leq \phi \leq 115^\circ$, domain switching induces positive stress intensity factor at the crack tip. This may lead to pure electric field-driven crack propagation. However, for $115^\circ \leq \phi \leq 180^\circ$, an applied electric field induces a negative stress intensity at the crack tip and thereby mechanically shields the tip. For the critical case of an electric field applied opposite to the poling direction ($\phi = 180^\circ$), the toughening effect is the largest.

Toughness variation under tension

Consider a crack under an applied stress intensity factor $K_I (>0)$. The shape of the domain switching zone is shown in Fig. 3.12(a) for a crack parallel ($\phi = 0^\circ$) and perpendicular ($\phi = 90^\circ$) to the poling axis for a mono-domain system. Switching zones corresponding to $\phi = 90^\circ$ are scaled by a factor of ten. Only $90^\circ$ domain switching occurs
Figure 3.11. (a) Switching zones induced by an electric field, (b) crack-tip stress intensity factor due to an electric field for different poling directions $\phi$. 
Figure 3.12. (a) Switching zones induced by an applied stress field, (b) crack-tip stress intensity factor due to an applied stress field for different poling directions $\phi$. 
and the switching zones are symmetric about the crack plane for both $\phi = 0^\circ$ and $\phi = 90^\circ$. The switching zone corresponds to a crack perpendicular to the poling direction ($\phi = 90^\circ$) is much smaller than that of a crack parallel to the poling axis ($\phi = 0^\circ$). Since the near-tip electric field is weak when compared to the near-tip stress field, crack-tip domain switching is mainly controlled by the stress field. This explains why only 90° switching is observed in Fig. 3.12(a). Normalized near-tip stress intensity factor $K_{IP}^{\phi}/K_I$ is shown in Fig. 3.12 (b) for different poling directions $\phi$. The magnitude of $\Delta K_I$ is in the order of 0–20% of the applied stress intensity factor $K_I$ and shows anisotropy. The largest amplification effect occurs at $\phi = 40^\circ$ and 140°.

**Toughness variation under combined loading**

A crack subjected to field intensity factors $K_I (> 0)$ and $K_E$ is considered. Fig. 3.13(a) and Fig. 3.13(b) show the switching zones corresponding to electric loading levels $\alpha_E = 0.5$ and $\alpha_E = 1.0$ respectively for three different poling directions $\phi = 0^\circ$, 90° and 180° ($\omega = \phi$). The switching zones corresponding to $\phi = 90^\circ$ are scaled by a factor of 5 and 1.5 in Fig. 3.13(a) and 3.13(b), respectively and the zone for $\phi = 0^\circ$ is magnified by three times in Fig. 3.13 (b). For a crack parallel to the poling axis ($\phi = 0^\circ$ or 180°), the switching zone is symmetric about the crack plane. For a crack perpendicular to the poling axis ($\phi = 90^\circ$), domain switching occurs mainly in the lower half plane. Both 90° and 180° domain switching occur under combined loading. The shape of the switching zone corresponding to $\alpha_E = 0.5$ is similar to that of $\alpha_E = 1.0$, but the zones are different in size.

Fig. 3.14 shows the variation of normalized near-tip stress intensity factor $K_{IP}^{\phi}/K_I$ with the poling angle $\phi$ for two different electric loading levels $\alpha_E = 0.5$ and $\alpha_E = 1.0$. For both cases, apparent fracture toughness may be increased or decreased depending on the crack orientation with respect to the poling direction. When
Figure 3.13. Switching zones induced by combined loading for different electric loading levels, (a) $\alpha_E = 0.5$, (b) $\alpha_E = 1.0$. 

98
an applied electric field forms an acute angle with the poling axis, effects of domain switching on fracture toughness variation is very small (±10% of $K_f$). The largest amplification effect occurs at $\phi$ between 120° and 150°. If the applied electric field is parallel or opposite to the poling axis ($\phi = 0°$ or 180°), switching induces a negative stress intensity factor and consequently shields the crack tip.

Fig. 3.14 shows the variation of normalized near-tip stress intensity factor $K_{I,\text{ip}}/K_f$ with the electric loading ratio $\alpha_E$ for a crack parallel ($\phi = 0°$) and perpendicular to the poling direction ($\phi = 90°$). For a crack perpendicular to the poling axis, the stress intensity $\Delta K_f$ induced by domain switching is positive and very small when compared to that corresponding to a crack parallel to the poling axis under the same loading. For a parallel crack, $K_{I,\text{ip}}$ decreases as the magnitude of electric loading ratio $\alpha$ increases. The magnitude of $\Delta K_f$ under a positive electric field is smaller than that under a negative electric field. If the near-tip stress intensity $K_{I,\text{ip}}$ corresponding to a pure
stress loading ($\alpha_E = 0$) is chosen as the intrinsic fracture toughness, both positive and negative electric field tend to increase the apparent fracture toughness and consequently shield the crack tip.

![Figure 3.15. Crack-tip stress intensity factors under combined loading for different electric loading levels.](image)

The characteristic fracture curve (Fig. 3.16) obtained by Heyer et al. [33] is used to further verify the present model. Note that the sign convention of Fig. 3.16 is opposite to that used in the present study, where an electric field is considered positive if directed along the poling direction. Heyer et al. proposed a fracture criterion for conducting cracks in PZT-PIC 151 as $G_{\text{tip}} = G_c$, where $G_{\text{tip}}$ denotes the total energy release rate in terms of local stress intensity factor and electric field intensity factor $K^{ip}_I$ and $K^{ip}_E$, and $G_c$ is a critical value to start crack growth. With known applied field intensity factors $K_I$ and $K_E$, the local stress intensity factor $K^{ip}_I$ and the local electric field intensity factor $K^{ip}_E$ can be determined by the theoretical approach described in this thesis. For a conducting crack, the total energy release rate can be expressed as [87],
Table 3.2 shows the local stress intensity factor $K_I^{tip}$ and the crack-tip total energy release rate $G_{tip}$ for the applied field intensity factors $K_I$ and $K_E$ based on the fracture curve shown in Fig. 3.16. Within the range of $0 \leq K_E \leq 12 \, \text{kV/m}^{1/2}$, the variation of near-tip stress intensity factor $K_I^{tip}$ is small. It implies that the fracture curve within this range can be explained by the present domain switching model coupled with a mode I stress intensity factor-based fracture criterion (3.27). However, the switching model overestimates the fracture toughness variation under a negative electric field (see the case $K_E = -5 \, \text{kV/m}^{1/2}$). Note that the total energy release rate $G_{tip}$ based on the localized field intensities $K_I^{tip}$ and $K_E^{tip}$ shows a small variation under an applied electric field within the
range of \(-3 \text{ kV/m}^{1/2} \leq K_E \leq 12 \text{ kV/m}^{1/2}\). It follows that, under small to moderate electric fields, the characteristic fracture curve of PZT PIC-151 can be explained by the total energy release rate criterion together with the current theoretical model. Further numerical results reveal that the current model fails to explain the experimental behavior under a large negative electric field. The effect of a negative electric field on the fracture load is more complicated than that of a positive field. Based on the experimental data shown in Fig. 3.16, a positive field always tends to increase the fracture load, whereas a negative field may increase or decrease the fracture load. Note that the negative field shown in Fig. 3.16 is considered here as a positive one since it was applied in the same direction as the poling axis, see [33].

