Continuum and Computational Modeling of Flexoelectricity

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Continuum and Computational Modeling of Flexoelectricity

Abstract
Flexoelectricity refers to the linear coupling of strain gradient and electric polarization. Early studies of this subject mostly look at liquid crystals and biomembranes. Recently, the advent of nanotechnology revealed its importance also in solid structures, such as flexible electronics, thin films, energy harvesters, etc. The energy storage function of a flexoelectric solid depends not only on polarization and strain, but also strain-gradient. This is our basis to formulate a consistent model of flexoelectric solids under small deformation. We derive a higher-order Navier equation for linear isotropic flexoelectric materials which resembles that of Mindlin in gradient elasticity. Closed-form solutions can be obtained for problems such as beam bending, pressurized tube, etc. Flexoelectric coupling can be enhanced in the vicinity of defects due to strong gradients and decay away in far field. We quantify this expectation by computing elastic and electric fields near different types of defects in flexoelectric solids. For point defects, we recover some well-known results of non-local theories. For dislocations, we make connections with experimental results on NaCl, ice, etc. For cracks, we perform a crack-tip asymptotic analysis and the results share features from gradient elasticity and piezoelectricity. We compute the J integral and use it for determining fracture criteria.

Conventional finite element methods formulated solely on displacement are inadequate to treat flexoelectric solids due to higher order governing equations. Therefore, we introduce a mixed formulation which uses displacement and displacement-gradient as separate variables. Their known relation is constrained in a weighted integral sense. We derive a variational formulation for boundary value problems for piezoe- and/or flexoelectric solids. We validate this computational framework against exact solutions. With this method more complex problems, including a plate with an elliptical hole, stationary cracks, as well as structures with periodic structures, can be studied consistently with the continuum theory. We also generate predictions of experimental merit and reveal interesting flexoelectric phenomena with potential for application.

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CONTINUUM AND COMPUTATIONAL MODELING OF
FLEXOELECTRICITY

Sheng Mao

A DISSERTATION
in
Mechanical Engineering and Applied Mechanics
Presented to the Faculties of the University of Pennsylvania
in
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Degree of Doctor of Philosophy
2016

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Sheng Mao
Who understands Tao seems dull of comprehension;
Who is advance in Tao seems to slip backwards.

Great music is faintly heard;
Great form has no contour.

‘Tao Te Ching’, Chapter 41
Translated by Yutang Lin
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# Contents

## Contents

List of Tables viii

List of Figures ix

Nomenclature xii

1 Introduction 1

1.1 Flexoelectricity in Hard Materials .......................... 1

1.1.1 Origins of flexoelectricity ................................... 2

1.1.2 Quantifying flexoelectric constants .......................... 4

1.1.3 Unique phenomenon due to flexoelectricity .................... 6

1.2 Continuum Treatment of Flexoelectricity ...................... 8

1.3 Scope of the thesis ........................................... 10

2 Continuum Theory of Flexoelectricity 11

2.1 Introduction .................................................. 11

2.2 Classical continuum field theory .............................. 12

2.3 Governing equations ......................................... 15

2.4 Linear constitutive relations .................................. 17

2.5 Isotropic flexoelectric material .............................. 19

2.6 Application .................................................. 21

2.6.1 Euler Bernoulli beam ....................................... 21

2.6.2 Torsion .................................................... 24

2.6.3 Cylinder under pressure .................................... 24

2.6.4 Cylinder under shear ....................................... 31

2.7 Concluding remarks .......................................... 33

3 Defects in Flexoelectric Solid 35

3.1 Introduction .................................................. 35

3.2 Flexoelectric Green’s function ................................ 36

3.3 Point defects .................................................. 39

3.4 Line defects ................................................... 41

3.4.1 Screw dislocation .......................................... 41

3.4.2 Edge dislocation ........................................... 43

3.5 Concluding remarks .......................................... 47
# Table of Contents

4 Fracture Mechanics of Flexoelectricity  
  4.1 Introduction .............................................. 48  
  4.2 Mode III crack ............................................ 49  
  4.3 Planar Cracks .............................................. 50  
    4.3.1 Mode I ............................................... 51  
    4.3.2 Mode II ............................................. 55  
    4.3.3 Mode D and Mode E ................................. 56  
    4.3.4 Mixed modes ....................................... 57  
  4.4 J integral ............................................... 59  
  4.5 Fracture criterion ...................................... 63  
  4.6 Concluding remarks .................................. 66  

5 Finite Element Analysis  
  5.1 Introduction ............................................ 67  
  5.2 Constitutive model ..................................... 68  
  5.3 The boundary value problem .......................... 70  
  5.4 A variational formulation ............................. 70  
  5.5 “Mixed” finite element formulation .................. 72  
  5.6 Applications .......................................... 74  
    5.6.1 Code validation .................................. 74  
    5.6.2 Elliptical hole in a plate ....................... 77  
    5.6.3 Stationary crack .................................. 79  
    5.6.4 Periodic structures ............................... 85  
  5.7 Concluding remarks .................................. 89  

6 Closure .................................................... 91  

A Appendix of Chapter 2  
  A.1 Example of reciprocity ................................. 95  
  A.2 Solution to a bimorph system ....................... 96  

B Appendix to Chapter 4 ...................................... 101  

C Modeling Pyro-paraelectricity .......................... 103  

D Tensorial Components in Polar Coordinates .......... 106  

Bibliography .................................................. 107
List of Tables

4.1 Leading order terms of crack tip asymptotics in different models. . . . . . . . . . . . 53
List of Figures

1.1 (a) Flexoelectricity induced by bending. When a slab of thickness $t$ is bent, it results in tension (blue) in one direction and compression (red) in the other, therefore a strain gradient. (b) the zoom-in of the locally bent lattices. Center of cations (light color circle) and anions (dark color circle) are displaced. A polarization is induced as a result. From Maranganti et al. (2006). Copyright 2006, American Physical Society. 

1.2 Two most common ways of measuring flexoelectric constants. (a) The cantilever beam and (b) the truncated pyramid compression. Gray parts are the electrodes used to measure charge flow. Here, $\hat{\mu}_{12} = \mu_{122}^{f}$ and $\hat{\mu}_{11} = \mu_{1111}^{f}$. From Zubko et al. (2013). Copyright 2013, Annual Review.

1.3 Illustration of mechanical writing of ferroelectric polarization by the use of AFM tip. Strong gradients exerted by the tip can reverse the polarization and hence result in different domain patterns. This method is purely mechanical without any charge injection. From Zubko et al. (2013). Copyright 2013, Annual Review.

2.1 A deformable dielectric body $V$ put in a coordinate system $\{x_1, x_2, x_3\}$ and subjected to traction $t(x_i)$ and electric loading $\phi(x_i)$ on its boundary $\partial V$.

2.2 Size dependent stiffening of flexoelectric beams. Flexoelectric calculations are carried out keeping $f_0/f_m = 0.25$ where $f_m = \sqrt{Ef_0^2}/\epsilon_0$ and $G$ is the effective bending rigidity.

2.3 A flexoelectric cylindrical tube/disk under pressure and voltage difference.

2.4 This figure plots a) potential and b) polarization with parameters as in Eqn.(2.71).

2.5 This figure plots a) radial strain $\varepsilon_{rr}$ and b) hoop strain $\varepsilon_{\theta \theta}$, with parameter as in Eqn.(2.71).

2.6 This figure plots a) radial stress $\sigma_{rr}$ and b) hoop stress $\sigma_{\theta \theta}$, with parameter as in Eqn.(2.71).

2.7 This figure plots in (a) the asymptotic behavior of SCF with $r_0/r_i \to \infty$ and in (b) the flexoelectric reduction of SCF with increasing $f$.

2.8 In this figure, (a) plots SCF as a function of potential $V$ holding mechanical loads fixed (b) plots polarization at the inner surface as a function of pressure $p_i$, holding $V = 0$.

2.9 (a) plots normalized shear strain and (b) the normalized displacement as functions of the radial coordinate. (c) plots the distribution of normalized azimuthal polarization. It reaches a minimum around the middle of the disk.
3.2 This figure plots the electric quantities due to an edge dislocation, at

4.3 The COD profile of mixed Mode I & Mode E cracks with different values of

4.2 Contours used in computation of the energy release rate. . . . . . . . . . . . . 60

5.3 Comparison of finite element and analytical solutions: (a) displacement

5.2 (a) A cylindrical flexoelectric tube with inner and outer radius

5.1 Schematic representation of finite element I9-87. . . . . . . . . . . . . . . . . . 73

5.4 Radial variation of the electric potential

5.8 (a) Mode I insulating crack loaded by uniform distributed load at infinity.

5.9 Log-log plot of (a) $u_2(r, \pi)$ and (b) $\Omega_3(r, \pi)$ for a Mode I insulating crack. . 82

5.7 Contour plots of (a) $\varepsilon_{22}$ and (b) $P_2$ for a plate with an elliptical hole as de-
5.10 Predicted polarization field compared to finite element calculation for Mode I insulating crack. (a) is the radial profile and (b) is the angular profile. The closer to the crack tip, the better the calculation agrees with the theory.

5.11 Predicted rotation $\Omega_3$ compared with finite element calculation (Mode D crack), in (a) radial and (b) angular direction. Note that $\omega_0$ is the surface charge density at bottom.

5.12 Periodic structure with a repeating unit cell $ABCD$.

5.13 Variation of the opening normal strain $\varepsilon_{22}$ (a) and polarization $P_2$ (b) along the $x_1-$ axis ahead of the void due to a macroscopic strain $\bar{\varepsilon}_{22}$ and an electric field $\bar{E}_2$ in the $x_2-$direction, unit-cell under tension.

5.14 Variation of shear strain $\varepsilon_{12}$ (a) and polarization $P_1$ (b) along the $x_2-$ axis above of the void due to a macroscopic strain $\bar{\varepsilon}_{12}$ and an electric field $\bar{E}_2$ in the $x_2-$direction, unit-cell under shear.

A.1 In (a), a point load $Q$ is applied, while in (b) there is a potential difference $V$ between the upper and lower surface over a portion of the beam.

A.2 Two different arrangements of the bimorph piezoelectric beams with flexoelectric effects. a) series b) parallel. Beams can be designed to be tail-to-tail (TT) and head-to-head (HH) in terms of poling direction. From Abdollahi & Arias (2015). Copyright 2015, American Society of Mechanical Engineers.

C.1 Strain-relaxation takes place at the interface of two crystalline materials, due to the mismatch of their lattice constants. The interfacial strain is $\varepsilon_0$. 

## Nomenclature

### Latin Notations

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a$</td>
<td>Isotropic Reciprocal Susceptibility Constant</td>
</tr>
<tr>
<td>$a_0$</td>
<td>Size of a Defect</td>
</tr>
<tr>
<td>$a_s$</td>
<td>Interatomic Spacing</td>
</tr>
<tr>
<td>$A$</td>
<td>Cross-section Area</td>
</tr>
<tr>
<td>$A_{ijklmn}$</td>
<td>Gradient Elastic Tensor</td>
</tr>
<tr>
<td>$b$</td>
<td>Body Force per Volume</td>
</tr>
<tr>
<td>$b_x, b_z$</td>
<td>Components of Burgers Vector</td>
</tr>
<tr>
<td>$C_3, C_{ij}$</td>
<td>Gradient Elastic Intensity Factors</td>
</tr>
<tr>
<td>$C$</td>
<td>Elastic Tensor</td>
</tr>
<tr>
<td>$C^3$</td>
<td>One Edge of $\partial\mathcal{V}$</td>
</tr>
<tr>
<td>$d$</td>
<td>Piezoelectric Tensor</td>
</tr>
<tr>
<td>$D$</td>
<td>Electric Displacement Vector</td>
</tr>
<tr>
<td>$D^s$</td>
<td>Surface Gradient Operator</td>
</tr>
<tr>
<td>$D_n$</td>
<td>Normal Gradient Operator</td>
</tr>
<tr>
<td>$E$</td>
<td>Electric Field Vector</td>
</tr>
<tr>
<td>$e$</td>
<td>Electron Charge</td>
</tr>
<tr>
<td>$e_i$</td>
<td>Orthonomal Cartesian Basis</td>
</tr>
<tr>
<td>$E$</td>
<td>Young’s Modulus</td>
</tr>
<tr>
<td>$f$</td>
<td>Flexoelectric coupling tensor</td>
</tr>
<tr>
<td>$f_1, f_2$</td>
<td>Flexoelectric Coupling Constants</td>
</tr>
<tr>
<td>$\hat{f}_b$</td>
<td>Effective Bending Flexoelectric Coupling Constant</td>
</tr>
<tr>
<td>$f$</td>
<td>Volumetric Flexoelectric Coupling Constant</td>
</tr>
<tr>
<td>$G_D, G_E$</td>
<td>Bending Rigidity</td>
</tr>
<tr>
<td>$G_{ij}, G_{\phi}$</td>
<td>Flexoelectric Green’s Function</td>
</tr>
<tr>
<td>$h$</td>
<td>Height</td>
</tr>
<tr>
<td>$H$</td>
<td>Enthalpy</td>
</tr>
<tr>
<td>$I$</td>
<td>Moment of Inertia</td>
</tr>
</tbody>
</table>
\( I_i(\cdot), K_i(\cdot) \)  \quad \text{ith order Modified Bessel Functions}

\( J_k \)  \quad \text{J Integral}

\( K_E, K_D, K_4^{I, II} \)  \quad \text{Electric Fracture Intensity Factors}

\( L \)  \quad \text{Geometric Length}

\( \ell \)  \quad \text{Unit Outward Normal of an Edge}

\( \ell \)  \quad \text{Gradient Elastic Length Scale}

\( \ell_1, \ell_2, \ell_0, \ell_f \)  \quad \text{Flexoelectric Length Scale}

\( \mathbf{m} = \mathbf{n} \cdot \hat{\mu} \)  \quad \text{Higher-order traction}

\( M \)  \quad \text{Bending Moment}

\( \mathbf{n} \)  \quad \text{Unit Outward Normal Vector}

\( p_i, p_o \)  \quad \text{Pressure}

\( p_{jk} = \hat{\mu}_{ijk,i} \)  \quad \text{Divergence of Higher-order Stress}

\( \mathbf{P} \)  \quad \text{Electric Polarization Vector}

\( q_e \)  \quad \text{Free charge per Volume}

\( q_i \)  \quad \text{Coordinates in Reciprocal Space}

\( \mathbf{Q} \)  \quad \text{Generalized Traction}

\( Q_{ij} \)  \quad \text{Energy Momentum Tensor}

\( r, \theta \)  \quad \text{Polar Coordinates}

\( r, \theta, z \)  \quad \text{Cylindrical Coordinates}

\( r_o, r_i \)  \quad \text{Geometric Radius}

\( \mathbf{R} \)  \quad \text{Higher-order Traction}

\( \mathbf{s} \)  \quad \text{Unit Tangent Vector of an Edge}

\( \mathbf{t} \)  \quad \text{Surface Traction}

\( \mathbf{u} \)  \quad \text{Displacement Field}

\( \mathbf{u}^C \)  \quad \text{Displacement on Edge } \mathbf{C}

\( \mathbf{v} \)  \quad \text{Shorthand of } u_{i,j} n_j

\( \mathcal{V} \)  \quad \text{Notation for a General Dielectric Body}

\( \partial \mathcal{V} \)  \quad \text{Boundary of That Body}

\( V \)  \quad \text{Voltage Difference}

\( w \)  \quad \text{Width}

\( \mathcal{W}, \mathcal{W}_L, \mathcal{W}_R \)  \quad \text{Energy Storage Density}

\( \mathcal{W}^{(\cdot)} \)  \quad \text{Work Done by Source } (\cdot)

\( x_i \)  \quad \text{Spatial Coordinates}

**Abbreviations**

xiii
AFM Atomic Force Microscopy
BC Boundary Condition
COD Crack Opening Displacement
LEFM Linear Elastic Fracture Mechanics
LPFM Linear Piezoelectric Fracture Mechanics
MEMS Micro-Electro-Mechanical System
PFM Piezoresponse Force Microscopy
SCF Stress Concentration Factor
SE Strain Energy
SGE Strain Gradient Elasticity

Greek and Other Symbols
α, β Non-dimensional Flexoelectric Coupling Constants
β Distortion Field
δ Variation
δ₀ Defect Mismatch Displacement
δ Identity Tensor
ε Dielectric Permittivity Tensor
ε₀ Permittivity of Vacuum
ε Isotropic Dielectric Permittivity
ε Linear Strain Tensor
ε' Deviatoric Strain
Γ A Closed Contour
κ Curvature of a Beam
λ, μ Lamé Constants
λe Line Charge Density
μ Higher-order Stress in SGE
μ Flexoelectric Tensor
μ₁₁₁ Longitudinal Flexoelectric Constant
μ₁₁₂ Transverse Flexoelectric Constant
η Concentration Factor
ω Surface Charge Density
Ω Curl of Displacement
Ω Out-of-plane Curl in Plane Problem
ϕ Electric Potential
\[ \varphi \quad \text{Angle of Twist per Length} \]
\[ \sigma = \frac{(1 - \nu)}{(1 - 2\nu)} \quad \text{Non-dimensional Modulus Ratio} \]
\[ \sigma^{(0)} \quad \text{Cauchy Stress} \]
\[ \sigma^{(2)} = -\nabla \cdot \tilde{\mu} \quad \text{Divergence of Higher-order Stress} \]
\[ \sigma \quad \text{True Stress Tensor} \]
\[ \tau_0 \quad \text{Shear Loads} \]
\[ \tau \quad \text{Cauchy Stress Tensor} \]
\[ \Theta \quad \text{Volumetric Strain or Dilatation} \]
\[ \chi \quad \text{Dielectric Susceptibility Tensor} \]
\[ \chi \quad \text{Isotropic Susceptibility Constant} \]
\[ \nabla \quad \text{Gradient Operator} \]
\[ \partial \quad \text{Partial Differentiation Operator} \]
\[ \mathcal{L}_i \quad \text{Operator } 1 - \ell_i \nabla^2 \]
\[ \nabla^2 \quad \text{Laplacian Operator} \]
\[ \tilde{\kappa} \quad \text{Double Displacement Gradient} \]
\[ \dddot{\cdot} \quad \text{Type I Formulation} \]
\[ \dddot{\cdot} \quad \text{SGE or Type II Formulation} \]
\[ (\cdot) \quad \text{Average of (\cdot)} \]
\[ (\cdot)^* \quad \text{Fourier Transform of (\cdot)} \]
\[ \overline{\cdot} \quad \text{Non-dimensionalized (\cdot)} \]
Chapter 1

Introduction

1.1 Flexoelectricity in Hard Materials

Coupled electro-mechanical phenomena are common in nature. For example, strains can be generated in dielectrics by the application of electric fields through electrostriction. Strains can also be generated in a special class of dielectrics by the phenomenon of piezoelectricity. Conversely, a piezoelectric material can be polarized when a stress is applied on it. The study of these phenomena has a long history in mechanics of materials and has been documented in quite a number of texts, including those of Landau et al. (1984), Maugin & Eringen (1990), Kovetz (2000) and many others.

A lesser known phenomenon, termed flexoelectricity, is the coupling between polarization and strain-gradient. Flexoelectricity was first proposed in theory half a century ago by Mashkevich & Tolpygo (1957), Tolpygo (1963), Kogan (1964) and shortly after, discovered in experiments by Scott (1968), Bursian et al. (1969). Even though flexoelectricity was first proposed and found in hard materials, it did not receive much attention within the field of mechanics of solids largely due to limited means of generating large strain gradients. As a result, from then on, the study of flexoelectricity has been extensively focused on soft materials, which can sustain large deformations. Among soft materials, flexoelectricity was first found to be prominent in liquid crystals Meyer (1969), followed by a systematical investigation from then on. Readers are referred to the review in Buka & Eber (2012) for detailed results. Later, the study of flexoelectricity was extended to biological soft materi-
als, like lipid bilayer membranes Raphael et al. (2010), Petrov (2002, 2006), Harland et al. (2010). It was found that flexoelectricity is related to the mechanism of hearing. Recently by incorporating fluctuation theory, Liu & Sharma (2013), Deng, Liu & Sharma (2014) also gave new insights to the subject. But, the origin of flexoelectricity in those materials differ from hard materials like crystalline solids.

Research on flexoelectricity in hard materials has surged in recent years, largely due to the advent of modern fabrication and characterization methods. Since gradients scale inversely as length scales, flexoelectric effects can be greatly enhanced in small specimens. Flexoelectric polarization also increases as the dielectric constant of a material increases. Taking account of these scalings, in the last decade high quality specimens of the above characteristics have been made possible, thanks to the new developments in fabrication techniques. This has led to a series of experimental efforts for measuring flexoelectric constants in different materials. Sophisticated apparatuses for nano-scale characterization, i.e. atomic force microscopy (AFM), piezoresponse force microscopy (PFM), etc., have enabled probing this effect at fine scales with high accuracy. In the mean time, significant growth in computing power stimulates better theoretical approaches to understand the origins of flexoelectricity. Also, improved numerical and computational tools bring new perspectives to flexoelectricity and are able to make predictions in more complex contexts. All these factors contribute to the current revival of interest into flexoelectric phenomena in hard materials.

1.1.1 Origins of flexoelectricity

Flexoelectricity, by definition, couples electric polarization $\mathbf{P}$ with strain gradient $\nabla \varepsilon$ in a linear fashion. Just as a piezoelectric material can be characterized by the piezoelectric tensor $\mathbf{d}$, flexoelectricity can be described by the flexoelectric tensor $\mathbf{\mu}^f$:

$$ P_i = \varepsilon_0 \chi_{ij} E_j + \mu^f_{ijkl} \varepsilon_{jk,i} \quad (1.1) $$

where $\varepsilon_0$ is the permittivity of vacuum, $\chi$ is the dielectric susceptibility tensor and $\mathbf{E}$ is the electric field. In piezoelectricity, $\mathbf{d}$ relates electric response ($\mathbf{P}$ or electric displacement $\mathbf{D}$) to strain $\varepsilon$, hence $\mathbf{d}$ is a third-order tensor. However, in flexoelectricity, $\mathbf{\mu}^f$ is a fourth-order
tensor because strain gradient is a third-order tensor which must be coupled to polarization vector, a first order tensor.

Early studies of flexoelectricity focused primarily on its microscopic origin. What gives rise to it? Can we estimate the magnitude of this $\mu^f$? In what kind of material can we expect large $\mu^f$? Kogan (1964) answered these questions by adopting a lattice description of solids, such as shown in Fig.1.1. Bending of a flat slab introduces a strain gradient along the cross-section that breaks the local symmetry of the lattice. As a result, the center of positive and negative charges are displaced, which induces net polarization. In his work, a straight-forward estimate was calculated by a simple scaling rule:

$$\frac{\mu^f}{\epsilon_0 \chi} \approx \frac{e}{4\pi \epsilon_0 a_s} \sim 1 - 10V$$

(1.2)

where $e$ is the charge of a single electron and $a_s$ is the interatomic spacing. The above equation shows that flexoelectricity is directly related to electric susceptibility of the material. In usual dielectrics, like sodium chloride, where $\chi \sim 10$, unless very sharp strain gradient is created, flexoelectric induced polarization is negligible. This equation also suggests that the ideal place to observe flexoelectricity is a material with high susceptibility (or high dielectric constant) that can suffer considerably large strain gradients.

Kogan’s lattice description has long dominated the understanding of flexoelectricity. Inspired by this, Askar et al. (1970) for the first time numerically calculated the flexoelectric constants based on shell models. Later, a rigid-ion model was systematically addressed in Tagantsev (1985, 1991). These works determined the possible contributions to the flexoelectric tensor and presented a more rigorous way to compute the ionic contribution to the relevant constants. Maranganti & Sharma (2009) developed this idea and employed a lattice dynamic simulation to calculate the flexoelectric constants. However, these works have been criticized by Resta (2010) since their derivation inevitably involves a surface contribution. In contrast, Resta (2010) built a more sophisticated physical model which argued that flexoelectricity, like piezoelectricity, is a purely bulk effect.

Resta’s argument is a first step towards a theory that accounts for both lattice and electronic contribution to the flexoelectric tensor. In fact, Kalinin & Meunier (2008) for the first time, showed that flexoelectricity can be entirely caused by electrons. They looked
Figure 1.1: (a) Flexoelectricity induced by bending. When a slab of thickness $t$ is bent, it results in tension (blue) in one direction and compression (red) in the other, therefore a strain gradient. (b) the zoom-in of the locally bent lattices. Center of cations (light color circle) and anions (dark color circle) are displaced. A polarization is induced as a result. From Maranganti et al. (2006). Copyright 2006, American Physical Society.

at a graphene sheet under symmetric bending and found that estimates of the flexoelectric tensor obtained by analytical calculation accounting for the electron clouds around the carbon atoms are within the range computed by first principles calculation. This was also the pioneering attempt that used first principles calculation to determine the flexoelectric tensor. Later, Hong et al. (2010) incorporated this method to study the flexoelectric properties in BaTiO$_3$, which has been known for its large flexoelectric constants. Subsequent papers of Hong & Vanderbilt (2011, 2013) systematically derived a complete theory and first principles simulation framework for general materials, ranging from usual dielectrics like carbon, diamond and silicon to perovskite ceramics. According to their calculation, electronic contribution to flexoelectric tensor actually prevails over the ionic contribution in most of these materials—even in perovskite ceramics for which it was long believed that flexoelectricity primarily arises from ionic charge separation. Their results significantly differ from those of Maranganti & Sharma (2009). Interestingly, although experimentalists often measured positive flexoelectric constants, their simulation yields negative values as well.
1.1.2 Quantifying flexoelectric constants

After Kogan (1964), there have been many efforts to measure the flexoelectric constants $\mu^f_{ijkl}$. As discussed above, an observable flexoelectric effect requires high dielectric constants and considerably large strain gradients. On the other hand, high dielectric constants can only be obtained through fabrication of high quality specimens. In the beginning of this century, Ma & Cross (2001, 2002, 2006) started to look at this problem in some ferroelectric perovskites in their paraelectric phase. In that phase, not only can we exclude piezoelectricity, but the dielectric constant of these materials can be huge—it can reach as high as $10^4 – 10^5$. Ma and Cross managed to measure the transverse flexoelectric constant $\mu^f_{1122}$ of these materials using cantilever bending approach, as shown in Fig.1.2(a). Shortly after, Zubko et al. (2007) used a three point bending system to carry out the measurement on paraelectric Strontium Titanate. Since bending can only determine $\mu^f$ in part even for simple cubic materials, as suggested in Zubko et al. (2007), to fully characterize the flexoelectric tensor, alternative methods must be employed. The truncated pyramid compression method is one alternative, as shown in Fig.1.2(b). It is employed by Fu et al. (2006), Baskaran et al. (2011) to measure the longitudinal flexoelectric constant $\mu^f_{1111}$. Another way of measuring flexoelectric constants is through Brillouin-scattering, like in Hehlen et al. (1998).

However, despite significant effort in quantifying these constants, there is still large
variability in the measurements. For example, the Brillouin scattering method by Hehlen et al. (1998) inevitably invokes a dynamic flexoelectric effect. The truncated pyramid compression method is also not reliable. It was intended to set up a uniform strain gradient, but in reality, as shown in Abdollahi, Millán, Peco, Arroyo & Arias (2015), due to the sharp edges, the strain field inside can be highly inhomogeneous. Theoretically, quantifying flexoelectric constants using beam bending is the most reliable method so far. However, measurements using this approach also do not converge. Ma & Cross (2001, 2002, 2006) reported unexpectedly high flexoelectric constants, on the order of $10^{-100} \mu C/m$ (exceeding Kogan’s limit), whereas Zubko et al. (2007) measured it to be on the order of nC/m (within Kogan’s limit). This discrepancy puzzled researchers for a long time. Not until very recently was it revealed by Narvaez & Catalan (2014), Garten & Trolier-McKinstry (2015), Narvaez et al. (2015) that this has to do with other effects due to material properties, such as residual polarization and flexoelectric poling effect. As observed in Müller & Burkard (1979), Strontium Titanate remains paraelectric at temperature as low as 4K, therefore free of these concerns. But for other perovskite materials, due to these effects, the flexoelectric constants measured can be erroneous. Tagantsev & Yurkov (2012) showed that sometimes, surface effects also perturb the measurement in a non-trivial way. In summary, reliable methods to determine flexoelectric constants accurately still remain a challenge.

1.1.3 Unique phenomenon due to flexoelectricity

Flexoelectricity, ever since its discovery, has been regarded as an alternative of piezoelectricity at small scales. In fact, as early as the 1960s, Koehler et al. (1962), Turcháni, G. et al. (1973), Whitworth (1975) found that edge dislocations in centrosymmetric materials, such as sodium chloride, carry charge. Later, Petrenko & Whitworth (1983) extended the observation to another kind of centrosymmetric material, ice. Piezoelectricity vanishes in these materials, therefore cannot be the source. Instead, a “pseudo-piezoelectric” effect was postulated by Evtushenko et al. (1987) for an explanation, which was later shown to be a result of flexoelectricity Mao & Purohit (2015).

Despite the strong gradient field created by dislocations, it is hardly controllable to utilize in applications. Sharma et al. (2007) introduced a continuum framework for studying flexoelectricity and suggested that flexoelectricity creates a size-dependent piezoelectric
response at small scales. Therefore, for piezoelectrics, flexoelectricity can enhance their piezoresponse. This idea was further demonstrated in simulation studies of Majdoub et al. (2008a,b) and experimental works of Lee et al. (2011), Qi et al. (2011). At the same time, Sharma et al. (2007) also predicted that for non-piezoelectrics, piezo-like response can be manifested through flexoelectric coupling. In fact, Ong & Reed (2012), Duerloo & Reed (2013) explored this idea using first-principles calculations. They predicted that by introducing non-centrosymmetric defects into 2D symmetric structures, like graphene, an overall piezoelectric response can be created. Even though introducing atomic size defects is quite challenging, Zelisko et al. (2014) managed to prove this concept in graphene nitride, experimentally. The response they measured agrees well with predictions made from flexoelectricity.

However, as noted in Zubko et al. (2013), “flexoelectricity is not just a substitute for piezoelectricity at the nanoscale; it also enables additional electromechanical functionalities not available otherwise”. Flexoelectricity opens up the possibility of “gradient engineering”, an innovative and unique way of optimizing functionalities of electronics. Convincing evidence of this possibility has already been demonstrated in materials. For instance, it was discovered that flexoelectricity leads to a gradient induced polarization rotation at a ferroelectric phase boundary, as shown in Catalan et al. (2011) and that this could lead to a new mechanism of electronic memory. Lu et al. (2012) further developed this idea by exerting stress on a BaTiO$_3$ ferroelectric thin film through AFM. In this way, the gradient can be controlled and flexoelectricity could enable a mechanical way of “writing” polarization into ferroelectrics as shown in Fig. 1.3. Built upon these results, Očenášek et al. (2015) explored the effects of perpendicular point load and sliding loads. Besides, flexoelectric interaction can also lead to negative domain wall energy as suggested in Borisevich et al. (2012). They attribute this negative domain wall energy to unusual periodic phase boundaries in an Sm-doped BiFeO$_3$. Fine structures of ferroelectric domain patterns due to flexoelectricity are discussed in Ahluwalia et al. (2014).

There has also been some progress in using flexoelectricity at device level. Deng, Kammoun, Erturk & Sharma (2014) proposed a flexoelectric energy harvester based on a cantilever beam system. Based on a similar idea, a flexoelectric microphone was demonstrated by Kwon et al. (2016). Pyro-paraelectricity, a phenomenon that arises due to flexoelectricity
Figure 1.3: Illustration of mechanical writing of ferroelectric polarization by the use of AFM tip. Strong gradients exerted by the tip can reverse the polarization and hence result in different domain patterns. This method is purely mechanical without any charge injection. From Zubko et al. (2013). Copyright 2013, Annual Review.

and strain relaxation, was utilized for thermal-electric conversion/detection devices as in Chin et al. (2015). A flexoelectric microelectromechanical system (MEMS) on silicon was fabricated by Bhaskar et al. (2015) with a performance comparable to the state-of-the-art. Later, Bhaskar et al. (2016) was able to demonstrate a proof-of-concept strain diode based on the unique interaction between piezoelectricity and flexoelectricity. Thus, the interest in novel and unique functionality based on flexoelectricity is increasing.

1.2 Continuum Treatment of Flexoelectricity

The surging interest in flexoelectricity demands a theoretical machinery that predicts electromechanical response under complex circumstances. The theory of continuum mechanics, including that of piezoelectricity has been successful in doing so, even in the non-linear regime. However, since flexoelectricity is a gradient effect, thus size-dependent, it cannot be directly incorporated into continuum mechanics, which does not possess an intrinsic length scale. Rather, flexoelectricity needs to be modeled under the framework of strain-
gradient elasticity (SGE) or gradient elasticity. The theory of gradient elasticity works well at small scales (especially sub-micron scales) when non-local phenomenon is prominent. And we expect the continuum theory of flexoelectricity will work well also within that range. Gradient elasticity was developed by Mindlin (1964), Toupin (1962), Koiter (1964), in which strain gradients are included in the elastic strain energy function. Under that assumption, they have shown that a consistent continuum theory can be derived similar to the classical one. Later Fleck et al. (1994), Fleck & Hutchinson (1997) extended the theory to strain-gradient plasticity. Various finite element formulations based on these ideas are also documented in the literature, e.g., Herrmann (1981), Ramaswamy & Aravas (1998a,b), Providas & Kattis (2002), Amanatidou & Aravas (2002).

To account for flexoelectricity, the above gradient elasticity framework needs to be extended to include general electromechanical coupling. Toupin (1956) proposed a variational principle which later was named after him, for such purposes. This principle was used by Mindlin (1968) to model other size-dependent electromechanical phenomena. Flexoelectricity can be treated in a similar fashion. Based on this idea, Maranganti et al. (2006) calculated the Green’s function for flexoelectric solids and used it to examine an Eshelby problem. Later, Majdoub et al. (2008b) looked at a flexoelectric nanobeam and predicted a size-dependent flexoelectric stiffening effect. Shen & Hu (2010) provided a general variational framework for flexoelectric solids including surface effects. Liu (2013) generalized the framework to large deformations. Besides, Liu & Sharma (2013), Deng, Liu & Sharma (2014) showed that fluctuation can also be incorporated in the continuum framework. In the mean time, mesh-free finite element analysis based on continuum models have also been carried out on more complicated geometries. Abdollahi, Millán, Peco, Arroyo & Arias (2015) revisited the truncated pyramid compression experiments and showed that it is not reliable by design. Abdollahi et al. (2014), Abdollahi & Arias (2015) gave some new insights and showed how we can further utilize flexoelectric beam structures. Abdollahi, Peco, Millán, Arroyo, Catalan & Arias (2015) looked at the asymmetry of fracture toughness in flexoelectric materials.

Despite all this theoretical and computational effort into the continuum theories of flexoelectricity, there has been some inconstistency in the treatment of the SGE terms. In fact, we have shown in Mao & Purohit (2014) that not only does the SGE length scale set
an intrinsic limit for the magnitude of flexoelectric constants, SGE is also essential to ensure that the energy storage function is positive definite. Finite element analysis in the presence of these SGE terms can also be tricky and needs careful treatment as stated in Mao et al. (2016). However, if these difficulties can be surmounted, many new and useful boundary value problems can be solved to inspire better application/experimental methods like in Mao & Purohit (2014), Mao et al. (2016). The interaction between defects and flexoelectricity can also bring some new insights into this subject as in Mao & Purohit (2015). This dissertation addresses all the above questions and is based on the aforementioned works (published or submitted). That said, it is important to point out that flexoelectricity is a rich subject and there are many other results that are beyond the scope of this thesis. For those, readers are directed to the following reviews: Nguyen et al. (2013), Zubko et al. (2013), Yudin & Tagantsev (2013).

### 1.3 Scope of the thesis

Following the introduction, Chapter 2 gives a systematic way of solving flexoelectric boundary value problems based on SGE models. First, we deal with general formulation of flexoelectricity combining SGE and electrostatics. Second, a reciprocal theorem is proved under linear constitutive law. Third, governing equations of the Navier type are obtained for isotropic materials. Chapter 2 is then completed by solving a few boundary value problems (BVP’s) based on this new model. Torsion, beam bending and axisymmetric plane problems are solved analytically.

Chapter 3 and Chapter 4 extend the framework of Chapter 2 to defects. Defects create strong discontinuities in a continua and hence large gradients. Flexoelectric interaction is expected to be prominent in the neighborhood of defects and die away quickly in the far field. We analytically quantify this expectation for typical types of defects. In particular, Chapter 3 deals with point defect and dislocation, where connections to various experimental results are made. Chapter 4 deals with cracks where unique fracture behaviors of flexoelectric solids are identified.

Chapter 5 provides a consistent finite element method for flexoelectricity. First, we introduce a mixed formulation based on the work of Amanatidou & Aravas (2002) to deal
with the higher-order differential governing equations due to flexoelectricity. This method is then implemented and validated against benchmark problems solved in Chapter 2. After validation, the finite element code is used to study problems involving complicated geometries: elliptical hole in a plate, edge crack panel, and materials with periodic unit cell.

Chapter 6 concludes the dissertation by summarizing and discussing the results of the preceding chapters. It also points out possible new developments in this field.
Chapter 2

Continuum Theory of Flexoelectricity

2.1 Introduction

In this chapter, we start our investigation from a general model of flexoelectricity in continua. In general, as pointed out in Kovetz (2000), Suo et al. (2008), governing equations of electromechanical phenomena are the Maxwell equations and conservation of linear and angular momentum. As a special case, electrostatics and linear elasticity combined suffice as a linear model of piezoelectricity. However, since flexoelectricity has to do with gradient effects, it has to be modeled with different governing equations and constitutive relations.

As discussed in the introduction, we need to invoke SGE theories to model flexoelectricity. Before doing so we will first review the classical field theory of a dielectric solid in Section 2.2. We will show the consistency between the classical theory and variational principles of Toupin (1956). In Section 2.3, we show how Toupin’s variational principles can be generalized to include general electromechanical coupling. To treat SGE consistently, we follow the treatment of Mindlin (1964), Toupin (1962), Koiter (1964), Fleck et al. (1994), Fleck & Hutchinson (1997), Aravas (2011). In these theories the energy density depends both on the strain and its gradient, and an intrinsic material length scale enters both the governing equations and constitutive relations. Another common feature of all these theories is the non-symmetry of the true stress tensor and the existence of couple and
higher order stresses. Some simplified theories, such as Yang et al. (2002), Hadjesfandiari & Dargush (2011), are also available to deal with special cases where certain components of the strain gradient can be neglected. In Section 2.4, we further develop the theory using a general linear constitutive model. A reciprocal theorem is proved. In Section 2.5, we deal with isotropic flexoelectric materials. Isotropic materials exclude piezoelectricity, hence isolating flexoelectricity as the source of linear electromechanical coupling. We derive a higher-order Navier Equation. All through this section, SGE is treated consistently. It is an essential part of flexoelectricity, without which the energy storage function loses its positive-definiteness. The SGE length scale also provides a bound for the flexoelectric coupling constants.

Following this general framework, we will use it to solve some one- and two-dimensional problems that are closely related to experiments. These problems include beam bending, torsion, cylinders under pressure and shear. We give closed form solutions to each of the problem. They can be used to interpret experiments on flexoelectric solids and can also provide a benchmark for verifying continuum based computational methods.

2.2 Classical continuum field theory

Now consider an elastic dielectric body occupying region $\mathcal{V}$ with a boundary $\partial\mathcal{V}$ in three-dimensional space, as shown in Fig.2.1. Without loss of generality, we will develop our theory in a Cartesian coordinate system with orthonormal basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ and respective coordinates $\{x_1, x_2, x_3\}$. The body is subject to some mechanical loads. As a response, a displacement field, $\mathbf{u}(\mathbf{x})$ is generated due to deformation. If we constrain ourselves to small deformations, the linear strain tensor $\mathbf{\varepsilon}$ is sufficient to describe the deformation field of the body:

$$\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}).$$

(2.1)

This body is dielectric and it has an electric response as well. As pointed out by Suo et al. (2008), the phenomenon can be intuitively thought of as every material point being connected to a battery that can pump (or withdraw) charge from it. Therefore, a scalar potential field $\phi(\mathbf{x})$ is created. In the Maxwell-Faraday theory of electrostatics, the electric
Figure 2.1: A deformable dielectric body $\mathcal{V}$ put in a coordinate system $\{x_1, x_2, x_3\}$ and subjected to traction $t(x_i)$ and electric loading $\phi(x_i)$ on its boundary $\partial \mathcal{V}$.

field is defined as:

$$E_i = -\phi_{,i},$$  \hspace{1cm} (2.2)

but as we will show shortly after, in more general electromechanical coupling problems, e.g. those associated with polarization gradient theories, Eqn (2.2) will need some modification.

The deformation and potential fields are the results of loads prescribed on the body. By the Cauchy postulate, for any continuous traction $t(\mathbf{x})$ on the surface, there is a second-order tensor $\sigma$ such that:

$$\sigma_{ij}n_j = t_i, \quad \text{on } \partial \mathcal{V},$$  \hspace{1cm} (2.3)

where $n$ is the unit outward normal vector of $\partial \mathcal{V}$. In classical continuum theory, true stress and Cauchy stress are equal to each other. But, in couple stress theory or gradient elasticity theory they are not equal, and we reserve the symbol $\sigma$ for the true stress. As alluded to earlier, the battery connected to the material pumps some charge on the surface, with a density $\omega$, a scalar. Correspondingly, a vector called electric displacement $\mathbf{D}$ is uniquely determined:

$$D_i n_i = -\omega,$$  \hspace{1cm} (2.4)

where a negative sign is kept to obey the convention of electrostatics. These relations keep the material in equilibrium states and can be generalized to the surface of any control volume inside the body, therefore, $\sigma$ and $\mathbf{D}$ are well-defined at all the material points.

The type of electric charge associated with $\mathbf{D}$ is the free charge, the charge that can be pumped up and down “freely” by the battery. There is also another source of charge, which
is due to polarization, the bound charge. These two types of charges summed together give the "total" charge. Hence,
\[ D_i = \varepsilon_0 E_i + P_i, \] (2.5)
where \( \varepsilon_0 \) is the permittivity of vacuum. For a linear rigid dielectric, we know
\[ D_i = \varepsilon_{ij} E_j, \] (2.6)
where \( \varepsilon = \varepsilon_0(\delta + \chi) \) is what we usually call a dielectric permittivity tensor. \( \chi \) is the susceptibility tensor and \( \delta \) is the identity tensor or Kronecker delta.