<table>
<thead>
<tr>
<th>(K_E) (kV/m(^{1/2}))</th>
<th>-5</th>
<th>-3</th>
<th>0</th>
<th>3</th>
<th>5</th>
<th>8</th>
<th>10</th>
<th>12</th>
<th>15</th>
</tr>
</thead>
<tbody>
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<td>0.900</td>
<td>0.930</td>
<td>0.949</td>
<td>0.979</td>
<td>0.998</td>
<td>1.017</td>
<td>1.046</td>
</tr>
<tr>
<td>(K_f^{pp}) (MPa m(^{1/2}))</td>
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<td>0.820</td>
<td>0.920</td>
<td>0.924</td>
<td>0.918</td>
<td>0.914</td>
<td>0.919</td>
<td>0.932</td>
<td>0.977</td>
</tr>
</tbody>
</table>

**3.6.4 Toughness variation of closed cracks**

As shown in the section 3.6.1, an insulating crack is closed under an electric field applied perpendicular to the crack and making an obtuse angle with the poling axis, while closure of a conducting crack occurs when the electric field is parallel to it and making an acute angle with the poling axis. Fig. 3.17 shows the switching zones of closed cracks in PZT-5H mono-domain systems (\(\phi = \omega\)) under an electric field applied parallel to the poling direction (conducting crack, \(\phi = 0^\circ\)), opposite to the poling direction (insulating crack, \(\phi = -90^\circ\)) and perpendicular to the poling axis (insulating crack, \(\phi = 0^\circ\); conducting crack, \(\phi = 90^\circ\)). For insulating cracks corresponding to \(\phi = -90^\circ, 90^\circ\) polarization switching occurs at the rear of the crack tip, while 180\(^\circ\) switching occurs at
the front. For a conducting crack corresponding to \( \phi = 0^\circ \), only \( 90^\circ \) polarization switching occurs behind the crack tip. For the other two cases, \( 90^\circ \) switching occurs ahead of the crack tip, while \( 180^\circ \) switching occurs behind it.

![Figure 3.17](image)

**Figure 3.17.** Switching zones around the tip of a closed insulating (conducting) crack under a pure electric field loading.

Fig. 3.18 shows the variation of mode I stress intensity factor of a closed insulating crack with the poling direction. When the poling axis is parallel to the crack plane, the applied electric field induces a zero stress intensity factor. However, for a crack perpendicular to the poling axis, the applied electric field induces the largest stress intensity factor. This case is the focus of previous experimental and theoretical investigations. The elevated tensile stress directly ahead of a crack tip can give rise to crack growth. This conclusion cannot be reached by using the conventional traction-free model, which predicts that an electric field does not produce any stress intensity factor. The effect of near-tip domain switching on the stress intensity factor is also shown in Fig. 3.18. The largest amplification occurs when the insulating crack is perpendicular to the
poling axis (i.e. an electric field applied opposite to the poling direction). Due to domain switching, the intensity of the near-tip can be increased by as high as 35%.

![Graph showing stress intensity factor vs. angle]

Figure 3.18. Model I stress intensity factor at the tip of a closed insulating crack due to an electric field.

Fig. 3.19 shows the changes of mode I stress intensity factor at the tip of a closed conducting crack with the direction of poling axis. A zero stress intensity factor is introduced by an applied electrical load for a crack perpendicular to the poling direction (\( \phi = -90^\circ \) and \( 90^\circ \)). When a closed conducting crack is parallel to the poling axis (\( \phi = 0^\circ \)), the applied electric field is in the poling direction and induces the largest stress intensity factor. This contradicts the conventional traction-free model, which predicts a zero stress intensity factor under pure electrical loading. The effect of polarization switching on the mode I stress intensity factor is also examined in Fig. 3.19. When the angle between the poling axis and the crack plane is less than 60°, the stress intensity factor at the crack tip is increased due to polarization switching. However, domain switching has negligible effect on the stress intensity when the angle between the poling axis and the crack plane is greater than 60°. The largest amplification is achieved when an
electric field is applied in the direction of poling. Due to crack closure, an applied electric field induces tensile stress directly ahead of a tip of an insulating or a conducting crack.

Figure 3.19. Model I stress intensity factor at the tip of a closed conducting crack due to an electric field.
Chapter 4

A MODEL FOR ELECTRODE-CERAMIC LAYER INTERACTION

4.1 Overview

Multilayer ceramic stack actuators are fabricated by cofiring internal electrode layers and unpoled ferroelectric ceramic layers. Without poling, ferroelectrics behave like dielectrics and possess no piezoelectric effect. To make a ceramic actuator useful, high voltages are applied to internal electrodes to polarize the ferroelectric ceramic between two electrodes. The poling of a ceramic layer is nonuniform, since internal electrodes do not extend completely toward the opposite edge (Fig. 1.4). However, the major portions of two neighboring ceramic layers are polarized nearly opposite to each other and perpendicular to an internal electrode. Experimental studies have shown that cracks leading to actuator failure initiate at the electrode tip and along the ceramic-electrode interface. It is therefore important to study the electrode tip field and related field intensity factors.

In this chapter, the near-tip stress and electric fields at an embedded electrode tip in two oppositely poled ferroelectric ceramic layers are investigated. The problem is formulated as a mixed boundary value problem within the scope of linear piezoelectricity. The elevated electroelastic field at an electrode-tip results in localized polarization switching of domains very close to the electrode, which induces incompatible strains and electric polarization due to constraint of the unswitched material. Based on a new fundamental solution for a semi-infinite electrode at the interface of two half-planes interacting with eigenstrains and eigen electric polarization, the effect of domain switching on the near-tip field is examined by an approach similar to that presented in the Chapter 3. Numerical results for the stress and the electric fields at a buried electrode tip are used to explain experimentally observed cracking patterns and design thickness of ceramic layers.
4.2 Theoretical Model

In order to reduce the electrode-ceramic interaction problem in a typical stack actuator to a form that is feasible for analytical treatment, each ceramic layer is idealized to have uniform remanent polarization perpendicular to the internal electrode. In view of the polar directions of two adjacent ceramic layers and the electric field vector directly ahead of an electrode tip, there are four different polarization configurations possible in two adjacent ceramic layers in an actuator (Fig. 4.1). An internal electrode is modeled as an infinitely thin conducting sheet with zero stiffness. This is acceptable since an electrode layer is thinner by about two orders of magnitude and more compliant than a ceramic layer. It is assumed that plane strain and plane electric field conditions \( (\varepsilon_{33} = \varepsilon_{31} = \varepsilon_{32} = 0, E_3 = 0) \) are applicable.

Consider a semi-infinite electrode (conducting sheet) with vanishing thickness embedded at the interface of two-bonded ferroelectric half-planes poled in opposite directions (Fig. 4.1). The electrode is subjected to a prescribed electric field \( E_0(x_1) \). The electrical and mechanical boundary conditions at the interface can be expressed as,

\[
\begin{align*}
  u^+_1 &= u^-_1, \\
  u^+_2 &= u^-_2, \\
  \psi^+ &= \psi^- \quad (\infty < x_1 < \infty \text{ and } x_2 = 0) \\
  \sigma^+_{12} &= \sigma^-_{12}, \\
  \sigma^+_{22} &= \sigma^-_{22} \quad (\infty < x_1 < \infty \text{ and } x_2 = 0) \\
  E^+_1 &= E^-_1 = E_0(x_1) \quad (\infty < x_1 < 0 \text{ and } x_2 = 0), \\
  D^+_2 &= D^-_2 \quad (0 < x_1 < \infty \text{ and } x_2 = 0)
\end{align*}
\]

where the superscripts ‘+’ and ‘-’ indicate the quantities on the upper and lower interfaces, respectively.

To facilitate the derivation, the general solution for the electroelastic field of a two-dimensional piezoelectric plane given by eqns. (2.3)-(2.6) is assembled into more compact forms as,

\[
\begin{align*}
  \mathbf{u} &= (u_1, u_2, \psi)^T = A\varphi(z) + \overline{A\varphi(z)} \\
  \mathbf{\sigma} &= (\sigma_{12}, \sigma_{22}, D_2)^T = B\Phi(z) + \overline{B\Phi(z)}
\end{align*}
\]

where \( \varphi(z) = (\varphi_1(z_1), \varphi_2(z_2), \varphi_3(z_3))^T \), \( \Phi(z) = (\varphi'_1(z_1), \varphi'_2(z_2), \varphi'_3(z_3))^T \) and
Figure 4.1. Simplified model for an embedded electrode tip in a multilayer actuator.

\[
\mathbf{A} = \begin{bmatrix} p_1 & p_2 & p_3 \\ q_1 & q_2 & q_3 \\ s_1 & s_2 & s_3 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} -\mu_1 & -\mu_2 & -\mu_3 \\ 1 & 1 & 1 \\ -\delta_1 & -\delta_2 & -\delta_3 \end{bmatrix}
\]  

(4.6)

Substituting the general solution (4.4) into the continuity conditions of displacement and electric potential (4.1) leads to the following relations,

\[
\mathbf{A}_I \Phi_I(x_I) + \overline{\mathbf{A}_I \Phi_I(x_I)} = \mathbf{A}_II \Phi_{II}(x_I) + \overline{\mathbf{A}_II \Phi_{II}(x_I)}
\]

(4.7)

or

\[
\mathbf{A}_I \Phi_I(x_I) - \overline{\mathbf{A}_II \Phi_{II}(x_I)} = \mathbf{A}_II \Phi_{II}(x_I) - \overline{\mathbf{A}_I \Phi_I(x_I)}
\]

(4.8)

where the subscripts 'I' and 'II' are used to identify the quantities in the upper and lower half planes respectively and \( \Phi_j(z) = \overline{\Phi_j(\bar{z})} \), \( j = I, II \). Since the functions \( \mathbf{A}_I \Phi_I(z) - \overline{\mathbf{A}_II \Phi_{II}(z)} \) and \( \mathbf{A}_II \Phi_{II}(z) - \overline{\mathbf{A}_I \Phi_I(z)} \) are analytic in the upper and the lower half-planes respectively and both approach zero at infinity, they should be equal to zero by the standard analytic continuity argument [93], i.e.
The substitution of general solution (4.5) into the continuity conditions (4.2) and (4.3) results in,

\[
\sigma^+ - \sigma^- = [B_i \Phi_i(x_1) + B_{ii} \Phi_{ii}(x_1)] - [B_{ii} \Phi_{ii}(x_1) + B_{ii} \Phi_{ii}(x_1)] \\
= [B_i \Phi_i(x_1) - B_{ii} \Phi_{ii}(x_1)] - [B_{ii} \Phi_{ii}(x_1) - B_i \Phi_i(x_1)] = (0 \ 0 \ \rho(x_1))^T
\]  

(4.11)

where \( \rho(x_1) \) is the jump of electric displacement \( D_2 \) across the interface of the two bonded piezoelectric half planes. After solving the eqn. 4.11, the following relations can be obtained [49],

\[
B_i \Phi_i(x_1) - B_{ii} \Phi_{ii}(x_1) = (0 \ 0 \ \tau(z))^T, \quad x_2 > 0
\]  

(4.12)

\[
B_{ii} \Phi_{ii}(x_1) - B_i \Phi_i(x_1) = (0 \ 0 \ \tau(z))^T, \quad x_2 < 0
\]  

(4.13)

where \( \tau(z) \) is a function which is related to the jump \( \rho(x_1) \) of the normal electric displacement \( D_2 \) across the electrode by,

\[
\tau(z) = \frac{1}{2\pi} \int_{-\infty}^{0} \frac{\rho(x_1)}{z-x_1} dx_1, \quad z = x_1 + ix_2
\]  

(4.14)

Using eqns. 4.9, 4.10, 4.12 and 4.13, the complex potential functions in the upper and lower half-planes can be expressed in terms of function \( \tau(z) \) as,

\[
\Phi_i(z) = iA_i^{-1}Y_i(Y_i + \overline{Y_{ii}})^{-1}\overline{Y_{ii}}(0 \ 0 \ \tau(z))^T, \quad x_2 > 0
\]  

(4.15)

\[
\Phi_{ii}(z) = iA_{ii}^{-1}Y_{ii}(Y_{ii} + \overline{Y_i})^{-1}\overline{Y_i}(0 \ 0 \ \tau(z))^T, \quad x_2 < 0
\]  

(4.16)

where \( Y_i = iA_iB_i^{-1} \) and \( Y_{ii} = iA_{ii}B_{ii}^{-1} \).