All of the above sets up the fundamentals for a continuum field theory of a dielectric solid. The influence of external sources is reflected by the change of the free energy of the solid. Suppose the density of the energy storage function is \( W \), then we have:
\[ \delta W = \sigma_{ij} \delta \varepsilon_{ij} + E_i \delta D_i, \] (2.7)
where \( \delta \) denotes some small changes or variation in the variable that follows it. Note that this means we are assuming \( W = W(\varepsilon, D) \) for the classical continuum theory. According to Eqn(2.5), we can also work with the polarization, if we remember that
\[ \delta W = \sigma_{ij} \delta \varepsilon_{ij} + E_i \delta P_i + \delta \left( \frac{\varepsilon_0}{2} E_i E_i \right), \] (2.8)
which is mathematically equivalent. In fact, Toupin’s variational principle is based on this formulation. To ensure consistency, the energy density he worked with is \( \mathcal{W}_L \):
\[ \mathcal{W}_L = \mathcal{W} - \frac{\varepsilon_0}{2} E_i E_i. \] (2.9)

Thus, the work conjugate of polarization is the electric field. We can start from a pure energetic point of view, that is, to assume the work conjugate of \( \varepsilon \) and \( P \) to be \( \sigma \) and \( \mathbf{E} \), respectively, so that
\[ \sigma_{ij} = \frac{\partial \mathcal{W}_L}{\partial \varepsilon_{ij}}, \quad E_i = \frac{\partial \mathcal{W}_L}{\partial P_i}. \] (2.10)
By adopting the principle, a field theory can be established in consistency with the classical
theories. In the classical context, we can write Toupin’s variational principle as

\[
\int_V \delta \left( W_L - \frac{1}{2} \varepsilon_{0,ij,i} \phi_{,i} + \phi_{,i} P_i \right) dV = \int_V (b_i \delta u_i - q_e \delta \phi) dV + \int_{\partial V} (t_i \delta u_i - \omega \delta \phi) dS,
\]

where, \( b \) is the body force per unit volume and \( q_e \) is the free charge volume density. Note that this is a general formulation that can deal with the case where \( E_i \neq -\phi_{,i} \), as in Mindlin (1968).

Substituting Eqn(2.10) into Eqn(2.11) and analyzing the variational form, we have the following governing equations:

\[
\begin{align*}
\sigma_{ij,j} + b_i &= 0, \quad (2.12) \\
E_i + \phi_{,i} &= 0, \quad (2.13) \\
-\varepsilon_{0,ii} \phi_{,i} + P_{i,i} - q_e &= 0, \quad (2.14)
\end{align*}
\]

which recovers the equilibrium equation and the Maxwell equation, and gives the following boundary conditions:

\[
\begin{align*}
\sigma_{ij} n_j - t_i &= 0, \quad \text{on} \ \partial V_t, \quad (2.15) \\
(\varepsilon_{0,ii} \phi_{,i} + P_i) n_i + \omega &= 0, \quad \text{on} \ \partial V_\omega, \quad (2.16)
\end{align*}
\]

which recovers those of Eqn(2.3, 2.4).

In the following section, we will generalize the above machinery to study flexoelectricity.

### 2.3 Governing equations

To generalize the above framework to flexoelectricity, the strain gradient \( \varepsilon_{jk,i} \) needs to be included in the energy density and we define the following pairs of work conjugates:

\[
\begin{align*}
\tau_{ij} &= \frac{\partial \hat{W}_L}{\partial \varepsilon_{ij}}, & \hat{\mu}_{ijk} &= \frac{\partial \hat{W}_L}{\partial \varepsilon_{jk,i}}, & E_i &= \frac{\partial \hat{W}_L}{\partial P_i},
\end{align*}
\]

where \( \tau \) is the Cauchy stress in the generalized theory and \( \hat{\mu} \) is the higher-order stress–the work conjugate of strain gradient. \( \hat{\cdot} \) denotes the strain gradient formulation.
Along with this higher-order stress, there must be a generalized surface load associated with it, whose conjugate must be related to the gradient of displacement on the surface. However, once the displacement is given on the boundary, the tangential part of displacement gradient is already determined. Only the normal derivative $\frac{\partial u}{\partial n}$ can be independent of the displacement on the boundary. Therefore, a higher-order load $\hat{R}$ conjugate to $\frac{\partial u}{\partial n}$ should enter the variational form. As a consequence, the variational form can be written as:

$$
\int_{\mathcal{V}} \delta \left( \hat{W}_L - \frac{1}{2} \epsilon_0 \phi, i, \phi, i + \phi, i P_i \right) d\mathcal{V} = \int_{\mathcal{V}} (b_i \delta u_i - q_e \delta \phi) d\mathcal{V} + \sum_{C_T^\beta} \hat{T}_i u_i ds + \int_{\partial \mathcal{V}} \left[ \hat{Q}_i \delta u_i + \hat{R}_i \delta (u_i, j n_j) - \omega \delta \phi \right] ds
$$

(2.18)

where $\hat{Q}$ is the generalized traction on $\partial \mathcal{V}$. The boundary integrals on $C_T^\beta$ are included in Eqn(2.18) when the outer surface $\partial \mathcal{V}$ is piecewise smooth; in such a case, the surface $\partial \mathcal{V}$ can be divided into a finite number of smooth surfaces $\partial \mathcal{V}^\beta (\beta = 1, 2, \ldots)$ each bounded by an edge $C^\beta = C^\beta_U \cup C^\beta_T (C^\beta_U \cap C^\beta_T = \emptyset)$.

With this we know that the governing equation will be:

$$
\tau_{jk,j} - \mu_{ijkl} b_k = 0,
$$

(2.19)

$$
-\epsilon_0 \phi, ii + P_{i,i} = q_e
$$

(2.20)

$$
E_i + \phi, i = 0
$$

(2.21)

In general, there is no free charge in an ideal dielectric, hence $q_e = 0$. Equation(2.21) can be put in a more compact form:

$$
D_{i,i} = 0.
$$

(2.22)

This equation, along with Eqn(2.19) constitutes the governing equation of a general dielectric with gradient effects, under small deformations. To model flexoelectricity, we need to add constitutive information. These governing equations admit six types of boundary conditions (BC’s):
1. displacement boundary condition

\[ u_i = \hat{u}_i, \quad \text{on } \partial \mathcal{V}_u, \quad (2.23) \]

2. normal derivative boundary condition

\[ D^n u_i = \hat{v}_i \quad \text{on } \partial \mathcal{V}_v, \quad (2.24) \]

3. traction boundary condition

\[ n_j (\tau_{jk} - \hat{\mu}_{ijk,i}) - D^j n_i \hat{\mu}_{ijk} - (D^j p) n_i n_j \hat{\mu}_{ijk} = \hat{Q}_k, \quad \text{on } \partial \mathcal{V}_Q, \quad (2.25) \]

4. higher-order traction boundary condition

\[ n_i n_j \hat{\mu}_{ijk} = \hat{R}_k \quad \text{on } \partial \mathcal{V}_R, \quad (2.26) \]

5. potential boundary condition

\[ \phi = \hat{\phi} \quad \text{on } \partial \mathcal{V}_\phi, \quad (2.27) \]

6. surface charge boundary condition

\[ n_i D_i = -\hat{\omega} \quad \text{on } \partial \mathcal{V}_\omega. \quad (2.28) \]

There are two additional conditions when \( \partial \mathcal{V} \) has edges:

\[ u_i = \hat{u}_i^C \quad \text{on } C^\beta_u, \quad (2.29) \]

\[ \left[ [\ell_j n_k \hat{\mu}_{jk}] \right] = \hat{T}_i \quad \text{on } C^\beta_T. \quad (2.30) \]

In all the above boundary conditions, \((\hat{u}, \hat{Q}, \hat{v}, \hat{R}, \hat{u}^C, \hat{T}, \hat{\phi}, \hat{\omega})\) are known functions, \(D^n = \mathbf{n} \cdot \nabla = n_i \frac{\partial}{\partial x_i}\) is the normal derivative, \(D^i = \nabla - \mathbf{n} D^n\) the “surface gradient” on \(\partial \mathcal{V}\), \(\partial \mathcal{V}_u \cup \partial \mathcal{V}_Q = \partial \mathcal{V}_v \cup \partial \mathcal{V}_R = \partial \mathcal{V}_\phi \cup \partial \mathcal{V}_\omega = \partial \mathcal{V}\), and \(\partial \mathcal{V}_u \cap \partial \mathcal{V}_Q = \partial \mathcal{V}_v \cap \partial \mathcal{V}_R = \partial \mathcal{V}_\phi \cap \partial \mathcal{V}_\omega = \emptyset\). The double brackets \([ [ \quad ] ]\) indicate the jump in the value of the enclosed quantity across \(C^\beta\), and an outward normal of the edge is defined as \(\ell = \mathbf{s} \times \mathbf{n}\), where \(\mathbf{s}\) is the unit vector tangent to \(C^\beta\).
2.4 Linear constitutive relations

So far, we have given the governing equations for a linear electromechanical theory of
dielectrics with gradient effects. Flexoelectric materials, which are our concern now, are in
the class for which \( \hat{W}_L \) is quadratic:

\[
\hat{W}_L(\varepsilon_{ij}, \varepsilon_{jk,i}, P_i) = \frac{1}{2} C_{ijkl} \varepsilon_{ij} \varepsilon_{kl} + \frac{1}{2} \hat{A}_{ijklmn} \varepsilon_{jk,i} \varepsilon_{mn,l} + \frac{1}{2} a_{ij} P_i P_j,
\]

(2.31)

\[
+ d_{ijk} \varepsilon_{ij} P_k + \hat{f}_{ijkl} \varepsilon_{jk,i} P_l,
\]

where \( C \) is the fourth order elasticity tensor, \( \hat{A} \) is the strain-gradient elasticity tensor, \( d \)
is the piezoelectric tensor, \( \hat{f} \) is the flexoelectric coupling tensor and \( a \) is the reciprocal
susceptibility tensor \( (a = \varepsilon_0^{-1} \chi^{-1}) \).

According to Eqn(2.17), we obtain the constitutive laws for a flexoelectric material:

\[
\tau_{ij} = C_{ijkl} \varepsilon_{kl} + d_{ijk} P_k,
\]

(2.32)

\[
\mu_{ijk} = \hat{f}_{ijkl} P_l + \hat{A}_{ijklmn} \varepsilon_{mn,l},
\]

(2.33)

\[
E_l = a_{lj} P_j + d_{ijl} \varepsilon_{ij} + \hat{f}_{ijkl} \varepsilon_{jk,i}.
\]

(2.34)

Using the governing equations and the linear constitutive relations above, we prove a re-
ciprocal theorem as follows. Consider the solutions to two different problems, the original
problem (problem 1) and the reciprocal problem (problem 2) which we differentiate by up-
per indices 1 and 2. The total work done by the original quantities through their reciprocal
conjugates is

\[
\mathcal{W}^{(12)} = \int_V \left[ \tau_{ij}^{(1)} \varepsilon_{ij}^{(2)} + \mu_{ijk}^{(1)} \varepsilon_{jk,i}^{(2)} + E_i^{(1)} D_i^{(2)} \right] dV.
\]

(2.35)

\( \mathcal{W}^{(21)} \), which is the work done by the reciprocal quantities through their original conjugates,
can be defined in a similar manner. Applying integration by parts and using the boundary
conditions, we obtain

\[
\mathcal{W}^{(12)} = \int_V \left[ -(\tau_{jk}^{(1)} - \hat{\mu}_{ijk}^{(1)}) \varepsilon_j \varepsilon_k^{(2)} + \phi^{(1)} D^{(2)}_{i,i} \right] dV + \int_{\partial V} \left[ \hat{Q}_i^{(1)} u_i^{(2)} + \hat{R}_i^{(1)} v_i^{(2)} + \phi^{(1)} \omega^{(2)} \right] dS.
\]

(2.36)
Plugging in the governing equations Eqn(2.19, 2.22) we get

$$ W^{(12)} = \int_{\partial V} b_k^{(1)} u_k^{(2)} d\mathbf{\Omega} + \int_{\partial V} \left[ \dot{Q}_i^{(1)} u_i^{(2)} + \dot{R}_i^{(1)} v_i^{(2)} + \phi^{(1)} \omega^{(2)} \right] dS. \quad (2.37) $$

Thus, $W^{(12)}$ is completely determined by the body force and boundary loads. Alternatively, $W^{(12)}$ can also be written by use of the constitutive laws:

$$ W^{(12)} = \int_{\partial V} \left[ C_{ijkl} \varepsilon_{kl}^{(2)} \varepsilon_{ij}^{(1)} + a_{ij} P_i^{(2)} P_j^{(1)} + \epsilon_0 E_i^{(2)} E_i^{(1)} + d_{ijk} \left( P_k^{(2)} \varepsilon_{ij}^{(1)} + P_k^{(1)} \varepsilon_{ij}^{(2)} \right) + \hat{f}_{ijkl} \left( P_i^{(2)} \varepsilon_{jk}^{(1)} + P_i^{(1)} \varepsilon_{jk}^{(2)} \right) + \hat{A}_{ijklmn} \varepsilon_{mn,l}^{(2)} \varepsilon_{jk,i}^{(1)} \right] d\mathbf{\Omega}. \quad (2.38) $$

Due to Maxwell relations $C$, $\hat{A}$ and $a$ have major symmetry, hence $W^{(12)}$ is symmetric with respect to its upper indices. In other words:

$$ W^{(12)} = W^{(21)}. \quad (2.39) $$

Furthermore, in the absence of body force and higher-order traction, the reciprocal theorem can be written in a compact form:

$$ \int_{\partial V} \left[ \dot{Q}_i^{(1)} u_i^{(2)} + \phi^{(1)} \omega^{(2)} \right] dS = \int_{\partial V} \left[ \dot{Q}_i^{(2)} u_i^{(1)} + \phi^{(2)} \omega^{(1)} \right] dS. \quad (2.40) $$

An example to demonstrate this result is shown in the Appendix A.1.

### 2.5 Isotropic flexoelectric material

The tensorial nature of the constitutive laws implies a rich variety of flexoelectric materials. However, in order to understand the general features of a flexoelectric material we must first study the simplest materials in this class. Therefore, we specialize to an isotropic flexoelectric material. Isotropic materials cannot be piezoelectric, so $d = 0$. Furthermore, under isotropic assumption and a simplified SGE model from Aravas (2011), which introduces
only one additional material length scale $\ell$, the energy density $W^L$ takes the following form:

$$\hat{\mathcal{W}}_L \left( \varepsilon_{ij}, \varepsilon_{jk,i}, P_i \right) = \frac{1}{2} \lambda \varepsilon_{ii} \varepsilon_{jj} + \mu \varepsilon_{ij} \varepsilon_{ij} + \frac{1}{2} \ell^2 \left( \lambda \varepsilon_{kk,i} \varepsilon_{nn,i} + 2 \mu \varepsilon_{jk,i} \varepsilon_{jk,i} \right) + \frac{1}{2} a P_i P_j + \left( \hat{f}_1 \varepsilon_{kk,i} P_i + 2 \hat{f}_2 \varepsilon_{ij,i} P_j \right), \tag{2.41}$$

where $\lambda$ and $\mu$ are Lamé constants and $\hat{f}_1$ and $\hat{f}_2$ are two flexoelectric coupling constants. $a$ is the reciprocal susceptibility which is related to the dielectric permittivity $\varepsilon$ and susceptibility $\chi$ through $a^{-1} = \varepsilon_0 \chi = \varepsilon - \varepsilon_0$. The above isotropic assumption leads to the following constitutive relations:

$$\tau_{ij} = \lambda \varepsilon_{kk} \delta_{ij} + 2 \mu \varepsilon_{ij}, \tag{2.42}$$

$$\hat{\mu}_{ijk} = \left( \lambda \varepsilon_{pp,i} \delta_{jk} + 2 \mu \varepsilon_{jk,i} \right) \ell^2 + \left( \hat{f}_1 \delta_{jk} P_i + \hat{f}_2 \delta_{ij} P_k + \hat{f}_2 \delta_{ik} P_j \right), \tag{2.43}$$

$$E_i = a P_i + \hat{f}_1 \varepsilon_{kk,i} + 2 \hat{f}_2 \varepsilon_{ij,i}. \tag{2.44}$$

Substituting the relations above into the governing equations Eqn(2.19, 2.22) and making use of Eqn(2.1) we get:

$$\partial_i \left( a \varepsilon \phi + \hat{f} u_{k,k} \right) = 0, \tag{2.45}$$

$$\left( \lambda + \mu \right) \left( 1 - \ell_1^2 \partial_{ii} \right) u_{k,kj} + \mu \left( 1 - \ell_2^2 \partial_{ii} \right) u_{j,kk} = 0, \tag{2.46}$$

where $\hat{f} = \hat{f}_1 + 2 \hat{f}_2$ and $\ell_1$, $\ell_2$ are some material length scales given by:

$$\ell_1^2 = \ell^2 - \frac{\varepsilon_0 \hat{f}^2}{\left( \lambda + \mu \right) a \varepsilon}, \quad \ell_2^2 = \ell^2 - \frac{\hat{f}^2}{a \mu}. \tag{2.47}$$

Note that Eqn(2.46) differs from that of Aravas (2011) in that we have two length scales $\ell_1$ and $\ell_2$ while he has only $\ell$. We observe from Eqn(2.47) that this is due to the flexoelectric effect. Interestingly, the form of Eqn(2.46) is the same as the Navier equation of general strain gradient elasticity proposed by Mindlin & Eshel (1968), but his length scales have nothing to do with electromechanical coupling. However, Mindlin’s argument concerning the positive definiteness of the energy still applies here.

Following that argument, in the isotropic flexoelectric material, to ensure positive-definiteness of the energy density $\mathcal{W}_L$, we basically need $\mathcal{W}_R = \mathcal{W}_L - \text{SE}$ to be positive-
definite (SE is the strain energy). This is because SE is already positive-definite due to the
constrains put on the Lamé constants:

\[ 3\lambda + 2\mu > 0, \quad \mu > 0. \tag{2.48} \]

Since flexoelectricity only has to do with the gradient terms and electric terms, bounds for
them should be derived from \( \mathcal{W}_R \). Volumetric strain or dilatation \( \Theta \) and deviatoric strain
\( \varepsilon'_{ij} \) are defined as:

\[ \Theta = \varepsilon_{kk}, \quad \varepsilon'_{ij} = \varepsilon_{ij} - \frac{1}{3} \Theta \delta_{ij}. \tag{2.49} \]

Now, we rewrite \( \mathcal{W}_R \) in terms of these two variables:

\[ \mathcal{W}_R = \frac{1}{2} \left( \lambda + \frac{2}{3} \mu \right) \ell^2 \Theta, \Theta + \left( f_1 + \frac{2}{3} f_2 \right) \Theta \delta_{ij} P_i + \mu \ell^2 \varepsilon'_{ij,ij} \varepsilon'_{ik,ik} + 2 f_2 \varepsilon'_{ik,ik} P_i + \frac{1}{2} a P_i P_i, \tag{2.50} \]

where the variation of \( \Theta, \varepsilon' \) and \( P \) can all be taken independently. As a result, to ensure
positive definiteness of the above quadratic form, we must have

\[ a \left( \lambda + \frac{2}{3} \mu \right) \ell^2 \geq \left( f_1 + \frac{2}{3} f_2 \right)^2, \quad \frac{1}{2} a \mu \ell^2 \geq f_2^2. \tag{2.51} \]

Therefore, in general, the thermodynamic constraints for the flexoelectric coupling constants
are

\[ \left| f_1 + \frac{2}{3} f_2 \right| \leq \ell \sqrt{\left( \lambda + \frac{2}{3} \mu \right) a}, \quad |f_2| \leq \ell \sqrt{\frac{\mu a}{2}}. \tag{2.52} \]

### 2.6 Application

In this section, several interesting 1D and 2D problems are examined for flexoelectric solids,
including beams, torsion and cylinders under pressure and shear. They are closely related
to experiments and insights are drawn from the closed-form solutions. Two other problems
are also shown in Appendix A.2 and C, to further extend the discussion.
2.6.1 Euler Bernoulli beam

Consider a slender beam on the $e_1-e_2$ plane, with length $L$ and thickness $2h$ (with width $w$ in $e_3$ direction). The coordinate $x_1$ runs along the length of the beam through the centroid of the cross-section and $x_2$ lies along the thickness of the beam. We assume $L \gg 2h$, so that gradients in the $e_2$ direction are much larger than the gradients in the $e_1$ direction, e.g. $E_2 \gg E_1$. As an approximation, we only work with the leading order terms here.

Suppose some distributed shear loads $q(x_1)$ and a voltage difference $V(x_1)$ are applied on the beam (with lower surface grounded). These loads will contribute to the deflection of the beam and create a curvature $\kappa(x_1) \approx u_{2,11}$. From the Euler-Bernoulli theory we have:

$$\varepsilon_{11} = -\kappa x_2, \quad \varepsilon_{22} = \varepsilon_{33} = \kappa \nu x_2, \quad \varepsilon_{ij} = 0 \text{ otherwise}$$  \hspace{1cm} (2.53)

where $\nu$ is the Poisson ratio. Under this deformation field, according to Eqn(2.45),

$$\phi = \frac{V}{2} (1 + \frac{x_2}{h}) = E_2 x_2 + \frac{V}{2},$$  \hspace{1cm} (2.54)

where $E_2 = -V(x_1)/2h$. Our objective is to determine the curvature $\kappa$ under given loads. Given the above strain and potential field, the energy density $W$ can be written in the following form:

$$\hat{W} = \frac{1}{2} \left( E x_2^2 + E \ell'^2 - \epsilon_0 \chi \hat{f}_b^2 \right) \kappa^2 + \frac{1}{2} \epsilon E_2^2$$  \hspace{1cm} (2.55)

where $E$ is the Young’s modulus and $\hat{f}_b = \hat{f}_1 - \nu \hat{f}$ is the effective bending flexoelectric coupling constant. This is the total energy stored in the flexoelectric solid. Based on the constitutive relations Eqn(2.5) and Eqn(2.44), we also know that

$$D_2 = \epsilon E_2 + \epsilon_0 \chi \hat{f}_b \kappa.$$  \hspace{1cm} (2.56)

This equation shows that present day experimental measurements using the beam approach, e.g. Ma & Cross (2001, 2002, 2006), Zubko et al. (2007) are actually quantifying $\mu_b^f = \epsilon_0 \chi \hat{f}_b$.

In the above experiments, the beams used for measurements are short-circuited to measure charge flow. Beams can also be made open-circuited to suffer purely mechanical loads. For short circuits, $V = 0$, while for open circuits, $D_2 = 0$. These two modes result in different
energy expressions, viz.

\[
\int_V \Delta \hat{W} d\nu = \frac{(\epsilon - \epsilon_0)^2 \hat{f}_b^2 A}{2\epsilon} \int_0^L \kappa^2 dx_1,
\]

(2.57)

where \( A \) is the cross-sectional area. Open circuit beams have larger energy for the same amount of deformation. This is the ‘flexoelectric stiffening’ effect which is an enhancement in the bending rigidity proportional to \( \hat{f}_b^2 \). This effect is also described in the works of Majdoub et al. (2008b), Yan & Jiang (2013). A similar effect is also observed in beams made of piezoelectric materials in Yang (2005) and is known in the literature as ‘piezoelectric stiffening’. To further elucidate this point, the governing equation for the beam can be obtained in the following fashion:

\[
M(x_1) = \frac{\partial}{\partial \kappa} \int_A \hat{W}(\kappa, D_2) dS = (EI + EA\ell^2 - \epsilon_0 \chi \hat{f}_b^2 A) \kappa + \frac{\epsilon_0 \chi \hat{f}_b A h V}{2h}.
\]

(2.58)

This relation shows that \( V \) causes a bending moment as a result of flexoelectric coupling. Therefore, the governing equation of this beam is

\[
\frac{d^2 M}{dx_1^2} = (EI + EA\ell^2 - \epsilon_0 \chi \hat{f}_b^2 A) \frac{d^2 \kappa}{dx_1^2} + \frac{\epsilon_0 \chi \hat{f}_b A d^2 V}{2h} \frac{d^2 \kappa}{dx_1^2} = q(x_1).
\]

(2.59)

Here, we let \( G_E = EI + EA\ell^2 - \epsilon_0 \chi \hat{f}_b^2 A \), which is the bending rigidity of the short-circuited beams. We can also find the bending rigidity of the open circuit beam, \( G_D \), in a similar way and get

\[
\frac{G_D - G_E}{EI} = \frac{3\epsilon_0^2 \chi^2 \hat{f}_b^2}{\epsilon E h^2}.
\]

(2.60)

Thus, flexoelectric stiffening is related to the flexoelectric coupling constants and the thickness of the material. If the thickness is small there could be a large flexoelectric stiffening. This is shown in Fig. 2.2.

Beam offer a simple but useful system to study flexoelectricity. There are many other ways of application, such as in Appendix A.2, where flexoelectricity can be used to alter the response of piezoelectric bimorph at small sizes.
Figure 2.2: Size dependent stiffening of flexoelectric beams. Flexoelectric calculations are carried out keeping $f_b/f_m = 0.25$ where $f_m = \sqrt{EI/\varepsilon_0}$ and $G$ is the effective bending rigidity.

2.6.2 Torsion

Torsion of circular shafts generates a constant strain gradient. Surprisingly, such a strain gradient does not polarize an isotropic flexoelectric material. To see why, let us start with the displacement field of a circular shaft under torsion with $e_3$ aligned with the axis of the shaft:

$$u_1 = -\varphi x_2 x_3, \quad u_2 = \varphi x_1 x_3, \quad u_3 = 0,$$

(2.61)

where $\varphi$ is the angle of twist per unit length. The strains are:

$$\varepsilon_{13} = -\frac{1}{2} \varphi x_2, \quad \varepsilon_{23} = \frac{1}{2} \varphi x_1.$$

(2.62)

The non-vanishing components of the strain-gradient are $\varepsilon_{13,2}$, $\varepsilon_{31,2}$ and $\varepsilon_{23,1}$, $\varepsilon_{32,1}$. The flexoelectric coupling energy can then be calculated:

$$\hat{f}_{ijkl}\varepsilon_{jk,i}P_l = f_1\varepsilon_{kk,i}P_i + 2\hat{f}_2\varepsilon_{ij,i}P_j = 0,$$

(2.63)
no matter which direction polarization takes. As a result a circular shaft made of isotropic flexoelectric material will not polarize under torsion even though strain gradient effects will lead to a size dependent torsional rigidity. This result also holds for cubic crystals, in which the flexoelectric tensor takes the following form:

\[ \hat{f}_{ijkl} = \hat{f}_1 \delta_{jk} \delta_{il} + \hat{f}_2 (\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl}) + \hat{f}_3 \delta_{ijkl}, \]  

(2.64)

where \( \hat{f}_3 \) is another flexoelectric constant and \( \delta_{ijkl} \) is the fourth order Kronecker Delta which is 1 when \( i, j, k, l \) are all equal and 0 otherwise. If the axis of the shaft is aligned with one of the sides of the cubic lattice then the flexoelectric coupling energy can be easily shown to still vanish. Similar results are also observed in screw dislocations in the later section. It is worthy of mention that for torsion of cross-section other than circular shape, the result can be very different.

2.6.3 Cylinder under pressure

Next we consider a cylindrical tube under pressure. Calculating the stress in a circular disk or tube with a central hole under internal and/or external pressure is a classic problem in linear elasticity, just as calculating the capacitance of a cylindrical capacitor is in electrostatics. The solution in this simple geometry offers not only a direct comparison to classical elasticity and SGE, but also some insights into the stress and polarization fields near point defects in flexoelectric materials. The geometry of the problem is illustrated in figure 2.3.

The cylinder is loaded by internal and external pressures \( p_i \) and \( p_o \), and a voltage difference \( V \) is applied across the inner and outer surfaces. The corresponding boundary conditions are:

\[ \hat{Q}_r = -p_i, \quad \hat{R}_r = 0, \quad \phi = 0, \quad \text{at} \quad r = r_i, \]  

(2.65)

\[ \hat{Q}_r = -p_o, \quad \hat{R}_r = 0, \quad \phi = V, \quad \text{at} \quad r = r_o. \]  

(2.66)

It is convenient to solve this axisymmetric problem in polar coordinates so that the only relevant component of displacement is \( u_r = u_r(r) \). Hence, the Navier equation (2.46) can
be simplified to:

\[
\left(1 - \epsilon_0^2 \nabla^2 + \frac{\ell_0^2}{r^2}\right)\left(\nabla^2 u_r(r) - \frac{u_r(r)}{r^2}\right) = 0,
\]

which is the characteristic length scale of this flexoelectric problem. The solution to the above BVP can be analytically obtained in the following form:

\[
u_r(r) = A r + \frac{B}{r} + C K_1\left(\frac{r}{\ell_0}\right) + D I_1\left(\frac{r}{\ell_0}\right),
\]

\[
\phi(r) = G + H \ln r - \frac{\hat{f}}{a \epsilon} \left(\frac{\partial u_r}{\partial r} + \frac{u_r}{r}\right),
\]

where \((A, B, C, D, G, H)\) are constants determined from the boundary conditions and \(I_i(x)\) and \(K_i(x)\) the \(i\)th order modified Bessel functions of the first and second kind respectively. For detailed component forms of all other quantities, refer to the procedure provided in Appendix D.

We can solve for these constants, but the expressions are lengthy and uninsightful. Instead, we plot the results for the polarization, stress and displacement fields for the
The following set of non-dimensional parameters:

$$\{ \hat{\nu}, \chi, \frac{\ell}{r_i}, \frac{r_o}{r_i}, \frac{p_o}{p_i}, \frac{\epsilon_0 \hat{f}^2}{E \ell^2} \} = \{ 0.3, 1, 2, 0.2, 2, 0.5^2 \}$$  \hspace{1cm} (2.71)$$

where in there we used the set of plane strain parameters that makes $$\lambda = \hat{E} / (1 + \hat{\nu}), \mu = \hat{E} \hat{\nu} / (2 - 2\hat{\nu}^2)$$. In here we also define $$\hat{f}_{\text{max}}$$ to be the maximum $$\hat{f}$$ that ensures $$\ell_0 \geq 0$$:

$$\hat{f}_{\text{max}} = \sqrt{\frac{a \epsilon (\lambda + 2\mu) \ell^2}{\epsilon_0}}.$$  \hspace{1cm} (2.72)$$

The electric quantities are plotted in Fig.2.4(a)-2.4(b). Clearly the polarization and electric potential are perturbed by the flexoelectric effect. Especially for polarization, we can see that gradient induced polarization is the dominating effect in here.

The strain fields are plotted in Fig.2.5. Due to the flexoelectric effect, the hoop strain $$\varepsilon_{\theta\theta}$$ is significantly reduced, see Fig.2.5(b). The variation of radial strain $$\varepsilon_{rr}$$ is smoothed out due to the flexoelectric effect, see Fig.2.5(a). Smaller strains imply higher rigidity of the disk. This is reminiscent of the increased rigidity we saw earlier in the flexoelectric beam.

Next, we will calculate the stresses. We recall the Cauchy stress $$\tau$$ no longer represents the “true” physical stress in materials with SGE effects. However, according to Mindlin & Eshel (1968), Aravas (2011), the true stress $$\sigma$$ can still be computed through the following
Figure 2.5: This figure plots a) radial strain $\varepsilon_{rr}$ and b) hoop strain $\varepsilon_{\theta\theta}$, with parameter as in Eqn.(2.71).

equation:

$$\sigma_{ij} = \tau_{ij} - \frac{2}{3} \hat{\mu}_{ijk,k} - \frac{1}{3} \hat{\mu}_{kij,k}. \quad (2.73)$$

A direct result of the above equation is that $\sigma$ (referred to as stress afterwards) is no longer symmetric. In general, $\sigma$ and $\tau$ can be very different, but there are cases where certain components of Cauchy stress can be a good approximation of those of the true stress. The two components of true stress are plotted in Fig.2.6. Comparing Fig.2.6(a) and Fig.2.6(b), it is clear that hoop stress is larger than the radial stress. The flexoelectric effect also significantly alters the magnitude of the hoop stress, which directly influences the stress concentration factor.

We define a stress concentration factor SCF as follows:

$$\text{SCF} = \left. \left( \frac{|\sigma_{ij}|_{\text{max}}}{p_i} \right) \right|_{r=r_i} = \left. \left( -\frac{\sigma_{\theta\theta}}{p_i} \right) \right|_{r=r_i}. \quad (2.74)$$

From Fig.2.6(b), it is apparent that flexoelectricity reduces the SCF compared to classical elasticity and SGE. This happens because in a flexoelectric material, part of the work done by the external loads is used to polarize the material. This is in contrast to elasticity where all the work done by the external loads is stored as elastic energy in the body.

SCF is clearly dependent on the geometry. In order to study its asymptotic behavior
when the size of the hole becomes much smaller—approaching a small defect in a material, we plot SCF as a function of \( r_o/r_i \), as shown in Fig.2.7(a), while keeping all the other parameters fixed. The SCF for the pure elasticity and SGE solutions are also plotted for comparison. We see that as \( r_o/r_i \to \infty \), SCF \( \to \) SCF\( ^\infty \), a constant. For a flexoelectric solid, SCF\( ^\infty _{\text{Flex}} \) = 2.89 < SCF\( ^\infty _{\text{SGE}} \) = 2.99 < SCF\( ^\infty _{\text{Elast}} \) = 3.00, so the SCF is clearly reduced. Intuitively, larger \( \hat{f} \) converts more mechanical energy into electrical energy, hence reduces SCF. To quantify this reduction, we plot SCF\( ^\infty \) as a function of \( \hat{f} \) in Fig.2.7(b). As \( \hat{f} \to 0 \) we recover SCF\( ^\infty _{\text{SGE}} \) = 2.99 and when \( \hat{f} \) approaches the limit \( \hat{f}_{\text{max}} \), SCF\( ^\infty \) reduces sharply (approximately proportional to \( \hat{f}^2 \)). Figure 2.7(b) shows that at \( \hat{f} = 0.9\hat{f}_{\text{max}} \), SCF\( ^\infty \) is reduced by more than 50%.

Even in cases where \( \hat{f} \) is not as large, it is possible to alter SCF by applying a stronger potential difference \( V \) between the inner and outer surfaces of the disk. This is shown in Fig.2.8(a), with different values of \( \hat{f} \). A linear reduction of SCF is observed as the potential \( V \) is increased. This reduction becomes more and more sensitive to \( V \) as \( \hat{f} \) becomes larger. From another perspective, this result implies that it is possible to modulate material strength through external electric fields. In fact, this modulation is proportional to the magnitude of external field and becomes stronger in materials with larger flexoelectric constants. Similarly, the electrical behavior can be controlled by changing the mechanical loading. Figure.2.8(b) shows that the magnitude of polarization (at \( r_i \)) increases propor-
tionally with $p_i$ while $V = 0$ is held fixed. This is a straightforward result of the dominating gradient induced polarization.

Figure 2.7: This figure plots in (a) the asymptotic behavior of SCF with $r_o/r_i \to \infty$ and in (b) the flexoelectric reduction of SCF$^\infty$ with increasing $\hat{f}$.

Figure 2.8: In this figure, (a) plots SCF$^\infty$ as a function of potential $V$ holding mechanical loads fixed (b) plots polarization at the inner surface as a function of pressure $p_i$, holding $V = 0$.

In order to see any of these effects in experiments it is important to get some estimates of $\hat{f}_{\text{max}}$. Note that flexoelectricity is prominent in those materials where $\chi \gg 1$. Since we
know $a\varepsilon \approx 1$. Lamé constants $\lambda, \mu \approx E$, by Eqn(2.72) we have:

$$\hat{f}_{\text{max}} \approx \sqrt{\frac{E}{\varepsilon_0}} \ell. \quad (2.75)$$

Thus, the magnitude of $\hat{f}_{\text{max}}$ is proportional to the SGE length scale. Unlike $\mu^f$, the flexoelectric constant, flexoelectric coupling constant $\hat{f}$ is not proportional to the susceptibility. As suggested in Nowacki (2006), $\ell$ is on the order of several to tens of nm, so this makes the estimates from the above equation consistent with the classical estimate for $\hat{f} \sim 1 - 10$ V by Kogan (1964).

Measurable flexoelectric effects have only been observed in materials with larger $\hat{f}$ and $\mu^f$. Perovskite materials, e.g. barium titanate, are good examples of such materials. These materials exhibit a high $\hat{f}$ as well as a high $\chi$ that can be several orders of magnitude greater than that of simple ionic crystals like sodium chloride. For these reasons, perovskite materials are now at the cutting edge of the research on flexoelectricity. Our predicted flexoelectric reduction of SCF and its interplay with elasticity should be observable in these materials.

We note here that the study of SGE and flexoelectricity are tightly connected. As in SGE our discussion of flexoelectricity is valid only when $r_i$ is comparable to $\ell$. In other words, this effect is important only at sub-micron length scales. If the inner diameter of the disk is on the order of centimeters, it can be shown that the solution we obtained converges to that of classical elasticity. Hence, our prediction of an electric field dependent enhancement of strength applies only to sub-micron scale specimens of flexoelectric solids.

### 2.6.4 Cylinder under shear

The disk of the previous example can also suffer in-plane shear, which is mimicking the uniform torsion of a hollowed nanowire. Suppose we are considering a hollowed wire whose inner edge is kept fixed (not allowed to rotate), then the boundary conditions are:

$$\hat{u}_\theta = 0, \quad \hat{R}_\theta = 0, \quad \phi = 0, \quad \text{at} \quad r = r_i, \quad (2.76)$$

$$\hat{Q}_\theta = \tau_0, \quad \hat{R}_\theta = 0, \quad \phi = 0, \quad \text{at} \quad r = r_o, \quad (2.77)$$
where $\tau_0$ is the shear applied on the outer edge.

The only important component of the displacement field in this problem is $u_\theta = u_\theta(r)$. As a result, the Navier equation for this problem is of the same type as the previous one:

$$
\left(1 - \ell_2^2 \nabla^2 + \frac{\ell_2^2}{r^2}\right) \left(\nabla^2 u_\theta(r) - \frac{u_\theta(r)}{r^2}\right) = 0,
$$

(2.78)

and

$$
\ell_2^2 = \ell^2 - \frac{f_2^2}{a \mu},
$$

(2.79)

is the characteristic length scale of this problem. The solution is given in a similar form to that of the pressurized case:

$$
u(r) = A r + \frac{B}{r} + C K_1 \left(\frac{r}{\ell_0}\right) + D I_1 \left(\frac{r}{\ell_0}\right),
$$

(2.80)

where $(A, B, C, D)$ are constants determined from the boundary conditions. Note that the electric potential is completely decoupled from this problem due to our assumption of short-circuited inner and outer edges. Hence, the potential vanishes in this problem and the calculation can be carried out using the following non-dimensional parameters:

$$
\left\{ \nu, \chi, \frac{\ell}{r_i}, \frac{r_o}{r_i}, \frac{\tau_0}{E}, \frac{f_2^2}{a \mu} \right\} = \left\{ 0.3, 1, 0.2, 2, 0.5 \right\}
$$

(2.81)

We plot the displacement, strain and polarization fields for a specific choice of parameters in Fig.2.9. The results confirm the features observed in earlier results: (a) smaller deformation for the same boundary loads, (b) smoother strain profiles compared to pure elasticity or strain gradient elasticity, and (c) increase in rigidity. We attribute these features to flexoelectricity.

Interestingly, in this problem the displacement field is divergence-free. As a result the governing equation for $\phi$ is completely decoupled from the deformation. However, the inhomogeneous strain field produces an azimuthal polarization $P_\theta$:

$$
P_\theta = -\frac{(\epsilon - \epsilon_0) f_2}{2 \ell_2^2} \left[ C I_1 \left(\frac{r}{\ell_2}\right) + D K_1 \left(\frac{r}{\ell_2}\right) \right].
$$

(2.82)

The magnitude of the azimuthal polarization shows an interesting variation – it is maximum
Figure 2.9: (a) plots normalized shear strain and (b) the normalized displacement as functions of the radial coordinate. (c) plots the distribution of normalized azimuthal polarization. It reaches a minimum around the middle of the disk.

at the boundaries and smaller inside. Note that the polarization is completely determined by $C$ and $D$ and it is only observable at length scales comparable to $\ell$. A piezoelectric problem with the same geometry and loading gives a radial polarization. The azimuthal polarization predicted here for a disk made of flexoelectric material can potentially be verified by experiments.

### 2.7 Concluding remarks

In this chapter, we start with a review on the classical treatment of electromechanics in a continua and an introduction of Toupin’s variational principle, which recovers the classical theories. Using this principle and extend it to include strain gradients, we are able to derive the governing equations and boundary conditions for general flexoelectric dielectrics. We then propose a linear constitutive law and prove a reciprocal theorem. An analogous theorem for piezoelectric materials is well known. Following that, we specialize to the study of isotropic materials and derive the governing Navier equations for the problem. Intrinsic length scales are introduced into the governing differential equations to raise the order of these equations. These intrinsic length scales are also different from the SGE ones due to the coupling effect. To ensure the uniqueness of the governing differential equations, an upper bound of flexoelectric coupling constant is then derived.
We have also used our theory to solve some boundary values problems for isotropic flexoelectric materials relevant to experiments and application. First we look at a flexoelectric beam. We give expressions for effective bending flexoelectric constant, which is a linear combination of transverse and longitudinal flexoelectric constant. A beam equation is derived where electric voltage will generate extra bending moment proportionally. Bending stiffness/rigidity is different in short and open circuited beams due to the coupling effect and that difference is size-dependent. Then we turn to the torsion of a cylindrical specimen but only to find that in isotropic and cubic materials, this deformation field will not create any flexoelectric coupling. Last we look into the hollow cylinders. Radially loaded cylinders offer insights into how the mechanical behavior of a flexoelectric material can be modulated at the nanoscale by the use of electric fields and vise versa. It demonstrates a way to control stress concentration by use of flexoelectric materials. Circumferentially sheared cylinder creates a unique azimuthal polarization field. Of course, there are many other problems that are of interests.

The methods discussed in this chapter is the starting point of studying flexoelectric solids, which we will use for the rest of the dissertation. It is also the fundamental of building continuum based computational methods for flexoelectric solids. Such methods will be required to compute displacement and polarization fields in complex geometries where close form solutions are not possible. Our solutions to various problems are useful in the interpretation of nanoscale experiments in the burgeoning field of flexoelectric materials. They are also useful in terms of providing benchmark problems to validate computational methods for flexoelectric solids.
Chapter 3

Defects in Flexoelectric Solid

3.1 Introduction

In this chapter, we will utilize the continuum framework in Chapter 2 to describe the stress and polarization fields near defects in flexo-electric solids. Defects are the spots where the effects of flexo-electricity are expected to be prominent due to the large strain gradients in their vicinity. As far as we know, there has been very few theoretical work that deals with this topic directly, but there is definitely a surging interests into it. In a computational study by Ong & Reed (2012), it is shown that overall piezoelectric behavior can be achieved by adopting defects into centrosymmetric graphene. This idea was later realized by Zelisko et al. (2014). According to their report, it is the interplay of non-centrosymmetric defects and flexoelectricity that creates this phenomenon. This indeed opens up the possibility of manipulating materials by flexoelectricity.