The electrical loading on the electrode (conducting sheet) is used to determine the unknown potential function \( \tau(z) \). With the aid of (4.15) and (4.16), the following non-homogenous Hilbert problem can be obtained.

\[
\gamma_1 \tau^+(x_1) + \gamma_2 \tau^-(x_1) = E_0(x_1)
\]  

(4.17)
where \( \gamma_1 = -(0 \ 0 \ 1)Y_1(Y_1 + \overline{Y}_2)^{-1}\overline{Y}_2(0 \ 0 \ 1)^T \) and \( \gamma_2 = -(0 \ 0 \ 1)Y_2(Y_2 + \overline{Y}_1)^{-1}\overline{Y}_1(0 \ 0 \ 1)^T \).

Note that \( \gamma_1 = \gamma_2 \) [49], the general solution to the above Hilbert problem is given by [91],

\[
\tau(z) = \frac{z^{-1/2}}{2\pi \gamma} \int_{-\infty}^{\infty} \frac{\sqrt{-x_1}E_0(x_1)}{x_1 - z} dx_1
\]

(4.18)

The electroelastic field at the electrode tip is finally determined by the general solutions in eqns. 4.4 and 4.5 together with the potential functions (4.15), (4.16) and (4.18). In view of eqn. 4.18, the elastic and electric fields near an embedded electrode tip show an inverse square root singularity which is identical to the cases of insulating and conducting cracks in piezoelectric media. Furthermore, the stress and electric field intensity factors at the electrode tip can be determined from the following relations.

\[
\langle \sigma_{22}, \sigma_{12}, E_1 \rangle = \langle K_I, K_{II}, K_E \rangle / \sqrt{2\pi} \ \ (0 < x_1 < \infty, \ x_2 = 0)
\]

(4.19)

It follows that,

\[
K_E = -\sqrt{\frac{2}{\pi}} \int_{-\infty}^{\infty} \frac{E_0(x_1)}{\sqrt{-x_1}} dx_1
\]

(4.20)

\[
K_I = \frac{(0 \ 1 \ 0)\text{Im}[(Y_1 + \overline{Y}_2)^{-1}\overline{Y}_2](0 \ 0 \ 1)^T}{(0 \ 0 \ 1)\text{Re}[Y_1(Y_1 + \overline{Y}_2)^{-1}\overline{Y}_2](0 \ 0 \ 1)^T} K_E
\]

(4.21)

\[
K_{II} = \frac{(1 \ 0 \ 0)\text{Im}[(Y_1 + \overline{Y}_2)^{-1}\overline{Y}_2](0 \ 0 \ 1)^T}{(0 \ 0 \ 1)\text{Re}[Y_1(Y_1 + \overline{Y}_2)^{-1}\overline{Y}_2](0 \ 0 \ 1)^T} K_E
\]

(4.22)

It is further shown in Section 4.4 that both the tensile and shear stress intensity factors \( K_I \) and \( K_{II} \) vanish at the electrode tip. Consequently, the singular electroelastic field can be uniquely characterized by the electric field intensity factor \( K_E \), which depends on both the applied electric voltage and the geometry of the actuator.
4.3 Effect of Domain Switching on Singular Field

To investigate the effect of domain switching on the variation of the stress and electric fields near an embedded electrode tip, a new fundamental solution for a semi-infinite electrode at the interface of two piezoelectric half-planes interacting with transformation strains and polarization is needed (Fig. 4.2). The new solution can be derived by using an approach analogous to that presented in Sec. 3.3 for an insulating (or a conducting) crack interacting with stress-free transformation strains and electric field-free polarization.

Consider a semi-infinite electrode interacting with a circular region of differential area $dA$ which has undergone a stress-free transformation strain $\varepsilon^*$ and an electric field-free polarization $D^*$ in the upper half-plane (Fig. 4.2). The poling directions of the upper and the lower half-planes are opposite to each other and normal to the electrode. The interaction problem can now be considered as the superposition of two sub-problems: (a) the circular region undergoes transformation strain $\varepsilon^*$ and polarization $D^*$ in the upper half-plane, resulting in an electric field $\hat{E}_1(x_1)$ on the line $x_2 = 0, x_1 < 0$; (b) the faces of an electrode at $x_2 = 0, x_1 < 0$ subjected to an electrical loading $E_0(x_1) = -\hat{E}_1(x_1)$. By superposition, the electrical and the mechanical boundary conditions on the embedded electrode are satisfied.

Figure 4.2. Electrode interacting with a circular spot with eigenstrains and eigenpolarization.
In the subproblem (a), a circular transformation inclusion is embedded in a bimaterial system. The solution to this problem can be constructed from the known solution for a piezoelectric inclusion embedded in an infinite homogeneous medium. Let \( \Phi_0(z) \) denote the potential function for a circular inclusion of differential area \( dA \) in an infinite homogeneous medium with properties identical to the upper half-plane, the potential function for the subproblem (a) can be expressed as,

\[
\Phi(z) = \begin{cases} 
\Phi_1(z) + \Phi_0(z), & x_2 > 0 \\
\Phi_\Pi(z), & x_2 < 0 
\end{cases}
\]

(4.23)

and \( \Phi_0(z) = (\varphi'_{01}(z_1^1), \varphi'_{02}(z_1^1), \varphi'_{03}(z_1^1))^T \) are derived from eqn. 3.11 as,

\[
\varphi'_n = \frac{G_n^1[1 + (\mu_n^1)^2]}{2\pi(z_n^1 - z_{n0})^2}, \quad n = 1, 2, 3
\]

(4.24)

where the superscript ‘1’ is used to identify the quantities corresponding to the upper half-plane.