Flexoelectricity can also interplay with dislocations and generate many interesting phenomena. One example could be the experiments by Koehler et al. (1962), Turchányi, G. et al. (1973), Whitworth (1975), as mentioned in the Introduction. They studied charged dislocations in cubic crystals, e.g. alkali halides. These solids have centrosymmetric lattices which rule out piezoelectricity as the cause for the charge carried by dislocations in them, but this symmetry does not rule out flexoelectricity. In fact, flexoelectric phenomena can be observed in dielectrics of any symmetry group, including isotropic ones. Charged dislocations were also observed in experiments on ice by Petrenko and co-workers in 1980s,
like in Petrenko & Whitworth (1983). They conducted a thorough study of the electromechanical properties of ice and attributed charged dislocations and other phenomena to a so-called “pseudo-piezoelectricity” as summarized in Petrenko & Whitworth (1999). This phenomenon assumed that the polarization in ice is proportional to the pressure gradient. In fact, Petrenko and co-workers studied point defects, dislocations and cracks in ice and arrived at their conclusions about pressure gradient dependent polarization from a microscopic viewpoint. This, as will be shown later, is a natural result of what is known today as flexoelectricity.

This chapter is organized as follows. First, we construct the Green’s function for a flexoelectric boundary value problem. We will use it in our studies of point defects and dislocations. Second, we give an analytic solution to the problem of a single point defect in an isotropic flexoelectric solid. Third, we solve for the polarization fields of screw and edge dislocations and connect our analysis to various experiments. In particular, we will show in this chapter that some of the results for charged dislocations can be qualitatively understood in terms of flexoelectricity.

### 3.2 Flexoelectric Green’s function

First, we present a quick recap of the continuum theory. Suppose we consider an isotropic flexo-electric solid in which the displacement field is $u(x)$ and the electric potential is $\phi(x)$. Such a solid is characterized by the Lamé constants, $\lambda$ and $\mu$, an SGE length scale $\ell$, two flexo-electric coupling constants $\hat{f}_1$ and $\hat{f}_2$ and the dielectric permittivity $\epsilon$. If the deformation and charge separation are sufficiently small then we can use a linearized theory and derive a Navier-type equation for the displacement field and the electric potential. With the absence of body force and free charge, the governing equations obtained in Chapter 2 are as follows:

\[
\partial_{ii}(a\epsilon\phi + \hat{f}u_{k,k}) = 0, \tag{3.1}
\]

\[
(\lambda + \mu)(1 - \ell_1^2\partial_{ii})u_{k,kj} + \mu(1 - \ell_2^2\partial_{ii})u_{j,kk} = 0, \tag{3.2}
\]
with some flexoelectric length scale \( \ell_1, \ell_2 \) and \( \ell_0 \) given by

\[
\ell_1^2 = \ell^2 - \frac{\epsilon_0 \hat{f}^2}{(\lambda + \mu)a\epsilon}, \quad \ell_2^2 = \ell^2 - \frac{\hat{f}_2^2}{a\mu}, \quad \ell_0^2 = \ell^2 - \frac{\epsilon_0 \hat{f}^2}{(\lambda + 2\mu)a\epsilon},
\]

(3.3)

with \( \hat{f} = \hat{f}_1 + 2\hat{f}_2 \) and \( a^{-1} = \epsilon - \epsilon_0 \), where \( \epsilon_0 \) is the permittivity of vacuum. Then the flexoelectric Green’s function for displacement \( G_{ij} \) due to a unit point load can be obtained by solving the following equation

\[
(\lambda + \mu)\mathcal{L}_1 G_{ik,kj} + \mu \mathcal{L}_2 G_{ij,kk} + \delta_{ij}\delta(r) = 0,
\]

(3.4)

where \( \mathcal{L}_i = (1 - \ell_i^2 \nabla^2) \), \( r = (x_1, x_2, x_3) \) is the position vector (with \( r = |r| \)) and \( G_{ij} \) corresponds to the displacement \( u_i \) in response to a unit point force in the \( j \) direction at origin.

Following the techniques of Phillips (2001), we employ the Fourier transform of the Green’s function, \( G_{ij}^* \). Then the equation above implies

\[
(\lambda + \mu)(1 + \ell_1^2 q^2)q_k q_j G_{ik}^* + \mu q^2 (1 + \ell_2^2 q^2)G_{ij}^* = \delta_{ij}.
\]

(3.5)

where \( q_i \) are the coordinates in the reciprocal space and \( q^2 \) is the square sum of all \( q \)'s. Multiplying by \( q_j \) on each side and summing over \( j \), we are able to solve for \( q_k G_{ik}^* \):

\[
q_k G_{ik}^* = \frac{q_i}{q^2 (1 + \ell_0^2 q^2)(\lambda + 2\mu)}.
\]

(3.6)

This intermediate result can be inverted to get

\[
G_{ik,k} = \partial_i \left[ \frac{1 - e^{-r/\ell_0}}{4\pi r(\lambda + 2\mu)} \right] = \frac{x_i}{4\pi r^2(\lambda + 2\mu)} \left[ 1 - \left( 1 + \frac{r}{\ell_0} \right) e^{-r/\ell_0} \right].
\]

(3.7)

We will use this result later in our analysis of a point defect. From (3.5) and (3.6), we solve for \( G_{ij}^* \) to get

\[
G_{ij}^* = \frac{\delta_{ij}}{\mu q^2 (1 + \ell_2^2 q^2)} - \frac{q_k q_j}{q^4} \left[ \frac{1}{\mu (1 + \ell_0^2 q^2)} - \frac{1}{(\lambda + 2\mu)(1 + \ell_0^2 q^2)} \right].
\]

(3.8)

We observe that due to flexoelectricity, \( \ell_0 \neq \ell_2 \). So, unlike in SGE, we have two different
material length scales in the problem. By inverting (3.8) we get:

\[ G_{ij} = \frac{1 - e^{-r/\ell_2}}{4\pi \mu r} \delta_{ij} - \partial_i \partial_j \left[ \frac{F_2(r)}{8\pi \mu} - \frac{F_0(r)}{8\pi (\lambda + 2\mu)} \right], \tag{3.9} \]

where the \( F_k \)'s are

\[ F_k(r) = r + \frac{2\ell_k^2}{r} \left( 1 - e^{-r/\ell_k} \right), \quad k = 0, 2. \tag{3.10} \]

On the other hand, the 2D Green’s function is given by

\[ G_{ij} = -\frac{\ln r + K_0(r/\ell_2)}{2\pi \mu} \delta_{ij} + \partial_i \partial_j \left[ \frac{F_2(r)}{8\pi \mu} - \frac{F_0(r)}{8\pi (\lambda + 2\mu)} \right], \tag{3.11} \]

where the \( F_k \)'s are given by

\[ F_k(r) = r^2 (\ln r - 1) + 4\ell_k^2 \left[ \ln r + K_0(r/\ell_k) \right], \quad k = 0, 2, \tag{3.12} \]

and \( K_0(x) \) is the 0-order modified Bessel function of the second kind. In both expressions we see the appearance of two distinct flexo-electric length scales. In the next section we will use the 3D Green’s function to compute the displacement field and potential near a point defect in a flexo-electric solid.

The Green’s function calculated above is the solution to a point force exerted at the origin in a flexoelectric solid. To work out the solution for \( \phi \) and \( u_i \) when a point charge is placed at the origin in a flexoelectric solid, the governing equation (2.45) must be modified to:

\[ \nabla^2 (\phi + \frac{\hat{f}}{a\epsilon} u_{k,k}) = \frac{q_e}{\epsilon}, \tag{3.13} \]

where \( q_e \) is the free charge volume density. As a consequence, the Navier equation (2.46) must also be modified as

\[ (\lambda + \mu)(1 - \ell_1^2 \nabla^2) u_{k,k} + \mu(1 - \ell_2^2 \nabla^2) u_{j,kk} = \frac{\hat{f}}{a\epsilon} \partial_j q_e, \tag{3.14} \]

which effectively creates a body force due to the free charge. So if the body has free charges inside, then the governing equations have to be adapted to take into account the effective body force they introduce. If they arise due to doping, residual polarization etc., it is important that these charges can be determined, otherwise they will strongly influence the
mechanical response.

Now, for a unit point charge, or to compute the Green’s function, we set \( q_e = \delta(r) \). By the same technique as we used for the Green’s function for a point force, we find that \( u_{k,k} \) is given by:

\[
 u_{k,k} = \frac{\hat{f}}{4\pi a\epsilon(\lambda + 2\mu)\ell_0^2} \frac{\exp(-r/\ell_0)}{r}. \tag{3.15}
\]

This is the flexoelectric contribution to the potential \( \phi \). By plugging the above into the electric governing equation and inverting it we get

\[
 G_\phi(r) = \frac{1}{4\pi \epsilon r} \left[ 1 - \frac{\hat{f}^2}{a^2 \epsilon(\lambda + 2\mu)\ell_0^2} \exp\left(-\frac{r}{\ell_0}\right) \right]. \tag{3.16}
\]

Clearly, we recover the classical electrostatic solution of a unit point charge in a dielectric when we let the flexoelectric coupling constant \( \hat{f} \) vanish. The above solution suggests that the flexoelectric contribution to the potential is of the Yukawa type. We will see this again in the analysis of a point defect. Essentially in the far field, the potential of point charge in a flexoelectric solid and a pure dielectric converge. We illustrate this in Fig.3.1.

### 3.3 Point defects

From the continuum perspective a point defect can be modeled as a spherical hole of some radius \( a_0 \), with prescribed radial displacement \( \delta_0 \) on the surface of that hole. Following the argument of Phillips (2001), the displacement field of an isotropic point defect is proportional to \( G_{ij,j} \)

\[
 u_i \propto G_{ij,j} = \frac{x_i}{4\pi r^3(\lambda + 2\mu)} \left[ 1 - \left(1 + \frac{r}{\ell_0}\right) e^{-r/\ell_0} \right], \tag{3.17}
\]

this actually suggests that \( u \) is radial. From the boundary condition at the surface of the hole, \( u_r(a_0) = \delta_0 \), we obtain:

\[
 u_r(r) = \frac{\delta_0 a_0^2}{r^2} \left[ \frac{1 - (1 + \gamma) e^{-\gamma}}{1 - (1 + \gamma_0) e^{-\gamma_0}} \right], \tag{3.18}
\]

where \( \gamma = r/\ell_0 \) and \( \gamma_0 = a_0/\ell_0 \). In the limit of \( a_0 \gg \ell_0 \), we recover the elastic result in Phillips (2001). A similar expression was obtained by Adler (1969) in the 1960s in an SGE calculation. Our result differs from that result only by a change of length scale \( (\ell_0 \text{ instead of } \ell_0) \).
of $\ell$ and $\ell_0 = \ell$ excluding flexo effects). Hence, in the limiting case of no flexoelectricity, our results converge to that of SGE. Intriguingly, Eringen (1984) arrived at a very similar expression for the displacement field around a point defect in a non-local piezo-electric solid. In the isotropic case his result differs from our only by a pre-factor (a different boundary condition was used in there). Note, however, that an isotropic solid cannot be piezo-electric. Hence, our result establishes an interesting connection between flexoelectricity and a non-local theory of electromechanics. This, as pointed out in Yang (2005), is by no means surprising since similar connections between gradient elasticity and the non-local elasticity theories are well-known.

We are interested in the variation of the electric quantities around this point defect. From eqn.(2.45) we can compute the potential due to its presence in an isotropic flexoelectric solid

$$
\phi^f = -\frac{\delta a_0^2 \hat{f}}{ae\ell^3 A_0} \left( \frac{e^{-\gamma}}{\gamma} \right) = -\phi^{fm} \left( \frac{e^{-\gamma}}{\gamma} \right),
$$

(3.19)

where $A_0 = 1 - (1 + \gamma_0) e^{-\gamma_0}$ and $\phi^f \sim e^{-\gamma}/\gamma$ is a Yukawa-type potential. This result was also reported in Eringen (1984). In that work the length scale that appeared in the expressions was interpreted as the Debye screening length, which was expected to shorten due to the presence of non-local piezoelectricity. In our case the length scale appearing in the expressions has its origins in SGE and flexoelectric effects. Since here we have $\ell_0 < \ell$, flexoelectricity shortens the SGE length scale. We have plotted the potential around a point defect as a function of distance in Fig.3.1(a). For comparison we have also plotted the potential field due to a point charge in a solid with the same dielectric constant as our flexoelectric solid. The field in the flexoelectric solid decays much faster. The effects of the flexo-electric constant $f$ and the defect size $a_0$ are analyzed in Fig.3.1(b). We find that the flexoelectric effect is prominent only when $a_0$ is comparable to the SGE length scale $\ell$ and at large $f$.

We can also work out the radial component of the polarization around this point defect

$$
P_r = \frac{\epsilon_0 \phi^{fm}}{\ell_0} \left[ \frac{(1 + \gamma) e^{-\gamma}}{\gamma^2} \right].
$$

(3.20)

Note that this potential and polarization field arises around a point defect even in an isotropic solid. This is because flexoelectricity arises in any dielectric irrespective of lattice
symmetry. In fact, Evtushenko et al. (1987) detected electric polarization around defects in ice, in a pursuit for the origins of electromagnetic radiation from glaciers. In a series of experimental and theoretical works by Petrenko and co-workers, summarized in Petrenko (1996), this radiation was attributed to “pseudo-piezoelectricity”, in which a material had induced electric fields in proportion to pressure gradients--which is exactly (2.45). They investigated the microscopic origins of this effect and showed that the potential field around static dislocations and cracks in ice could be consistently explained beginning with this idea. This idea was further employed to quantify the stress and potential fields around moving/growing cracks. We will come back to this point when we analyze cracks.

Finally, with the advent of 2D flexoelectric materials, such as graphene, carbon nitride and many others, it is now possible to study the polarization field around the defects in them, like in Zelisko et al. (2014). The polarization fields in this case must be computed using the 2D Green’s functions that we discussed in the previous section. This could be a way to validate the analytic solutions presented in this paper and others.
3.4 Line defects

3.4.1 Screw dislocation

We showed in Chapter 2.6.2 that even though torsion of an isotropic circular rod produces a strain gradient, it does not polarize the rod due to the symmetry of the flexoelectric coupling tensor $\hat{f}_{ijkl}$. A similar result also holds for a material with cubic symmetry which has three flexoelectric coupling constants. We show here that the result can be extended to screw dislocations in such materials. If the axis of the screw dislocation is along the $e_3$ direction then the only non-zero displacement field is $u_3$. Hence, the field equations for an isotropic flexoelectric solid reduce to

$$(1 - \ell_2^2 \nabla^2) \nabla^2 u_3 = 0, \quad \nabla^2 \phi = 0.$$ \hfill (3.21)

These equations are the same as those in the SGE problems studied by Lazar (2013), except for a different length scale. Applying his method, the relevant 2D Green’s function is

$$G_{33} = -\frac{1}{2\pi \mu} \left[ \ln r + K_0 \left( \frac{r}{\ell_2} \right) \right],$$ \hfill (3.22)

then the distortion of a screw dislocation with a Burgers vector $(0, 0, b_z)$ can be constructed as

$$\beta_{31} = \mu b_z G_{33,2} = \frac{b_z x_2}{2\pi r^2} \left[ 1 - \frac{r}{\ell_2} K_1 \left( \frac{r}{\ell_2} \right) \right],$$ \hfill (3.23)

$$\beta_{32} = -\mu b_z G_{33,1} = \frac{b_z x_1}{2\pi r^2} \left[ 1 - \frac{r}{\ell_2} K_1 \left( \frac{r}{\ell_2} \right) \right],$$ \hfill (3.24)

By changing to cylindrical coordinates $(r, \theta, z)$ we get

$$\beta_{z\theta} = \frac{b_z}{2\pi r} \left[ 1 - \frac{r}{\ell_2} K_1 \left( \frac{r}{\ell_2} \right) \right], \quad \beta_{zr} = 0,$$

\hfill (3.25)

Therefore, strain $\varepsilon$ can be written as $\varepsilon = \text{sym} \beta = f(r) (e_\theta \otimes e_z + e_z \otimes e_\theta)$. In other words, the $\theta$ component of strain is a function of only $r$ while all other components vanish. According
to Sharma & Ganti (2005), we know

$$\nabla \otimes S = \frac{df(r)}{dr} (e_\theta \otimes e_z + e_z \otimes e_\theta) \otimes e_r - \frac{f(r)}{r} (e_r \otimes e_z + e_z \otimes e_r ) \otimes e_\theta. \quad (3.26)$$

These non-vanishing gradient terms do not induce any polarization in the isotropic flexoelectric solid due to the symmetry of the isotropic \( \tilde{f}_{ijkl} \) (no terms of the above have any repeated index). The same holds for cubic materials by doing the same exercise as in Chapter 2.6.2. This result is consistent with the results documented in Whitworth (1975), that in cubic ionic structures, screw dislocations do not carry charge. For details of the experimental setup, please refer to that work. We consider edge dislocations in the following section.

### 3.4.2 Edge dislocation

In the case of the edge dislocation one could follow Lazar (2013) to construct the displacement field using the Green’s function. However, following Eshelby (1966), we find it more convenient to work with the divergence \( \Theta \) and rotation \( \Omega \), which are defined as

$$\Theta = u_{i,i}, \quad \Omega_i = \frac{1}{2} e_{ijk} \partial_j u_k, \quad (3.27)$$

where \( e_{ijk} \) is the permutation symbol. The displacement field can be reconstructed through the following equation

$$\nabla^2 u_i = \Theta_{,i} + e_{ijk} \Omega_{j,k}. \quad (3.28)$$

This is just the Helmholtz decomposition of \( \nabla^2 u_i \), which splits it into a rotation-free part \( \Theta_{,i} \) and a divergence free part \( e_{ijk} \Omega_{j,k} \). In this problem \( \Omega = \Omega_3 e_3 \) can be treated as a scalar and let \( \Omega_3 = \Omega \). Eshelby (1966) used this idea to solve elasticity problems. In linear elasticity, \( \Theta^0 \) and \( \Omega^0 \) are governed by the following equations

$$\frac{\partial(\sigma \Theta^0)}{\partial r} = \frac{1}{r} \frac{\partial \Omega^0}{\partial \theta}, \quad \frac{1}{r} \frac{\partial (\sigma \Theta^0)}{\partial \theta} = - \frac{\partial \Omega^0}{\partial r}, \quad (3.29)$$

where \( \sigma = (1-\nu)/(1-2\nu) \) is a material constant. This means that \( \sigma \Theta^0 \) and \( \Omega^0 \) are harmonic conjugates. Now, in our problem with the isotropic flexoelectric solid, dilatation and
rotation are each governed by a distinct length scale
\begin{equation}
(\sigma L_0 \Theta)_{,j} + e_{j3k} L_2 \Omega_{,k} = 0, \quad j, k = 1, 2,
\end{equation}
where $L_0 = (1 - \ell_0^2 \nabla^2)$ and $L_2 = (1 - \ell_2^2 \nabla^2)$ are linear operators. More explicitly, in polar coordinates
\begin{align}
\frac{\partial (\sigma L_0 \Theta)}{\partial r} - \frac{1}{r} \frac{\partial (L_2 \Omega)}{\partial \theta} &= 0, \\
\frac{1}{r} \frac{\partial (\sigma L_0 \Theta)}{\partial \theta} + \frac{\partial (L_2 \Omega)}{\partial r} &= 0.
\end{align}
Therefore, if we replace $L_0 \Theta$ and $L_2 \Omega$ with $\Omega^0$ and $\Theta^0$, we recover (3.29). As a consequence, a solution of our problem can be constructed by solving
\begin{equation}
L_0 \Theta = \Theta^0, \quad L_2 \Omega = \Omega^0.
\end{equation}
The solution for $\Theta$ and $\Omega$ can be obtained by inverting the operators $L_0$ and $L_2$. Now, suppose we have an edge dislocation with burgers vector $(b_x, 0, 0)$, then the well known elasticity solution is given by
\begin{align}
\Theta^0 &= -\frac{b_x}{2\pi \sigma} \frac{\sin \theta}{r} \\
\Omega^0 &= -\frac{b_x}{2\pi} \frac{\cos \theta}{r}.
\end{align}
Following the methods used in Lazar & Maugin (2006) we obtain
\begin{align}
\Theta &= -\frac{b_x}{2\pi \sigma} \frac{\sin \theta}{r} \left[ 1 - \frac{r}{\ell_0} K_1 \left( \frac{r}{\ell_0} \right) \right] \\
\Omega &= -\frac{b_x}{2\pi} \frac{\cos \theta}{r} \left[ 1 - \frac{r}{\ell_2} K_1 \left( \frac{r}{\ell_2} \right) \right].
\end{align}
It can be shown that the above results converge to classical linear elasticity when $\ell \to 0$, $f_1, f_2 \to 0$ and to SGE when $f_1, f_2 \to 0$. A direct consequence of the above solution is the associated electric potential due to this deformation field:
\begin{align}
\phi^f &= \hat{f} b_x \frac{\sin \theta}{2\pi \alpha \sigma} \frac{1}{r} \left[ 1 - \frac{r}{\ell_0} K_1 \left( \frac{r}{\ell_0} \right) \right] = \phi^f_{m} \left[ \frac{\ell_0}{r} - K_1 \left( \frac{r}{\ell_0} \right) \right] \sin \theta,
\end{align}
where $\phi^f_{m} = \hat{f} b_x / (2\pi \alpha \sigma \ell_0)$. This potential is only related to $\ell_0$. It reaches its maximum around $\ell_0$, as plotted in figure 3.2(a), and decays to 0 in the both limits of $\frac{r}{\ell_0} \gg 1$ and
Generally speaking, as revealed by Maranganti & Sharma (2007), in single crystals the length scale \( \ell_0 \) and \( \ell \) are comparable to \( b_x \), in orders of nm. Therefore, strain-gradient induced electric potential is significant only in the vicinity of the core, namely when \( r \sim \ell \). Moreover, the electric field, as the negative gradient of this potential, has the appearance of a Lennard-Jones potential—the field decays strongly when \( r < \ell_0 \), reaches a minimum, and then increases slowly for \( r > \ell_0 \). The magnitude of the electric field dies down in the far field, but reaches a maximum in the vicinity of \( r \sim 2\ell_0 \), still in the range \( r \sim \ell \). In that region,

\[
\phi_{fm} \sim 1 - 10 \text{ V, } |E|^m \approx 1 \times 10^7 - 1 \times 10^8 \text{ V/cm},
\]

(3.38)

using the following estimates: \( \ell_0 \approx 10^{-9}\text{m} \) and \( \tilde{f} \sim 1-10\text{V} \) (this is a conservative estimate of \( \tilde{f} \) by Kogan (1964)). Interestingly, Turchányi, G. et al. (1973) reported from their experiments decades ago, that in alkali halide crystals, the field generated by a “charged” dislocation is in the range of \( 3.5 \times 10^6 \sim 1.05 \times 10^7 \text{V/cm} \). This is in good agreement with our rough estimates above. The electric field was measured by dislocation photoconduction spectrum (DSP). The method can capture the electric field in the vicinity of dislocation.

These dislocations are called “charged” because they create non-zero electric field and electric potential. This does not violate Eqn(2.45) since the “free charge” density \( q_e \) is still zero. Since the total charge is the sum of free charge and polarized (or bound) charge, it is possible that the dislocation generates non-vanishing electric field without carrying any free charge. Here the polarized charge arises due to the flexoelectric effect.

We can also compute the polarization field around the dislocation using the isotropic constitutive equations in Chapter 2.5

\[
P_i = -a^{-1} \left[ \phi_i + \tilde{f}_1 u_{k,ki} + \tilde{f}_2 (u_{j,ji} + u_{i,jj}) \right] = -a^{-1} \left( \phi_i + \tilde{f} \Theta_i + \tilde{f}_2 \varepsilon_{ij} \Omega_{ij} \right).
\]

(3.39)
Figure 3.2: This figure plots the electric quantities due to an edge dislocation, at \( \theta = \pi/2 \). a) plots radial distribution of electric potential with various \( f \)'s. b) plots the radial polarization field with different dielectric constants. The curves almost overlap when dielectric constant is larger than 5. Also in here, \( \phi_0 = \sqrt{(\lambda + 2\mu)a\epsilon\ell^2/\epsilon_0} \).

In polar coordinates the polarization field is:

\[
\begin{align*}
P_r &= -\frac{P^m\sin\theta}{(r/\ell)^2} \left\{ \frac{\epsilon_0}{\epsilon\sigma} \left[ 1 + \frac{r}{\ell_0} K_1 \left( \frac{r}{\ell_0} \right) \right]^2 K_0 \left( \frac{r}{\ell_0} \right) - \frac{\hat{f}_2}{f} \left[ 1 + \frac{r}{\ell_2} K_1 \left( \frac{r}{\ell_2} \right) \right] \right\}, \\
P_\theta &= \frac{P^m\cos\theta}{(r/\ell)^2} \left\{ \frac{\epsilon_0}{\epsilon\sigma} \left[ 1 + \frac{r}{\ell_0} K_1 \left( \frac{r}{\ell_0} \right) \right] - \frac{\hat{f}_2}{f} \left[ 1 + \frac{r}{\ell_2} K_1 \left( \frac{r}{\ell_2} \right) + \frac{r}{\ell_2} K_0 \left( \frac{r}{\ell_2} \right) \right] \right\},
\end{align*}
\]

where \( P^m = b_x \hat{f}/(2\pi a\ell^2) \). Unlike the potential, we have both \( \ell \) and \( \ell_2 \) present in these equations. However, in most cases, the polarization will be dominated by the \( r/\ell_2 \) and hence \( \hat{f}_2 \) terms. This is evident from Fig.3.2(b) in which we see that curves for dielectric constant of 5 and 10 are almost identical. For most solids in which flexoelectricity is prominent, dielectric constant is \( 10^2 \) or more. In perovskite materials, for which it is more than \( 10^3 \), we can safely claim that the polarization field around an edge dislocation is determined by \( \hat{f}_2 \).

From the polarization field, we are able to estimate the line charge density of the dislocation and compare it with the experiments done by Petrenko & Whitworth (1983) on charged dislocations in ice. Again, as indicated above, the “charge” that we are referring to is the charge due to polarization rather than the free charge. The polarized line charge
density $\lambda_\text{e}$ can be written as:

$$\lambda_\text{e} \approx P^m \ell_0 \approx \frac{1.6b_x \hat{f}_2}{\pi \ell_0}. \tag{3.42}$$

Hobbs et al. (1966) measured the dielectric constant of ice to be around 100. From the data given in Petrenko & Whitworth (1983), we know $\ell_0 \approx 50 \mu m$, $b_x \approx 0.73a_s \approx 10^{-9} m$ with $\hat{f} \sim 1 - 10 V$, hence

$$\lambda_\text{e} \approx 0.01 - 0.1 \text{pC/m} \sim 10^{-4} - 10^{-3} e/a_s, \tag{3.43}$$

where $a_s$ is the inter-atomic spacing and $e$ is the electron charge. The line charge density measured in the experiments is $\lambda_\text{e} = 3.0 \times 10^{-3} e/a_s$, reasonably close to our rough estimate. This suggests that flexoelectricity could provide a plausible reason for charged dislocations in ice.

Besides ice, perovskite materials like barium titanate and strontium titanate (STO) are good candidates to observe interplay between dislocations and flexoelectricity. These materials, according to Maranganti & Sharma (2007), have larger flexoelectric and dielectric constants and much shorter screening length scale $\ell_0$ (especially in single crystal). For example, Zubko et al. (2007) measured the flexoelectric constant of STO to be around $1 - 10 \text{nC/m}$. This suggests that the charges around a dislocation would be on the order of $10^4 - 10^5 \mu \text{C/m}^2$ at room temperature in STO. At lower temperatures the dielectric constant is even higher, so there will be more charge near the dislocation. This is a prediction from our analysis that could be verified against experiments.

### 3.5 Concluding remarks

In this chapter we have analyzed the stress and polarization fields near point defects, screw and edge dislocations in flexoelectric solids. We have shown that flexoelectricity plays an important role in the immediate vicinity of these defects where there are large strain gradients. For point defect, a Yukawa type of electric potential is produced as a result of mechanical distortion. This potential field decays away exponentially. Hence the region of action will have to be within the same range as the characteristic length scale. For screw dislocation in cubic or isotropic flexoelectric materials, the distortion does not produce polarization. For edge dislocation, that will result in net polarization. This result can
be connected to the experiments about charged dislocation in alkali halides. It can also be connected to the experiments on electromechanical phenomena in ice. The electrical behavior of defects in ice had been explained earlier by a “pseudo-piezoelectricity”, which we now recognize as flexoelectricity. Qualitative agreement of the experimental data and theoretical estimates are observed.
Chapter 4

Fracture Mechanics of Flexoelectricity

4.1 Introduction

In this chapter, we extend our analysis to cracks in flexoelectric solids. Cracks are special kind of defect that is closely related to the fracture behavior of materials. Since crack tip fields are singular there are large gradients near the tip. Thus, we expect flexoelectricity to play a prominent role in determining the fracture criterion.

The study of fracture mechanics of flexoelectricity is almost untouched. However, on the other hand, that in closely related piezoelectricity has developed very fast in the last two decades, as summarized in Kuma (2010). A primary motivation for these studies was to better understand damage and failure of piezoelectric devices. In particular, mathematical techniques from linear elastic fracture mechanics (LEFM) were used to find analytic solutions for a variety of crack problems in piezoelectric solids such as Sosa (1992), Suo et al. (1992), Pak (1992), which are now referred to as linear piezoelectric fracture mechanics (LPFM). Parallel experimental studies were also conducted, as summarized in Schneider (2007). It was realized that both mechanical failure and electric breakdown are responsible for damage in piezoelectric devices due to the singular nature of the stress and electric fields near a crack tip. For example, an “electric-yielded” zone in ferroelectrics was proposed by Gao et al. (1997), Wang (2000), which is analogous to the plastic zone in fracture mechan-
ics. Other important developments in this field involve treatment of boundary conditions, anisotropy, mode mixing etc., as summarized in Kuna (2010). All these studies have led to the development of a powerful continuum framework to study electromechanical effects in cracks. Some insights from this literature are used in our analysis. In the mean time, since strain gradient elasticity (SGE) is also an important ingredient of flexoelectricity, we draw upon literature of Zhang et al. (1998), Aravas & Giannakopoulos (2009) on asymptotic solutions of crack tip fields in gradient elasticity.

In the sequel, we perform an asymptotic analysis of crack tip fields in flexoelectric solids to tease out the contribution of flexoelectricity. We expect that the effects of flexoelectricity will die out far enough away from the crack tips just as we observed for point defects and dislocations. We first examine the simple Mode III crack and then into the Planar cracks. For that we isolated four modes, Mode I, Mode II, Mode D and Mode E, which has to do with the conducting and insulating boundary conditions at crack faces. Mixed modes are also discussed in sequence. Following that, path independent J integral is computed for each mode. Finally, we discuss new fracture criteria that could be used for predicting failure in flexoelectric solids.

4.2 Mode III crack

We start by considering a semi-infinite Mode III crack along the $x_1$ axis with crack tip located at the origin. This is an anti-plane shear problem with out-of-plane displacement $u_3 = u_3(x_1, x_2)$ and an electric potential $\phi = \phi(x_1, x_2)$. They are homogeneous along the $x_3$ axis but functions of in-plane coordinates, $x_1$ and $x_2$. The only surviving stresses are shear stresses $\tau_{3i}$ and $\tau_{3i}$ with $i = 1, 2$. Recall that the antiplane shear version of the governing equation is

$$\nabla^2 \phi = 0, \quad (1-\ell^2 \nabla^2) \nabla^2 u_3 = 0. \quad (4.1)$$

It is easier to work this problem out using cylindrical coordinates $(r, \theta, z)$. As for the boundary conditions, we require that the crack faces are traction and higher-order traction
free, so that at \( \theta = \pm \pi \):

\[
\tau_{23} - \hat{\mu}_{123,1} - \hat{\mu}_{223,2} - \hat{\mu}_{213,1} = 0, \quad (4.2)
\]
\[
\hat{\mu}_{223} = 0. \quad (4.3)
\]

We also impose the impermeable electric boundary condition at \( \theta = \pm \pi \):

\[
D_2 = 0 \quad (4.4)
\]

For example, this is a good approximation for cracks in ceramics with air between the open crack faces. We also require that far away from the crack tip the electric field and electric displacement decay to zero. The above imply that the in-plane component of \( E \) and \( D \) admit only the trivial solution, thus being irrelevant for our problem.

To find the asymptotic crack tip solution we assume that \( u_3 = r^s F_s(\theta) \). Then the leading order solution is

\[
u_3(r, \theta) = C_3 \sqrt{\frac{r}{\ell}} \left[ \frac{\theta}{2} - \frac{5}{3} \frac{s}{3} \frac{\alpha^2}{2} \sin \frac{3\theta}{2} \right], \quad (4.5)
\]

where \( \alpha^2 = \dot{\hat{f}}_2^2 / \mu a \ell^2 \), note that \( \alpha^2 \leq 1/2 \) by Eqn(2.52). \( C_3 \) is an undetermined constant which generally depends on \( \ell \). In fact, \( C_3 \) is related to the stress intensity factor. Note in the above asymptotic solution that as \( \ell \) and \( \alpha \) tend to 0, \( u_3(r, \theta) \) tends to the classical solution from linear elastic fracture mechanics. This idea will come up again when we compute the J integral. When we let \( \alpha \to 0 \), the solution converges to the SGE version of the crack problem, as in Zhang et al. (1998).

An interesting result emerging from this displacement field is that an out-of-plane polarization is expected:

\[
P_3 = - (\epsilon - \epsilon_0) \dot{f}_2 \nabla^2 u_3 = \frac{\dot{f}_2 C_3}{2a \sqrt{r} \ell} \sin \frac{\theta}{2} \quad (4.6)
\]

This polarization is independent of \( z \). This prediction could perhaps be verified in an experiment.
4.3 Planar Cracks

The solution of the asymptotic crack tip fields in Mode III involves solving a simpler problem than Mode I and Mode II. But, in the Mode III solution we saw some essential features of the crack-tip fields that will be present also for Mode I and Mode II cracks. The key difference between plane cracks of Mode I and II as opposed to Mode III is that the dilatation gradient (which is directly proportional to the hydro-static pressure gradient) induces a non-trivial electric field around plane cracks.

For simplicity, we will discuss only the plane strain version of this problem. Here we have, \( u_i = u_i(x_1, x_2), \ i = 1, 2, \ u_3 = 0 \) and \( \phi = \phi(x_1, x_2) \). Again it is easier to work in cylindrical coordinates in the planar cracks. We will follow the approach of Aravas & Giannakopoulos (2009) and obtain the asymptotic solution in the form of \( u_i = r^s F_s^{(i)}(\theta) \) and \( \phi = r^s G_s(\theta) \) and take the leading order asymptotics.

Due to flexoelectric coupling, there are four separate modes, two mechanical modes, Mode I (symmetric opening) and Mode II (anti-symmetric shear) and two electric ones, Mode D (electric loading with insulating condition) and Mode E (electric loading with conducting condition). For Mode I and Mode II we will also need to discuss the effect of two electric boundary conditions (insulating or conducting condition). Mixed type electric boundary condition is beyond the scope of this dissertation. We will also discuss the mixture of electrical and mechanical modes.

4.3.1 Mode I

For a Mode I crack we require that \( u_r(r, \theta) = u_r(r, -\theta) \) and \( u_\theta(r, \theta) = -u_\theta(r, -\theta) \). In here we do not assume any symmetric properties of \( \phi \). Without loss of generality, we can assume the following fields,

\[
\begin{align*}
  u_r &= \sqrt{\frac{-3}{\ell}} (A_1 + A_2 \cos \theta + A_0 \cos 2\theta) \cos \frac{\theta}{2}, \\
  u_\theta &= \sqrt{\frac{-3}{\ell}} (A_3 + A_4 \cos \theta - A_0 \cos 2\theta) \sin \frac{\theta}{2}, \\
  \phi &= -\frac{f}{ae} \left[ \sqrt{\frac{r}{\ell}} \left( A_5 \cos \frac{\theta}{2} + A_6 \sin \frac{\theta}{2} \right) + \Theta \right],
\end{align*}
\]
where $A_i$’s are all unknown constants. Our goal is to determine these constants by insisting that the governing equations and boundary conditions are satisfied.

Note by Eqn(2.19) that without body force, the equilibrium equation can be written as

$$
\tau_{jk,j} - \hat{\mu}_{ijk,ij} = 0.
$$

(4.10)

Suppose $p_{jk,i} = \hat{\mu}_{ijk,i}$, then to leading order of the above equation boils down to

$$
p_{rr,\theta} + r^{-1}(p_{r\theta,\theta} + p_{rr} - p_{\theta\theta}) = 0,
$$

(4.11)

$$
p_{r\theta,r} + r^{-1}(p_{\theta\theta,\theta} + 2p_{r\theta}) = 0.
$$

(4.12)

As in LEFM, here we assume traction free boundary conditions along the faces of our semi-infinite crack. So, the traction and higher order traction are both zero on the crack faces, as in Aravas & Giannakopoulos (2009). We have not put any restrictions on electric parts of the solution other than the governing equation it has to satisfy. From the traction free conditions, we find that at $\theta = \pm \pi$:

$$
\hat{Q}_r = -p_{r\theta} - \hat{\mu}_{r\theta,rr} = 0,\quad (4.13)
$$

$$
\hat{Q}_\theta = -p_{\theta\theta} - \hat{\mu}_{\theta\theta,\theta} = 0,\quad (4.14)
$$

$$
\hat{R}_r = \hat{R}_\theta = 0.\quad (4.15)
$$

The second and third of these boundary conditions boil down to

$$
\hat{Q}_\theta = -\frac{\alpha \beta \mu A_6}{4} \left( \frac{r}{\ell} \right)^{-\frac{3}{2}} = 0,\quad (4.16)
$$

$$
\hat{R}_\theta = \frac{\alpha \beta \mu \ell A_6}{2} \left( \frac{r}{\ell} \right)^{-\frac{1}{2}} = 0.\quad (4.17)
$$

Hence, if we insist on the traction-free boundary condition then $A_6$ must vanish.

Now, we turn to the electric part of the solution. By Eqn(2.45), we can write the equation to

$$
\nabla^2 (a e \phi + \hat{f} \Theta) = 0
$$

(4.18)

which is already included in Eqn(4.9). Electric field and electric displacement can be derived
accordingly. For detailed component form, please refer to the Appendix D.

In terms of the boundary conditions, one is called impermeable/insulating crack boundary condition

$$D_\theta(r, \pm \pi) = 0, \quad D_\theta(r, 0) = 0. \quad (4.19)$$

this boundary condition, as previously discussed, corresponds to the case where the dielectric constant of the crack is much larger than the medium in between the crack faces. For example, a finite crack inside a Barium Titanante with air stuffed in between cracks.

Another type of boundary condition is the pure conducting case, the boundary conditions are

$$E_r(r, 0) = 0, \quad E_r(r, \pm \pi) = 0. \quad (4.20)$$

this corresponds to the case where the medium stuffed in between is conductive. For example, if the crack inside Barium Titanante is filled with conductive liquid instead. Then we will need this type of boundary condition. Other types of boundary condition also exists and there have been different arguments over what is the correct electric boundary condition in the literature of LPFM. But these two conditions are good enough as a starting point of theoretical studies.

Before any analysis, we introduce the following non-dimensional material constants:

$$\alpha = \frac{\hat{f}_2}{\ell^2 \sqrt{a\mu}}, \quad \beta = \frac{\hat{f}/(\ell \sqrt{a\mu})}{\nu}$$

and $\nu$ the Poisson ratio. We will also use the relation $a\varepsilon \approx 1$, which is typical for solids with large dielectric constants and are the main focus of this study. Following (Aravas & Giannakopoulos 2009), we define intensity constants, $C_{11}$ and $C_{12}$, which are given by:

$$C_{11} = -\lim_{r \to 0} \frac{u_\theta(r, \pi)}{\sqrt{r^3/\ell}}, \quad C_{12} = -\lim_{r \to 0} \frac{\Omega(r, \pi)}{\sqrt{r/\ell}}. \quad (4.21)$$

Here, $\Omega$ as defined in (3.27), is the rotation of the displacement field. Two intensity constants are needed for characterizing Mode I crack whereas for LEFM, we only need one. The additional one is to account for the gradient effects. The singular behavior of all relevant quantities are summarized in the following table

Note that it is still possible to define the conventional intensity factors as in LEFM, but since the order of singularity has changed, it needs to be done in a different fashion. The
Table 4.1: Leading order terms of crack tip asymptotics in different models.

calculation is carried out in Appendix B.1.

By imposing the pure insulating boundary condition, the solution to $D_\theta$ is:

$$
\frac{D_\theta}{\sqrt{\mu/\epsilon}} = \frac{\alpha(3C_{11} - 2C_{12})}{8(1 - \alpha^2)} \left(\sin \frac{\theta}{2} + \sin \frac{3\theta}{2}\right) \sqrt{\frac{\ell}{r}}.
$$

(4.22)

Note that the $D_\theta$ component of electric displacement is 0 behind and ahead of the crack tip. Even though $D_\theta$ vanishes, the corresponding electric field component at $\theta = \pm \pi$ does not:

$$
\frac{E_\theta(r, \pi)}{\sqrt{\mu/\epsilon}} = \frac{(3C_{11} - 4C_{12})(2\nu - 1)\beta + 4C_{12}(1 - \nu)\alpha}{4(1 - \nu)} \sqrt{\frac{\ell}{r}}.
$$

(4.23)

If pure conducting boundary condition is imposed instead, we have the following

$$
\frac{E_r(r, \theta)}{\sqrt{\mu/\epsilon}} = \frac{(3C_{11} - 2C_{12})}{16\sigma} \beta \left(\cos \frac{\theta}{2} - \cos \frac{3\theta}{2}\right) \sqrt{\frac{\ell}{r}},
$$

(4.24)

where $\sigma = (1 - \nu)/(1 - 2\nu)$ is a material constant which we used for the edge dislocation. Along the crack faces, $E_\theta(r, \pi)$ is given by

$$
\frac{E_\theta(r, \pi)}{\sqrt{\mu/\epsilon}} = \frac{\beta(3C_{11} - 4C_{12})}{4\sigma} \sqrt{\frac{\ell}{r}}.
$$

(4.25)

The fact that the electric field perpendicular to the crack face does not vanish and is proportional to $1/\sqrt{r}$ asymptotically is of interest. Imagine a steadily growing crack so that, $r = r(t)$ and $E_\theta$ is a function of time $t$ as well. If the crack is moving quasistatically along the $x_1$ axis at a slow speed $\dot{r}(t)$, then we know $\dot{E}_\theta \propto r^{-3/2}\dot{r}(t)$. According to the Maxwell equations, this will induce a magnetic field. Hence a growing crack in a flexoelectric solid
will emit radiation. This was observed in a series of experiments by Petrenko and co-workers for cracks in ice, as documented in Petrenko (1996). The simple model they used postulated that the electric field is proportional to the hydro-static pressure gradient. In our analysis it is the flexoelectric coupling constant \( \hat{f} \) that relates them. Hence, the experiments carried out by Petrenko and co-workers strongly support their idea that “pseudo-piezoelectricity” (or flexoelectricity) is responsible for radiation emitted from sliding glaciers.