From eqn. 4.2, the continuity of normal and shear tractions and normal electric displacement requires that,

\[
B_1[\Phi_1(x_1) + \Phi_0(x_1)] + B_{11}[\Phi_1(x_1) + \Phi_0(x_1)] = B_{11}\Phi_\Pi(x_1) + B_{11}\Phi_{\Pi}(x_1)
\]

(4.25)

or

\[
B_1\Phi_1(x_1) + B_1\Phi_0(x_1) - B_{11}\Phi_\Pi(x_1) = B_{11}\Phi_{\Pi}(x_1) - B_1\Phi_0(x_1) - B_1\Phi_1(x_1)
\]

(4.26)

The functions on the left-hand and the right-hand sides are analytic in the upper and lower half-planes respectively and they both approach zero at infinity. By the standard analytic continuity argument, both functions are identical to zero. Therefore,

\[
B_1\Phi_1(z) + B_1\Phi_0(z) - B_{11}\Phi_\Pi(z) = 0, \quad x_2 > 0
\]

(4.27)

\[
B_{11}\Phi_\Pi(z) - B_1\Phi_0(z) - B_1\Phi_1(z) = 0, \quad x_2 < 0
\]

(4.28)

Similarly, in view of eqn. 4.3, the continuity of displacements and electric potential across the interface leads to,
\[ A_1 \Phi_1(z) + A_1 \Phi_0(z) - \overline{A_1 \Phi_1}(z) = 0, \quad x_2 > 0 \]  
\[ A_1 \Phi_1(z) - A_1 \Phi_0(z) - \overline{A_1 \Phi_1}(z) = 0, \quad x_2 < 0 \]  

In view of eqns. 4.27, 4.28, 4.29 and 4.30, the potential functions \( \Phi_1(z) \) and \( \Phi_0(z) \) are obtained as,
\[ \Phi_1(z) = B_1^{-1}(Y_1 + Y_0)^{-1}(Y_1 - Y_0)B_1 \Phi_0(z), \quad x_2 > 0 \]  
\[ \Phi_0(z) = B_1^{-1}(Y_1 + Y_0)^{-1}(Y_1 + Y_0)B_1 \Phi_0(z), \quad x_2 < 0 \]  

The electric field \( \hat{E}_1(x_1) \) on the line \( x_2 = 0, x_1 < 0 \) due to the transformation field of the inclusion can be expressed as,
\[ \hat{E}_1(x_1) = 2 \text{Re} \sum_{n=1}^{3} \frac{s_n T_n}{(x_1 - z_n^0)^2} \]  

where the superscript ‘II’ is used to identify the quantities corresponding to the lower half-plane and,
\[ (T_1^{II}, T_2^{II}, T_3^{II})^T = \frac{1}{2\pi} B_1^{-1}(Y_1 + Y_0)^{-1}(Y_1 + Y_0)B_1 (G_1^{I})(1 + (\mu_1^I)^2) \]
\[ G_2^{I+} \text{[1 + (\mu_2^I)^2]} \]
\[ G_3^{I+} \text{[1 + (\mu_3^I)^2]} \]  

The solution to subproblem (b) is hence determined. When the faces of a semi-infinite electrode are subjected to electrical loading \( E_0(x_1) = -\hat{E}_1(x_1) \), the electric field intensity factor is derived as (eqn. 4.20),
\[ dK_E = \sqrt{\frac{2}{\pi}} \int_{-\infty}^{0} \frac{\hat{E}_1(x_1)}{\sqrt{-x_1}} dx_1 = \text{Re} \sum_{n=0}^{3} \frac{\sqrt{2\pi} s_n T_n}{(z_n^0)^{3/2}} \]  

and the normal and shear stress intensity factors are related to the electric field intensity factor by eqns. 4.21 and 4.22, respectively.

Similarly the electric field intensity corresponding to an inclusion in the lower half-plane subjected to an eigen field is derived as,
Without switching, the nominal near-tip electric and stress fields can be characterized by the electric field intensity factor \( K_E \) as derived in the previous section. After switching, the electroelastic field in the vicinity of an electrode tip approaches a level characterized by a local electric field intensity factor \( K'_E = K_E + \Delta K_E \), where \( \Delta K_E \) denotes the additional electric field intensity due to polarization switching. \( \Delta K_E \) can be estimated using an approach analogous to that presented in Chapter 3. For a given domain orientation, the switching zone around a buried electrode tip is determined by the domain switching criterion (3.4) coupled with the singular stress and electric fields (eqns. 4.18) characterized by the applied electric field intensity factor \( K_E \). By integrating the fundamental solutions (4.35) and (4.36) over switching zones in the upper and the lower half-planes, the contribution of an individual domain orientation to the field intensity \( \Delta K_E \) is obtained. Using eqn. 3.25, switching induced field intensity \( \Delta K_E \) due to all possible domain orientations can be determined. This leads to a Reuss-type approximation for poly-domain ferroelectrics with details given in Section 3.5.

4.4 Numerical Results and Discussion

In this section, the electroelastic field at the tip of an embedded electrode at the interface of two-bonded piezoelectric half-planes is investigated (Fig. 4.1). The effect of domain switching on the near-tip field is also examined and PZT-5H is used in the numerical study.

Fig 4.3 shows switching zones around an embedded electrode tip for a mono-domain system. The coordinates in the figure are normalized by \( r_0 = [K_E/(2\sqrt{\pi E_s})]^2 \), where \( K_E \) is the applied nominal electric field intensity factor. For the cases I and II (Fig. 4.1), the switching zones are identical and only 90° domain switching occurs in front of
the electrode tip. For the cases III and IV, 90° switching is predicted to occur ahead of the electrode tip and 180° switching occurs behind the tip. The different domain switching behavior between case I (or II) and case III (or IV) can be explained by the argument that ferroelectric domains tend to align their spontaneous polarization closer to the local electric field vector. By examining the field vector around an embedded electrode tip, the different switching types for case I (or II) and case III (or IV) can be justified. Domain switching induced electric field intensity factor $\Delta K_E$ is predicted to be $-0.443K_E$ and $0.743K_E$ for case I (or II) and case III (or IV), respectively.