However, unlike in the work of Petrenko (1996) who simply use the results from LEFM to deduce the potential field, here we have provided a solution that satisfies both the mechanical and electrical governing equations. We see that the field produced around the crack tip is indeed asymptotically similar to that in the piezoelectric case, both \( r^{-1/2} \).

However, ice is not piezoelectric, so the flexoelectric effect could very likely be the cause behind the effects seen by Petrenko and co-workers. Aside from the postulates about the coupling between the gradients of hydrostatic pressure/dilatation and polarization, there are also couplings that come from the gradients of shear stresses/strains which are also prominent around the crack tip and included in our analysis.

### 4.3.2 Mode II

For a Mode II crack we require that \( u_r(r, \theta) = -u_r(r, -\theta) \) and \( u_\theta(r, \theta) = u_\theta(r, -\theta) \). Without loss of generality, we can assume the following:

\[
u_r = \sqrt{\frac{r^3}{\ell}} (B_1 + B_2 \cos \theta + B_0 \cos 2\theta) \sin \frac{\theta}{2},
\]

\[
u_\theta = \sqrt{\frac{r^3}{\ell}} (B_3 + B_4 \cos \theta + B_0 \cos 2\theta) \cos \frac{\theta}{2},
\]

\[
\phi = -\frac{\hat{f}}{ae} \left[ \sqrt{\frac{\tau}{\ell}} \left( B_5 \sin \frac{\theta}{2} + B_6 \cos \frac{\theta}{2} \right) + \Theta \right],
\]

where \( B_i \)'s are all unknown constants. In order to find all \( B_i \)'s we carry out the same calculations as in the Mode I case. The crack faces \( \theta = \pm \pi \) are again assumed to be free of tractions and higher order tractions. At \( \theta = 0 \) we assume that all the fields are continuous.
Again, due to the traction free boundary conditions:

\[ \hat{Q}_r = -\frac{\beta^2 \mu B_6}{4} \left( \frac{r}{l} \right)^{\frac{3}{2}} = 0, \quad (4.29) \]
\[ \hat{R}_\theta = \frac{\beta^2 \mu \ell B_6}{2} \left( \frac{r}{l} \right)^{\frac{1}{2}} = 0, \quad (4.30) \]

so that \( B_6 = 0 \). For the same reason as in Mode I, the displacement field can be fully determined by the following intensity constants to \( C_{21} \) and \( C_{22} \):

\[ C_{21} = \lim_{r \to 0} \frac{\varepsilon_{\theta r} (r, \theta = 0)}{\sqrt{r/l}}, \quad C_{22} = -\lim_{r \to 0} \frac{\Omega (r, \theta = 0)}{\sqrt{r/l}}. \quad (4.31) \]

Now, consider the pure insulating and pure conducting crack boundary conditions just as we did in Mode I. For the pure insulating case, we have the following solution for \( D_\theta \):

\[ \frac{D_\theta (r, \theta)}{\sqrt{\mu \varepsilon}} = -\frac{\alpha C_{21}}{1 + \alpha^2 (2\nu - 3)} \left( \cos \frac{\theta}{2} - \cos \frac{3\theta}{2} \right) \sqrt{\frac{\ell}{r}}. \quad (4.32) \]

For the pure conducting case, we have:

\[ \frac{E_r (r, \theta)}{\sqrt{\mu \ell}} = \frac{\alpha C_{21} (1 - \alpha^2) \beta (2\nu - 1)}{2 + 2\alpha^2 (2\nu - 3)} \left( \sin \frac{\theta}{2} + \sin \frac{3\theta}{2} \right) \sqrt{\frac{\ell}{r}}. \quad (4.33) \]

### 4.3.3 Mode D and Mode E

Just as in Mode I and Mode II cracks, the displacement fields for Mode D (insulating, zero traction) and Mode E (conducting, zero traction) are determined by \( C_{ij}, i, j = 1, 2 \).

Generally, when a crack is conducting, we define the electric field intensity factor \( K_E \) as:

\[ K_E = \lim_{r \to 0} \sqrt{2\pi r} E_r (r, 0). \quad (4.34) \]

For insulating cracks we define \( K_D \) as:

\[ K_D = \lim_{r \to 0} \sqrt{2\pi r} D_\theta (r, 0). \quad (4.35) \]
The boundary conditions for Mode D are at \( \theta = 0 \)

\[
\hat{Q}_\theta = \hat{Q}_r = 0, \quad D_\theta = \frac{K_D}{\sqrt{2\pi r}},
\]

\[
\hat{R}_r = \hat{R}_\theta = 0.
\]  

This is the case in which the relevant stresses and higher-order stresses are zero along crack line, therefore The sole contribution to the J integral comes from the electrical part. All of the above lead to:

\[
C_{11} = C_{12} = C_{21} = 0, \quad (4.38)
\]

\[
C_{22} = \frac{K_D}{\sqrt{2\pi \mu \ell}} \left[ 2\alpha(1 - \nu) - \beta(1 - 2\nu) \right].
\]  

The boundary conditions for Mode E are, at \( \theta = 0 \):

\[
\hat{Q}_\theta = \hat{Q}_r = 0, \quad E_r = \frac{K_E}{\sqrt{2\pi r}},
\]

\[
\hat{R}_r = \hat{R}_\theta = 0.
\]  

On the crack faces, \( \theta = \pm \pi \), traction and higher-order traction are zero and \( E_r = 0 \). These conditions give:

\[
C_{21} = C_{22} = 0, \quad (4.42)
\]

\[
C_{11} = \frac{(K_E/3)}{\sqrt{2\pi \mu \ell/\epsilon}} \left[ \frac{2\alpha(1 - \nu) - \beta(1 - 2\nu)}{1 - \alpha^2 - (1 - 2\nu)(\beta - \alpha)^2} \right], \quad (4.43)
\]

\[
C_{12} = \frac{(K_E/2)}{\sqrt{2\pi \mu \ell/\epsilon}} \left[ \frac{2\alpha(1 - \nu) - \beta(1 - 2\nu)}{1 - \alpha^2 - (1 - 2\nu)(\beta - \alpha)^2} \right].
\]  

4.3.4 Mixed modes

The classification above separates mechanical and electrical boundary loads. In practice, when we are dealing with cracks in electromechanically active materials, it is difficult to completely separate mechanical modes and electrical modes. As mentioned in a recent review by Kuna (2010) of closely related piezoelectric fracture, “mechanical and electrical quantities are inherently coupled at the crack” and “there is always a mixture of (mechanical
and electrical) crack opening modes”. For this reason we give some results on mixed modes below.

Recall the boundary conditions of the pure conducting case which result in $K_E = 0$, and the pure insulating case which result in $K_D = 0$. Now, let us imagine a crack under Mode I loading. From the fact that $A_6 = 0$ (traction-free faces), we know that $D_\theta (r, 0) = 0$ before we impose any electric boundary condition (as discussed in Mode I pure insulating crack). Also, recall that in Mode D all constants related to Mode I, i.e. $C_{11}, C_{12}$ are zero. This means that in a flexoelectric solid, Mode I cannot be mixed with Mode D (under the traction free faces assumption). If we forcefully introduce Mode D together with Mode I, then $C_{22}$ will be non-zero, and the crack will have a Mode II component too. A similar argument shows that Mode II cannot be mixed with Mode E under the current framework.

On the other hand, since the Mode I solution does not exclude the possibility of non-zero $K_E$, we can have a crack in which Mode I pure conducting conditions are mixed with Mode E. Then, the boundary condition is different from that of the Mode I pure conducting case, viz.,

$$E_r(r, \pm \pi) = 0, \quad E_r(r, 0) = \frac{K_E}{\sqrt{2\pi r}}.$$  \hspace{1cm} (4.45)

We have computed the strain profiles for this boundary condition. For the purposes of illustration we picked a particular set of material parameters: $\alpha = 0.5, \beta = 0.6, \nu = 0.3$. Then, the strain profile is

$$\varepsilon_{rr} = \left[ (0.009C_{11} - 0.11C_{12} + 0.21K_4^1) \cos \frac{\theta}{2} + (0.76C_{11} + 0.51C_{12}) \cos \frac{3\theta}{2} \right] + \left[ (1.04C_{11} - 0.87C_{12} - 0.043K_4^1) \frac{5\theta}{2} \sqrt{\frac{r}{\ell}} \right],$$

$$\varepsilon_{r\theta} = \left[ (-0.043C_{11} + 0.098C_{12} - 0.24K_4^1) \sin \frac{\theta}{2} + (0.56C_{11} - 0.37C_{12}) \sin \frac{3\theta}{2} \right] + \left[ (0.87C_{11} - 0.043C_{12} - 1.04K_4^1) \frac{5\theta}{2} \sqrt{\frac{r}{\ell}} \right],$$

$$\varepsilon_{\theta\theta} = \left[ (0.21C_{11} - 0.60C_{12} + 0.13K_4^1) \cos \frac{\theta}{2} + (0.55C_{11} - 0.37C_{12}) \cos \frac{3\theta}{2} \right] + \left[ (-1.04C_{11} + 0.87C_{12} + 0.043K_4^1) \cos \frac{5\theta}{2} \sqrt{\frac{r}{\ell}} \right].$$

These are plotted in Fig.4.1(a) for $r = \ell$. Notice that instead of using $K_E$ we introduce, for convenience, an non-dimensinal constant $K_4^1$, which is a linear combination of $C_{11}, C_{12}$ and
$K_E$ (detailed expression in Appendix B.1). It is defined as

$$K^I_4 = \lim_{r \to 0} \frac{r}{\mu \epsilon \ell} D_\theta (r, \pi). \quad (4.49)$$

We also compute true stress $\sigma_{22}$ (as defined in Aravas (2011)) for the above mentioned material parameters, as depicted in Fig.4.1(b). The similarity between the SGE solution and the flexoelectric solution is clear. Interestingly enough, the $\sigma_{22}$ plot suggests compression just behind the crack tip, a feature also observed by Aravas & Giannakopoulos (2009).

For the same material parameters the strain profile for a Mode II pure insulating crack mixed with Mode D is

$$\varepsilon_{rr} = \left[ (-0.03 C_{21} + C_{22} - 0.63 K^{II}_4) \sin \frac{\theta}{2} - 2.67 \sin \frac{3\theta}{2} + (2.61 C_{21} + 0.125 K^{II}_4) \sin \frac{5\theta}{2} \right] \sqrt{\frac{r}{\ell}}, \quad (4.50)$$

$$\varepsilon_{r\theta} = \left[ (-0.34 C_{21} - 0.13 K^{II}_4) \cos \frac{\theta}{2} - 1.95 C_{21} \cos \frac{3\theta}{2} + (2.61 C_{21} - 0.13 K^I_4) \cos \frac{5\theta}{2} \right] \sqrt{\frac{r}{\ell}}, \quad (4.51)$$

$$\varepsilon_{\theta\theta} = \left[ (-0.72 C_{21} + C_{22} - 0.38 K^{II}_4) \sin \frac{\theta}{2} + 1.92 \sin \frac{3\theta}{2} - (2.61 C_{21} + 0.13 K^{II}_4) \sin \frac{5\theta}{2} \right] \sqrt{\frac{r}{\ell}}. \quad (4.52)$$

Here again, for convenience, a non-dimensionalized intensity $K^{II}_4$ is used instead of $K_D$:

$$K^{II}_4 = K_D / \sqrt{2\pi \mu \epsilon \ell}. \quad (4.53)$$

As discussed in the beginning of this section, Mode II cannot be mixed with Mode E.

Notice that we have not used the conventional intensity factors $K_1$, $K_{11}$ etc., because their expressions are lengthy and cumbersome. However, those conventional intensity factors can be written in terms of $C_{11}, C_{12}, K^I_4$ and $C_{21}, C_{22}, K^{II}_4$ as shown in the Appendix B.1. Using the constants defined above we can work out the displacement, strain and stress profiles. The expressions are long and are not reproduced here.
Figure 4.1: In this figure, it plots in a) the angular profile of strain at $r = \ell$ and in b) the $\sigma_{22}$ at $\theta = \pi/2$ for a Mode I & Mode E crack with $K_1^I = 1.0$. Material constants are $\alpha = 0.5$, $\beta = 0.6$, $\nu = 0.3$. The intensity factors are from Tsantidis & Aravas (2011) and kept at a constant energy release rate for flexoelectric cases.

4.4 J integral

In analogy to piezoelectricity, the flexoelectric energy momentum tensor can be written as

$$Q_{ik} = H\delta_{ik} - \tau_{ij}u_{j,k} - \hat{\mu}_{ijk}u_{l,jk} - D_i\phi_{,k}, \quad (4.54)$$

where $H$ is the enthalpy of the system defined as:

$$dH = \tau_{ij}d\varepsilon_{ij} + \hat{\mu}_{ijk}d\varepsilon_{jk,i} - D_i dE_i. \quad (4.55)$$

The J integral $J_k$ is related to $Q_{ik}$ through

$$J_k = \lim_{\varepsilon \to 0} \int_{\Gamma_\varepsilon} Q_{ik}n_i ds, \quad (4.56)$$

where $\Gamma_\varepsilon$ is a closed contour around the crack tip whose outward normal is $n$. The J integral is path independent, so any curve that includes the crack tip would yield same result. But, we take $\varepsilon \to 0$ since we use an asymptotic solution which is only valid near the crack tip.

We are interested in $J_1$, which is the energy release rate. It can be computed by using any closed contour around the crack tip. One such contour consists of an infinitesimally
small closed circle that goes to the crack face, as shown in Fig. 4.2. Another one is the box contour as in Aravas & Giannakopoulos (2009), also shown in Fig. 4.2. Let us start with the circular contour for the Mode III crack. Using the constitutive relations, $J_{I}^{III}$ has the following relation with $u_3$:

\begin{align}
J_{I}^{III} &= \frac{G}{2} \lim_{r \to 0} \int_{-\pi}^{\pi} \left\{ (u_{3,2}^2 - u_{3,1}^2) \cos \theta - 2u_{3,1}u_{3,2} \sin \theta \\
&+ \ell^2 \left[ (\nabla^2 u_3)^2 \cos \theta + 2u_{3,1}(\nabla^2 u_3),r - 2u_{3,1,r} \nabla^2 u_3 \right] \right\} r \, d\theta.
\end{align}

By substituting our asymptotic solution into the integral for $J_{I}^{III}$ we find that

$$J_{I}^{III} = 2\pi \mu \ell C_3^2 (1 - \alpha^2)(3 - 4\alpha^2) \geq \pi \mu \ell C_3^2.$$  

This is a positive quantity, exactly as shown by Rice & Drucker (1967) in LEFM. In what follows we show that the form of the energy release rate for Mode I and Mode II cracks in flexoelectric solids is similar to that in piezoelectric materials. The constant $C_3$ above is a function of the material constants and is related to the stress intensity $K_{III}$. In the limiting case of $\alpha, \beta, \ell \to 0$ we know that

$$\lim_{\alpha, \beta, \ell \to 0} J_{I}^{III} = \frac{K_{III}^2}{2\mu}.$$  

Thus, if we remove all the SGE and flexoelectric effects from the material, the energy release rate converges to the results from linear elastic fracture mechanics. Now, for an infinite medium with a semi-infinite crack, we know that far away from the crack tip the
fields should be the same as those of linear elasticity. Hence, by using the path independence of the J integral we can write

\[ C_3 = \frac{K_{III}}{2\mu\sqrt{\pi\ell}} \left[ (1 - \alpha^2)(3 - 4\alpha^2) \right]^{-\frac{1}{2}}. \] (4.60)

In the case of \( \alpha \to 0 \), we get

\[ C_3 = \frac{K_{III}}{2\mu\sqrt{3\pi\ell}}, \] (4.61)

which recovers the result of Zhang et al. (1998) using couple stress theory, except that they used a length scale that is half of our’s.

An alternative way of calculating J integral is to use the box contour as in Freund (1972). For planar cracks, this can be written as

\[ J_1 = -2 \lim_{\varepsilon \to 0} \int_{-\varepsilon}^{\varepsilon} \left[ \hat{Q}_1 u_{1,1} + \hat{Q}_2 u_{2,1} + \hat{\mu}_{221} u_{1,12} + \hat{\mu}_{222} u_{2,12} + D_2 \phi_1 \right] \bigg|_{x_2=0^+} dx_1. \] (4.62)

For Mode I purely insulating(ID) and purely conducting(IE) conditions, the J-integrals are respectively given by:

\[ J_{1,ID} = \frac{\mu\pi\ell}{16(1-\nu)} \left[ \frac{(5 - 4\nu) - (7 - 6\nu)\alpha^2}{1 - \alpha^2} (3C_{11} - 2C_{12})^2 + 8C_{12}^2 \right], \] (4.63)

\[ J_{1,IE} = \mu\pi\ell \left[ \frac{(5 - 4\nu) - (7 - 6\nu)\alpha^2}{16(1-\nu)(1-\alpha^2)} (3C_{11} - 2C_{12})^2 + \frac{1 - \alpha^2 - (\alpha - \beta)^2(1 - 2\nu)}{1 + (1 - 2\nu)(1 - \beta^2)} C_{12}^2 \right]. \] (4.64)

For Mode II purely insulating(IID) and purely conducting conditions(IIE), they are respectively:

\[ J_{1,IID} = \mu\pi\ell \left[ \frac{4(1 - \alpha^2)(1 - \nu) \left[ (5 - 4\nu) - (7 - 6\nu)\alpha^2 \right] C_{21}^2}{(2\alpha^2\nu - 3\alpha^2 + 1)^2} + \frac{C_{22}^2}{1 - 2\nu} \right], \] (4.65)

\[ J_{1,IIE} = \mu\pi\ell(1 - \alpha^2) \left[ \frac{4(1 - \nu) \left[ (5 - 4\nu) - (7 - 6\nu)\alpha^2 \right] C_{21}^2}{(2\alpha^2\nu - 3\alpha^2 + 1)^2} + \frac{1 - \alpha^2 - (\alpha - \beta)^2(1 - 2\nu)}{(1 - \alpha\beta)(1 - 2\nu)} C_{22}^2 \right]. \] (4.66)

The above expressions, in the limiting case of \( \alpha, \beta \to 0 \), reduce to the results of Aravas & Giannakopoulos (2009).
For Mode D:
\[ J_1^D = \frac{K_D^2}{2\varepsilon} \left[ 1 - \alpha^2 - (1 - 2\nu)(\beta - \alpha)^2 \right], \tag{4.67} \]
and for Mode E:
\[ J_1^E = \frac{\varepsilon K_E^2}{2} \left[ 1 - \alpha^2 - (1 - 2\nu)(\beta - \alpha)^2 \right]^{-1}. \tag{4.68} \]

For the mixed modes, Mode I & Mode E we have:
\[ J_{IE}^1 = \frac{\mu \pi \ell}{16(1 - \nu)} \left[ \frac{(5 - 4\nu) - (7 - 6\nu)\alpha^2}{1 - \alpha^2} (3C_{11} - 2C_{12})^2 + 8C_{12}^2 - 8(2 - \beta^2 - 2\nu + 2\beta^2\nu)(K_{11}^I)^2 \right], \tag{4.69} \]
and for Mode II & Mode D:
\[ J_{II&D}^1 = \mu \pi \ell \left\{ \frac{4(1 - \alpha^2)(1 - \nu)\left[ (5 - 4\nu) - (7 - 6\nu)\alpha^2 \right] C_{21}^2}{(2\alpha^2\nu - 3\alpha^2)^2} + \frac{(C_{22} - \alpha K_{II}^I)^2}{1 - 2\nu} - (1 - \alpha^2)(K_{II}^I)^2 \right\}. \tag{4.70} \]

There are a few points that we note. First, unlike Mode III, the planar cracks have more intensity constants resulting from SGE, \( C_{11}, C_{12} \), or \( C_{21}, C_{22} \). Just as in Aravas & Giannakopoulos (2009) for the case of SGE cracks, these intensity factors are needed to characterize the fracture behavior. For example, \( C_{12} \) can be a good measure of the rotation intensity factor at the crack face. Second, in the mixed modes, flexoelectricity reduces the energy release rate compared to the SGE crack. We also note that the form of the above equations is similar to those for piezoelectric materials, where the electric intensity also reduces the energy release rate of a crack.

### 4.5 Fracture criterion

The present asymptotic analysis serves as a staring point for the study of crack propagation, but with some limitations. In our cases, the asymptotics is only valid within a region around the crack tip that is on the order of the flexoelectric length scale or the SGE length scale. We will apply some simple fracture criteria using the asymptotic solution.