![Figure 4.3. Localized switching zone around an embedded electrode tip.](image)

The variation of normal and shear stresses $\sigma_{11},\sigma_{22}$ and $\sigma_{12}$ with the polar angle $\theta$ defined at the electrode tip is presented in Figs. 4.4, 4.5 and 4.6 respectively. Fig. 4.4 shows the variation of normal stress $\sigma_{11}$ with the polar angle $\theta$. Directly ahead of the electrode ($\theta=0^\circ$), the normal stress $\sigma_{11}$ vanishes. The largest normal stress parallel to the electrode ($\sigma_{11}$) occurs at the electrode-ceramic interfaces ($\theta = -180^\circ$ and $180^\circ$). If there
are micro-cracks developed in the interfaces during manufacturing or the poling process, segmentation cracks can easily be initiated due to the intensified normal stress $\sigma_{11}$. In their experiments, Schneider et al. [22] found that segmentation cracks were formed during the first few cycles of applied electric loading prior to the occurrence of electrode tip cracks and electrode delamination.

![Figure 4.4. Variation of normal stress $\sigma_{11}$ with polar angle $\theta$.](image)

Fig. 4.5 shows the variation of normal stress $\sigma_{22}$ with the polar angle $\theta$. At the electrode-free interface ($\theta = 0^\circ$), the normal stress $\sigma_{22}$ vanishes. It implies that the mode I stress intensity factor $K_1$ is equal to zero and a crack can not emanate along the bonded interface, which is supported by experimental observations [20-22]. However, at the electrode-ceramic interfaces, the normal stress is intense and can lead to electrode delamination in multilayer actuators as observed in experiments. When an applied electric field reverses it sign, i.e. from case I to case III, or from case II to case IV, the normal stress $\sigma_{22}$ changes its sign from compressive to tensile. This implies that a delamination can propagate in only half of the cycle under a bipolar cyclic electric field.
The sign of $\sigma_{22}$ can be deduced by considering the constraint of the interface on the expansion (or contraction) of the upper and lower ceramic layers. For example, the elongation of the upper and lower half planes in case I is impeded by the interface, which consequently results in a compressive normal stress.

![Diagram showing variation of normal stress $\sigma_{22}$ with polar angle $\theta$.](image)

Figure 4.5. Variation of normal stress $\sigma_{22}$ with polar angle $\theta$.

Fig. 4.6 shows the variation of shear stress $\sigma_{12}$ with the polar angle $\theta$. The shear stress $\sigma_{12}$ vanishes at both the electrode-free and the electrode-ceramic interfaces for the four cases in consideration. Therefore the mode II stress intensity factor $K_{II}$ vanishes. Note that the shear stress changes sign at around +/- 120° and the maximum shear stress is achieved at +/- 60°. Fig. 4.7 shows the variation of hoop stress $\sigma_{\theta\theta}$ with the polar angle $\theta$. At the electrode-free interface ($\theta = 0^\circ$), the hoop stress vanishes, whereas the largest hoop stress happens at the electrode-ceramic interface ($\theta = -180^\circ$ and 180°). Due to domain switching, the near-tip electroelastic field is intensified for the cases III and IV, while decreased for the cases I and II. In view of the stress distributions shown in Figs.
4.4 to 4.7, the maximum tensile stress occurs behind an embedded electrode tip. Therefore, the present model fails to predict the large tensile stress leading to the observed Y-shaped crack pattern ahead of an internal electrode tip [20-22]. This may be a consequence of the modelling assumption of uniform poling in ceramic layers. In fact, the poling of ferroelectric materials ahead of an electrode tip can be nonuniform and not exactly perpendicular to the internal electrode. Moreover, the residual stress induced in multilayer actuators by the poling process can also play an important role in fracture of ceramic actuators. This effect is not included in the present model.

![Figure 4.6. Variation of shear stress $\sigma_{12}$ with polar angle $\theta$.](image)
Investigation of the concentrated electric field around an internal electrode tip is important to understanding of dielectric failure of ferroelectric actuators. Figs. 4.8 and 4.9 show the variation of electric field $E_1$ and $E_2$ with the polar angle $\theta$ respectively. As shown in Fig. 4.8, the electric field $E_1$ vanishes at an electrode layer. Directly ahead of an electrode tip, i.e. along the electrode-free interface, $E_1$ reaches its maximum value. Due to domain switching, the electric field is increased for case III and IV by about 75 percent, while it decreases for Cases I and II by about 45 percent. As shown in Fig. 4.9, along the electrode-free interface, $E_2$ vanishes. It reaches the maximum value at the electrode-ceramic interface. The maximum value of the electric field perpendicular to the electrode is very close to that of the electric field parallel to it. Note that the electric field $E_2$ has a jump across the electrode layer, which is proportional to the stored electric charge in the electrode. The elevated electric field near an electrode layer can lead to dielectric breakdown of actuators.
Figure 4.8. Variation of electric field $E_1$ with polar angle $\theta$.

Figure 4.9. Variation of electric field $E_2$ with polar angle $\theta$. 

Cases I-IV, no switching
Cases I & II, with switching
Cases III & IV, with switching
The solutions for the near-tip stresses maybe helpful to establish a critical thickness for the ceramic layer in order to prevent cracking of multilayer actuators [48]. In view of Figs. 4.4-4.7, the ratio of the maximum tensile stress to the nominal electric field is about 30 Nm/V. It follows that the mode I stress intensity ($K_I$) of a crack emanating from the electrode tip may be approximated by 30 times the nominal electric field intensity $K_B$. For a stacked actuator as shown in Fig. 1.4, $K_E \approx E_{appl} \sqrt{2H}$, where $E_{appl}$ is the applied electric field and $H$ the thickness of a ceramic layer [48]. To prevent cracking of an actuator, $K_I$ should be less than the intrinsic fracture toughness $K_{IC}$ ($\approx 1$ MPa m$^{1/2}$) of the material. If $E_{appl}$ is half of the coercive field $E_C$ ($\approx 1$ MV/m), a critical layer thickness of $H=2.22$ mm is predicted in order to suppress cracking. In practice, $H$ is much smaller than this value. If $E_{appl}$ approaches the coercive field, the critical thickness is predicted to be 556 $\mu$m, which falls into the order of layer thicknesses used in practical multilayer actuators (100–300 $\mu$m).
Chapter 5

CONCLUSIONS

5.1 Summary

The major findings and conclusions of the present study are summarized as follows:

1. Two-dimensional piezoelectric Eshelby tensor can be obtained in closed form for an elliptic inclusion with specified eigenstrains and eigenelectric displacement and its symmetric properties can be established. Based on the derived constraint tensor, the potential energy due to the introduction of an elliptic crystallite into a poled ferroelectric material is derived and applied to establish an energy criterion for polarization switching of the crystallite. The resulting switching criterion takes into account full electromechanical coupling, the changes of spontaneous strains and spontaneous polarization, and electroelastic properties of the crystallite before and after switching. It is found that the switching criterion can be reduced to the work energy based switching criterion of Hwang et al. [15] under certain assumptions. The switching criterion can be used to predict the nonlinear process zone around a crack tip and the change of orientation of a ferroelectric crystallite under varying applied electric and stress fields. By employing appropriate homogenization techniques, the evolution of average strains and polarization can be traced as applied electric and stress fields change. By this approach, the nonlinear material characteristics of ferroelectrics such as dielectric hysteresis and butterfly loops can be reproduced.

2. A new Gibbs free energy expression due to the introduction of an elliptic nucleus into a large parent ferroelectric domain is derived and used to simulate the evolution of 180° and 90° domain nuclei under electromechanical loading. Numerical results
for 180° and 90° domain evolution in single crystal BaTiO₃ reveal that the domains tend to grow in paths with higher aspect ratios \((b/a)\). This explains the experimentally observed spike-like domain growth behavior in single crystal materials or polycrystal materials of very large grain size [81, 94]. However, ferroelectric domains in fine-grained ferroelectric ceramics such as PZTs are not typically needle-shaped. Electromechanical coupling and material anisotropy are shown to play important roles in the domain evolution. 180° domain nucleus tend to evolve in a path with even a higher aspect ratio when the material is modeled as a piezoelectric instead of an isotropic elastic dielectric. It is also found that a compressive stress applied parallel to the polar direction has a trivial effect on 180° domain evolution. For 90° domain evolution, the effects of electromechanical coupling and material anisotropy are less pronounced as compared to 180° domain nucleus. An electric field applied perpendicular to the polar direction is shown to enhance the evolution of a 90° domain nucleus.

3. The piezoelectric Eshelby tensor derived in the present study is also applied to derive the electroelastic field and the energy release rate of an elliptic flaw in poled ferroelectrics. Self-similar propagation is assumed in this study to derive the energy release expressions. The remanent strains and remanent polarization have a minor effect on the stress field and can have a pronounced effect on the electric field and on the energy release rate, depending on the geometry and dielectric properties of the elliptic flaw. For the case of a conducting flaw, the remanent field has no effect on the electroelastic field and consequently the energy release rate. It is clear from this study that the energy release rates of a flaw in a poled ferroelectric with and without the consideration of remanent strains and remanent polarization are different. The residual stain energy and the depolarization energy can significantly affect the fracture behavior of poled ferroelectric ceramics.

4. Effects of domain switching on the electroelastic field at the tip of an insulating (or a conducting) crack are investigated in the spirit of transformation toughening. A
theoretical model is proposed to calculate domain switching induced electric and stress field intensity factors under electromechanical loading. The two basic building blocks for the theoretical model are the domain switching criterion proposed in the present study and a fundamental solution for the electroelastic field intensity factors of a semi-infinite insulating (or conducting) crack interacting with stress-free transformation strains and electric field-free polarization in a piezoelectric solid. Domain switching zone near a crack tip is predicted by the switching criterion derived in the present study coupled with the singular near-tip field provided by linear piezoelectricity. The solution of switching induced field intensities of a polycrystalline ferroelectric ceramic is obtained by a Reuss-type approximation, which assumes that every domain in the same continuum element is subjected to identical stress field and electric field.

5. The influence of electrical loading and the poling direction on the change of mode I stress intensity factor (toughness variation) of insulating and conducting cracks is investigated numerically. For an insulating crack, both positive and negative electric fields are shown to enhance the propagation of a crack perpendicular to the initial poling direction. This finding is consistent with some experimental observations, but disagrees with others. For a conducting crack, both positive and negative fields tend to shield the tip of a crack parallel to the poling axis. Under small to moderate electric fields, the characteristic fracture curve obtained experimentally for a conducting crack in PZT PIC-151 [33] can be explained by the current domain switching model coupled with the total energy release rate criterion. The poling direction with respect to the crack orientation and the direction of an applied electric field also affect domain switching at a crack tip and consequently apparent fracture toughness.

6. Conditions are established for closure of insulating and conducting cracks in piezoelectric solids under electrical and mechanical loading. Under pure electrical loading, an insulating crack is closed when an electric field is applied perpendicular
to the crack and forming an obtuse angle with the poling axis, while a conducting crack is closed by an electric field applied parallel to it and making an acute angle with the poling direction. Due to electric field triggered crack closure, large tensile stress is induced directly ahead of an insulating (or a conducting) crack. This can lead to electric field-driven crack growth. Numerical studies show that a pure electric loading results in the largest mode-I stress intensity when an electric field applied opposite to the poling direction for an insulating crack, or parallel to the poling axis for a conducting crack. Due to polarization switching, the mode I stress intensity factor of an electric field-induced closed crack may be increased or decreased, depending on the crack face electric boundary conditions and the direction of poling axis with respect to the applied electric field.

7. A simplified mathematical model is presented to investigate the electric and stress fields at the tip of an internal electrode in a multilayer ferroelectric actuator. It is found that the stress and electric fields show inverse square root singularity at an embedded electrode tip. Directly ahead of an electrode tip, the normal and shear stresses vanish, which implies that a crack cannot emanate at the electrode-free interface. However, intensified normal stress is developed at the electrode-ceramic interface, which can result in segmentation cracks and electrode debonding as observed in experiments. The effect of domain switching on the electroelastic field near an internal electrode tip is calculated in the spirit of transformation toughening with the aid of a new fundamental solution for an electrode interacting with eigenstrains and eigenelectric displacement. The magnitude of the near tip field can increase or decrease by up to seventy percent depending on the poling directions of two adjacent ceramic layers with respect to the applied electric field. To suppress cracking of a piezoelectric multilayer actuator, the thickness of each ceramic layer should be lower than a critical value, which depends on the material properties, magnitude of operating field and geometry of an actuator.
5.2 Suggestions for Future Work

To further improve the understanding of fracture behavior of ferroelectric materials and to improve the design of ferroelectric electromechanical devices, the following suggestions are made for future work.

1. The near-tip domain-switching model proposed in the present study has been used to investigate the effect of polarization switching on the electroelastic field of a stationary crack. It can be further extended to study stable growing cracks and to explain the experimentally observed R-curve behavior of ferroelectric materials. As a crack tip advances, the fracture toughness of a ferroelectric increases with the crack length until it attains a plateau where the crack reaches a stable growth state. The toughening effect is generally believed to be attributed to a domain-switching wake behind the advancing crack tip. The present theoretical model can be employed to estimate the modified stress intensity factor (toughness variation) induced by the switching wake. The effects of an applied electric field and the poling direction on the R-Curve behavior need to be investigated both experimentally and theoretically.

2. The remanent strains and remanent polarization introduced in ferroelectric ceramics after the poling process play an important role in the electroelastic field and energy release rate of a crack tip. After poling, residual stress and residual electric field can be induced in a ceramic along with remanent strains and remanent polarization. This may significantly affect the fracture behavior of ferroelectrics and the cracking of multilayer ceramic actuators. To fully resolve the residual field and the remanent field effects, coupled-field finite element programs with nonlinear constitutive models for ferroelectric materials are needed. With the aid of such programs, nonlinear fracture mechanics of ferroelectrics can be established. The variation of electric and stress fields at cracks or internal electrodes with applied loading can be fully understood. Such programs are indispensable for improving the design of ferroelectric actuators.
3. In the present study, domain switching is modeled as an on-off (instantaneous) process. Such an approach may not be adequate to address the complex thermodynamic process of polarization switching. In fact, domain switching occurs through the nucleation of domain walls and subsequent domain wall propagation. It is indeed a non-instantaneous process. Micromechanics-based non-instantaneous domain switching models with detailed description of domain wall dynamics may be helpful to gain a better understanding of the constitutive behavior of ferroelectric materials. However, the intensive computational burden will preclude such models from applying to study macroscopic fracture behavior. A more feasible solution is to devise phenomenological constitutive models for ferroelectrics, similar to yielding models in plasticity. Such phenomenological models can be implemented in finite element codes and applied to study macroscopic failure of electromechanical devices.

4. More experimental tests are needed to investigate the fracture behavior of ferroelectric materials and electromechanical failure of ferroelectric actuators. To better understand the exact nature of electric boundary condition on crack surfaces, the measurement of electric potential at the upper and lower crack faces is needed. As shown in the present study, the poling direction may have remarkable influence on apparent fracture toughness. Therefore, the effect of poling direction on fracture of ferroelectric materials needs to be experimentally investigated. However, the previous experiments were always focusing on a crack parallel or perpendicular to the poling axis. Note that even with identical electrical and mechanical loading, the effect of poling direction on the crack-tip electroelastic field is rather subtle.
Bibliography


APPENDIX A

The complex roots \( \mu_n \) (n = 1, 2, 3) appearing in the general solution [eqns. (2.3)-(2.6)] with positive imaginary parts are determined by the following characteristic equation:

\[
l_1(\mu)l_2(\mu) + l_3^2(\mu) = 0 \quad (A1)
\]

\[
l_1(\mu) = \beta_{11}\mu^2 - 2\beta_{12}\mu + \beta_{22} \quad (A2)
\]

\[
l_2(\mu) = S_{11}\mu^4 - 2S_{13}\mu^3 + (2S_{12} + S_{33})\mu^2 - 2S_{23}\mu + S_{22} \quad (A3)
\]

\[
l_3(\mu) = g_{11}\mu^3 - (g_{21} + g_{13})\mu^2 + (g_{12} + g_{23})\mu - g_{22} \quad (A4)
\]

where \( S_{ij}, g_{ij} \) and \( \beta_{ij} \) are the elements of the constitutive matrices \( S, g \) and \( \beta \), respectively.

The complex constants appearing in the formulations for two-dimensional electroelastic field of piezoelectrics [eqns. (2.3)-(2.6)] are given by

\[
\delta_n = l_3(\mu_n) / l_1(\mu_n) \quad (A5)
\]

\[
p_n = S_{11}\mu_n^2 - S_{13}\mu_n + S_{12} + \delta_n(g_{11}\mu_n - g_{21}) \quad (A6)
\]

\[
q_n = (S_{12}\mu_n^2 - S_{23}\mu_n + S_{22} + \delta_n g_{12}\mu_n - \delta_n g_{22}) / \mu_n \quad (A7)
\]

\[
s_n = g_{11}\mu_n^2 - g_{13}\mu_n + g_{12} - \delta_n(\beta_{11}\mu_n - \beta_{12}) \quad (A8)
\]

\[
t_n = g_{21}\mu_n^2 - g_{23}\mu_n + g_{22} - \delta_n(\beta_{12}\mu_n - \beta_{22}) \quad (A9)
\]

The derivation of eqn. (2.45) is given in the following.

In view of eqns. (2.31), (2.32) and (2.33),

\[
(\Sigma_1^1)^T L_2^{-1}\Sigma_2^1 = (\Sigma_1^1)^T L_2^{-1}L_2 (L^{-1}\Sigma^0 - Z_2^p + QZ_2^p')
\]
\[-(\Sigma_1^1)^T Z_2^p + [\Sigma^0 + L(Q - I)Z_1^*]^T (L^{-1} \Sigma^0 + QZ_2^*) \]

\[-(\Sigma_1^1)^T Z_2^p + (\Sigma_2^1)^T L^{-1} \Sigma^0 + (\Sigma_2^1)^T QZ_2^* + (\Sigma^0)^T (Q - I) Z_1^* + (Z_1^*)^T [L(Q - I)]^T QZ_2^* \]  

(A10)

Similarly,

\[(\Sigma_1^1)^T L_1^{-1} \Sigma_2^1 = -(\Sigma_2^1)^T Z_1^p + (\Sigma_2^1)^T L^{-1} \Sigma^0 + (\Sigma^0)^T QZ_1^* + (\Sigma^0)^T (Q - I) Z_2^* + (Z_2^*)^T [L(Q - I)]^T QZ_1^* \]  

(A11)

Therefore,

\[\Delta U = U_1 - U_2 = U_1^f - U_2^f = \frac{\pi ab}{2} [(\Sigma^0)^T Z_2^* + (\Sigma_2^1)^T Z_2^p - (\Sigma_2^1)^T Z_1^* - (\Sigma_1^1)^T Z_2^p] \]

\[= \frac{\pi ab}{2} [(\Sigma_1^1 + \Sigma_2^1)^T (Z_2^p - Z_1^p) + (\Sigma_1^1)^T (L_2^{-1} - L_1^{-1}) \Sigma_2^1] \]  

(A12)