As a well-known example, we recall the classical Griffith postulate regarding a critical energy release rate \( G_c \) for the crack to advance Griffith (1921)

\[ J_1 = G_c. \tag{4.71} \]
Figure 4.3: The COD profile of mixed Mode I & Mode E cracks with different values of $K_E$. $K_E$ is normalized against $\sqrt{2\pi\mu/\epsilon}$. Other normalized intensity factors are from Tsantidis & Aravas (2011) so as to keep the energy release rate fixed.

With the equations for various $J_1$ on hand, it is possible to connect flexoelectric parameters at the crack tip to the far field quantities that can be measured to calculate $J_1$. For example, in the mixed Mode I & Mode E crack, we have $J_1 = f(C_{11}, C_{12}, K_I^4) = \hat{f}(C_{11}, C_{12}, K_E)$, so fracture criteria of this type can be written as:

$$\hat{f}(C_{11}, C_{12}, K_E) - G_c = 0.$$  \hspace{1cm} (4.72)

We recall the above criterion resembles that in piezoelectric materials Schneider (2007), except that the function $\hat{f}$ for piezoelectrics depends on only two constants, while for flexoelectric materials we have three. In both mixed modes, flexoelectricity tends to reduce the energy release rate. Hence, with the same $G_c$ it requires more loading/energy to achieve the minimum condition for the crack to advance/grow if the material is flexoelectric versus when it is not.

Another important criterion for crack propagation depends on the crack opening displacement (COD). According to Aravas & Giannakopoulos (2009), the small-scale cohesive zone assumed by Barenblatt (1962) can be well modeled by the cusp-like curve of the COD produced by the SGE asymptotic analysis. Similarly, the flexoelectric COD criterion for
Figure 4.4: This figure plots the electric yielded zone near crack tips for a) Mode I & Mode E crack, (b) Mode II & Mode D crack. In both cases, $\overline{D}_{Y} = 1.0$ and the crack tip is located at $x = 0$. All material constants are the same as those in Fig.4.1 and Fig.4.3. Notice the similarity of the shape of the electric yielded zone with that of the plastic yielded zone for these cracks.

crack propagation can be worked out as

$$\text{COD} \approx 2u_{1}(\ell, \pi) = 2C_{11} \ell = \delta_{c}. \quad (4.73)$$

where $\delta_{c}$ is some critical crack opening displacement. In the above equation only $C_{11}$ is explicitly involved. This is in contrast to the energy release rate criterion in which all three intensity factors are involved. Hence, measuring the COD could be a more practical way of determining the critical condition for crack growth. Recall that the critical opening for propagation of the crack is $\delta_{c}$ which is a material property. As mentioned in Aravas & Giannakopoulos (2009), the critical value $C_{11c}$ could serve as the measure which determines when crack growth occurs without assuming the length of the cohesive zone. The parameter $C_{11}$ in SGE can be calculated through finite element simulation of a finite crack. But, in order to illustrate the applicability of this idea to flexoelectric materials we adopt a data set obtained from Tsantidis & Aravas (2011) as a zero order approximation and hold the loading/energy release rate fixed. We want to see how $C_{11}$ changes if we change $K_{E}$. This is shown in Fig.4.3. From this figure it is apparent that for larger $K_{E}$ we need to supply more energy in order to achieve the critical COD at a given $r$ and cause the crack to grow.
Lastly, a flexoelectric material is a dielectric, therefore failure also arises from the electric properties of the material. For example, since \( K_E \) or \( K_D \) is itself a measurable quantity, a simple failure condition could be:

\[
K_E = K_{Ec}
\] (4.74)

where \( K_{Ec} \) is a critical intensity factor for the electric field (governed, for example, by the condition for electric breakdown).

Since the electric displacement field is singular near the crack tip we can expect some non-linearity to overwhelm the linear constitutive laws much like the plastic zone in small-scale yielding. As advocated by Gao et al. (1997), a simple non-linear model of ferroelectric solids behaves like an elastic-perfectly plastic material where the stress stays the same irrespective of strain after reaching a yield stress. For the simple non-linear ferroelectric the electric displacement stays the same irrespective of the increasing electric loads. Just like the plastic zone in small-scale yielding we will have a zone around the crack in a flexoelectric solid in which the electric displacement is a constant, so that

\[
\frac{D_1^2 + D_2^2}{\mu \epsilon} = \tilde{D}_Y^2,
\] (4.75)

where \( \tilde{D}_Y \) is a non-dimensional yielding electric displacement parameter. Electric yielding of this type is an important aspect of piezoelectric fracture as pointed out in Gao et al. (1997), Wang (2000), Schneider (2007), Kuna (2010). Similar to the plastic zone in elasticity, this phenomenon protects the material from singularities in the presence of a crack. The electric yielded zones of mixed modes cracks are shown in Fig.4.4. These zones are associated with phase transition and domain switching, an analysis of which is beyond the scope of this work.

### 4.6 Concluding remarks

This chapter is devoted to asymptotic solutions for crack tip fields in flexoelectric solids. While there is a wealth of literature on cracks in piezoelectrics, little is known about cracks in flexoelectric materials. Our’s is a first attempt to learn something about the nature of singularities near cracks in flexoelectric solids. The usual \( r^{1/2} \) singularity of the displacement
in both LEFM and LPFM is replaced by higher order $r^{3/2}$ singularity due to gradient effects. Gradient effects also introduce new intensity factors which could not be computed in our analysis. Using the finite element methods in the following chapters, this is amendable. To fully characterize the fracture behavior, these intensity factors are crucial. The crack opening profile is also altered from the classical parabolic shape to a cusp-like one. By employing the J integral, we found that, similar to piezoelectric solids, electric coupling reduces the energy release rate so that more energy must be supplied in order for a crack to grow. There are four separate modes of flexoelectric cracks, depending on the boundary conditions. Mixing Mode I and Mode D or Mode II and Mode E will result in a change of the symmetric properties of the asymptotic deformation fields.
Chapter 5

Finite Element Analysis

5.1 Introduction

In the preceding chapters we have discussed a theoretical continuum framework that can be used for solutions of useful boundary value problems. We have looked at beam bending, torsion, axis-symmetric problems and even problems with strong discontinuity, like defects and cracks. But still our understanding towards flexoelectricity in complex geometries is still limited and there is a demand that a finite element computational tool be developed for this purpose.

Finite element studies have also been conducted by Abdollahi et al. (2014), Abdollahi, Peco, Millán, Arroyo, Catalan & Arias (2015), Abdollahi, Millán, Peco, Arroyo & Arias (2015), Abdollahi & Arias (2015). They studied several non-trivial geometries, e.g. beam and truncated pyramid structures, which have been extensively used for experimental measurements. Their studies have led to important insights. For example, the non-uniform strain-gradient distribution in a truncated-pyramid around sharp edges significantly influences the measurements of flexoelectric constants. To use the finite element method with piecewise continuous shape functions to solve problems for flexoelectric solids one must confront the difficulties arising from higher-order differential equations. Abdollahi et al. avoided the use of these piecewise continuous functions by applying a mesh-free technique. For 2D problems they needed to discretize only three degrees of freedom, so their method is computationally efficient. In contrast, our approach still uses the shape function, so it
is compatible with the framework of a majority of the current finite element codes. Our method can be easily incorporated into software packages such as ABAQUS. Therefore, it can be used by non-expert engineers for the analysis of complex geometries.

In this chapter, we will introduce a general framework for finite element solutions of problems for an elastic dielectric with flexoelectricity and/or piezoelectricity. The generalized gradient theory developed by Mindlin (1964) is used to model the gradient effect of elasticity. Piezoelectric as well as flexoelectric coupling are introduced into the formulation by adding polarization as a variable in the energy storage function. The energy storage function depends on the strain tensor, second gradient of displacement, and polarization. To avoid using $C^1$ finite elements in our numerical solution, a mixed formulation based on the work of Amanatidou & Aravas (2002) is developed. In this formulation, displacement and displacement gradient are treated as separate degrees of freedom and their relationship is enforced in the variational form. This framework is entirely consistent with the continuum theory of flexoelectricity and is capable of capturing fine structures due to gradient effects. The finite element code is validated against benchmark problems with known analytical solutions. Then it is employed to study three important classes of problems: plate with an elliptical hole, stationary crack, and periodic metastructures. In the static crack problem, for which an asymptotic solution has been developed in Chapter 4, the validity and region of dominance of the asymptotics is determined. The elliptical hole and periodic structure provide an alternative means of generating large strain gradients; the finite element results show how these large gradients influence classical observations and generate crucial insights that can lead to better measurement in experiments as well as improved functionality in applications.

### 5.2 Constitutive model

Here we follow the problem set up like in Chapter 2. A fixed Cartesian coordinates is introduced with orthonormal basis $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ and spatial coordinates given as $(x_1, x_2, x_3)$. The body occupies a region $\mathcal{V}$ in a fixed reference configuration with boundary $\partial \mathcal{V}$ and outward unit normal vector $\mathbf{n}$.

The constitutive model in this chapter is slightly different but equivalent to that used in
the preceding chapters. Here we use the Type I gradient elasticity model. It is is based on
an energy function per unit volume $\tilde{W}_L$, which depends on the infinitesimal strain tensor $\varepsilon$
and the second gradient of displacement $\tilde{\kappa} = \nabla(\nabla \mathbf{u})$ (i.e., $\tilde{W}_L = \tilde{W}_L(\varepsilon, \tilde{\kappa}, \mathbf{P})$).
We notice that the difference is between strain gradients and double displacement gradients.
It is shown in Mindlin (1964) that these two are totally equivalent to each other. Quantities
associated with SGE (Type II) have been denoted by $\hat{\cdot}$ and those with Type I will generally
be denoted by $\tilde{\cdot}$.

Now the corresponding constitutive equations for the Cauchy stress $\sigma^{(0)}$, the double-
stress $\tilde{\mu}$ (conjugate of $\tilde{\kappa}$) and the electric field $\mathbf{E}$ are:

$$\sigma_{ij}^{(0)} = \frac{\partial \tilde{W}_L}{\partial \varepsilon_{ij}}, \quad \tilde{\mu}_{ijk} = \frac{\partial \tilde{W}_L}{\partial \tilde{\kappa}_{ijk}}, \quad E_i = \frac{\partial \tilde{W}_L}{\partial P_i}. \quad (5.1)$$

Following Toupin (1956) we write the variation of the electric enthalpy in the form

$$\delta W^{\text{int}} = \int_V \delta \left( \tilde{W}_L(\varepsilon, \tilde{\kappa}, \mathbf{P}) - \frac{1}{2} \varepsilon_0 \phi_i \phi_i + P_i \phi_i \right) dV =$$

$$= \int_V \left[ \sigma_{ij}^{(0)} \delta \varepsilon_{ij} + \tilde{\mu}_{ijk} \delta \tilde{\kappa}_{ijk} + (E_i + \phi_i) \delta P_i + (-\varepsilon_0 \phi_i + P_i) \delta \phi_i \right] dV, \quad (5.2)$$

where $\phi$ is the electric potential associated with the dielectric and $\varepsilon_0$ the permittivity of vacuum. The above expression is general and can be used to include other gradient effects
like Mindlin (1968). The virtual work of the external sources can be written as

$$\delta W^{\text{ext}} = \int_V b_i \delta u_i dV + \int_V \tilde{Q}_i \delta u_i dS + \int_{\partial V_R} \tilde{R}_i \delta (u_{ij} n_j) dS + \sum_{\beta} \int_{\partial V_{\beta}} \tilde{T}_i \delta u_i ds -$$

$$- \int_V q_e \delta \phi dV - \int_{\partial V_{\omega}} \tilde{\omega} \delta \phi dS, \quad (5.3)$$

where $\mathbf{b}$ is the body force per unit volume, $q_e$ the free charge per unit volume, $(\tilde{Q}, \tilde{R}, \tilde{T})$
are generalized forces, and $\tilde{\omega}$ is the surface charge density. The boundary integrals on $C_T^\beta$
are included in Eqn(5.3) when the outer surface $\partial V$ is piecewise smooth; in such a case, the
surface $\partial V$ can be divided into a finite number of smooth surfaces $\partial V^\beta$ ($\beta = 1, 2, \ldots$) each
bounded by an edge $C^\beta = C_u^\beta \cup C_T^\beta$ ($C_u^\beta \cap C_T^\beta = \emptyset$).
5.3 The boundary value problem

The field equations of the corresponding boundary value problem are

\[
\left(\sigma_{ji}^{(0)} - \tilde{\mu}_{kij,k}\right)_{,j} + b_i = 0, \quad (5.4)
\]
\[
D_i, i = q_e, \quad (5.5)
\]
\[
E_i = -\phi, i, \quad (5.6)
\]
\[
D_i = \varepsilon_0 E_i + P_i, \quad (5.7)
\]

where \(D\) is the electric displacement (not to be confused with the “surface gradient” operator \(D^s\) used in the following). The corresponding boundary conditions are

\[
u_i = \tilde{u}_i \quad \text{on} \ \partial V_u, \quad (5.8)
\]
\[
\left(\sigma_{ji}^{(0)} - \tilde{\mu}_{kij,k}\right) n_j + \left[(D^s_i n_p) n_k - D^s_k\right] (n_m \tilde{\mu}_{mk}^i) = \tilde{Q}_i \quad \text{on} \ \partial V_Q, \quad (5.9)
\]
\[
D^n u_i = \tilde{d}_i \quad \text{on} \ \partial V_d, \quad (5.10)
\]
\[
n_j n_k \tilde{\mu}_{jki} = \tilde{R}_i \quad \text{on} \ \partial V_R, \quad (5.11)
\]
\[
u_i = \tilde{v}_i \quad \text{on} \ \partial V_u, \quad (5.12)
\]
\[
[[\ell_j n_k \tilde{\mu}_{jki}]] = \tilde{T}_i \quad \text{on} \ C^\beta_u, \quad (5.13)
\]
\[
\phi = \tilde{\phi} \quad \text{on} \ \partial V_\phi, \quad (5.14)
\]
\[
D_i n_i = -\tilde{\omega} \quad \text{on} \ \partial V_\omega, \quad (5.15)
\]

where \((\tilde{u}, \tilde{Q}, \tilde{d}, \tilde{R}, \tilde{v}, \tilde{T}, \tilde{\phi}, \tilde{\omega})\) are known functions, \(D^n = n \cdot \nabla = n_i \frac{\partial}{\partial x_i}\) is the normal derivative, \(D^s = \nabla - n D^n\) the “surface gradient” on \(\partial V\), \(\partial V_u \cup \partial V_Q = \partial V_d \cup \partial V_R = \partial V_\phi \cup \partial V_\omega = \partial V\), and \(\partial V_u \cap \partial V_Q = \partial V_d \cap \partial V_R = \partial V_\phi \cap \partial V_\omega = \emptyset\). The double brackets \([[]\text{]}\) indicate the jump in the value of the enclosed quantity across \(C^\beta\), and \(\ell = s \times n\), where \(s\) is the unit vector tangent to \(C^\beta\).

5.4 A variational formulation

Following the works of Amanatidou & Aravas (2002), Yang (1992), Yang & Batra (1995) we can show that the boundary value problem defined in Section 5.3 can be formulated
alternatively by the stationarity condition $\delta \Pi = 0$ of the functional

$$
\Pi \left( u, \alpha, \tilde{\sigma}^{(2)}, \phi, P \right) = \int_V \left[ \tilde{W}_L \left( u_{(i,j)}, \tilde{\kappa}(\alpha), P \right) - \frac{1}{2} \varepsilon_0 \phi, i \phi, i + P_i \phi, i \right] d\mathcal{V} + 
$$

$$
+ \int_V \left( u_{i,j} - \alpha_{ij} \right) \tilde{\sigma}^{(2)}_{ij} d\mathcal{V} + \int_{\partial \mathcal{V}} \left( D_j^t u_i - \alpha_{ij}^t \right) n_k \tilde{\mu}_{kji}(u, \alpha, P) dS - 
$$

$$
- \int_{\partial \mathcal{V}} b_i u_i d\mathcal{V} - \int_{\partial \mathcal{V}} \bar{Q}_i u_i dS - \int_{\partial \mathcal{V}} \bar{R}_i \alpha_{ij} n_j dS - \sum_{\beta} \oint_C \bar{T}_i u_i ds + 
$$

$$
+ \int_{\partial \mathcal{V}} g_e \phi d\mathcal{V} + \int_{\partial \mathcal{V}} \bar{\omega} \phi dS,
$$

(5.16)

where $\tilde{\sigma}^{(2)}_{ij} = -\tilde{\mu}_{kij,k}$, $\tilde{k}_{ijm}(\alpha) = \alpha_{jm,i}$, $\alpha^t = \alpha - (\alpha \cdot n)n$ is the “tangential part” of $\alpha$ on $\partial \mathcal{V}$, with $\delta u = 0$ on $\partial \mathcal{V}_u$ and $C_u^\beta$, $\delta \alpha \cdot n = 0$ on $\partial \mathcal{V}_d$, and $\delta \phi = 0$ on $\partial \mathcal{V}_\phi$. Using the “surface divergence theorem”

$$
\int_{\partial \mathcal{V}} D_j^t q_j dS = \int_{\partial \mathcal{V}} \left( D_j^t n_k \right) n_j q_j dS + \sum_{\beta} \oint_C \left[ \ell_j q_j \right] ds,
$$

(5.17)

for $q_j = \tilde{m}_{ij} \delta u_i$ and taking into account that $(D_j^t \delta u_i) \tilde{m}_{ik} = \delta u_{i,j} \tilde{m}_{ik}^t$, with with $\tilde{m}_{ik} = n_j \tilde{m}_{ik}$ and $\tilde{m}_{ik}^t = \tilde{m}_{ik} - \tilde{m}_{ij} n_j n_k$, we conclude

$$
\int_{\partial \mathcal{V}} \left\{ \left( D_j^t n_p \right) n_k - D_k^t \tilde{m}_{ki} \right\} \delta u_i dS = \int_{\partial \mathcal{V}} \tilde{m}_{ik}^t \delta u_{i,k} dS - \sum_{\beta} \oint_C \left[ \ell_k \tilde{m}_{ki} \right] \delta u_i ds.
$$

(5.18)

Using the above identity we can readily show that the stationarity condition $\delta \Pi = 0$ implies the field equations

$$
\left( \sigma^{(0)}_{ij} + \tilde{\sigma}^{(2)}_{ij} \right)_{,j} + b_i = 0,
$$

(5.19)

$$
\tilde{\sigma}^{(2)}_{ij} = -\tilde{\mu}_{kij,k},
$$

(5.20)

$$
\alpha_{ij} = u_{i,j},
$$

(5.21)

$$
E_i = -\phi, i,
$$

(5.22)

$$
(-\varepsilon_0 \phi, i + P_i)_{,i} = g_e,
$$

(5.23)
and the boundary conditions

\[
\begin{align*}
\left( \sigma_{ij}^{(0)} + \tilde{\sigma}_{ij}^{(2)} \right) n_j + \left[ \left( D_p n_p \right) n_k - D_k \right] (n_m \bar{\mu}_{mki}) &= \tilde{Q}_i \quad \text{on } \partial \mathcal{V}_Q, \\
n_j n_k \bar{\mu}_{kji} &= \tilde{R}_i \quad \text{on } \partial \mathcal{V}_R, \\
\left[ [\ell_j n_k \bar{\mu}_{kji}] \right] &= \tilde{T}_i \quad \text{on } C_T, \\
\left( -\epsilon_0 \phi_i + P_1 \right) n_i &= -\tilde{\omega} \quad \text{on } \partial \mathcal{V}_\omega, \\
\alpha_i^{ij} &= D_j^i u_i \quad \text{on } \partial \mathcal{V},
\end{align*}
\]

with \( \sigma_{ij}^{(0)} = \frac{\partial \tilde{V}_i}{\partial u_{(i,j)}}, \bar{\mu}_{ij} = \frac{\partial \tilde{V}_i}{\partial \bar{\mu}_{ij}}, \) and \( E_i = \frac{\partial \tilde{V}_i}{\partial P_1}. \)

In the above functional, the quantities \( \tilde{\sigma}_{ij}^{(2)} \) and \( n_k \bar{\mu}_{kij} \) are Lagrange multipliers that enforce the corresponding constraints in \( \mathcal{V} \) and on \( \partial \mathcal{V}. \)

### 5.5 “Mixed” finite element formulation

Functional (5.16) forms the basis for a “mixed” finite element formulation, in which \( u, \alpha, \tilde{\sigma}^{(2)}, \phi, \) and \( P \) are the nodal variables. The stationarity condition \( \delta \Pi \) leads to

\[
\begin{align*}
\int_{\mathcal{V}} \left( \sigma_{ij}^{(0)} + \tilde{\sigma}_{ij}^{(2)} \right) \delta u_{ij} d\mathcal{V} + \int_{\mathcal{V}} \left( -\tilde{\sigma}_{ij}^{(2)} \delta \alpha_{ji} + \bar{\mu}_{ij} \delta \kappa_{ij} \right) d\mathcal{V} + \\
\int_{\mathcal{V}} (u_{i,j} - \alpha_{ij}) \delta \tilde{\sigma}_{ji}^{(2)} d\mathcal{V} + \int_{\partial \mathcal{V}} \left[ \bar{m}_k^t (\delta u_{i,k} - \delta \alpha_{ik}) + (u_{i,k} - \alpha_{ik}) \delta \bar{m}_k^t \right] dS + \\
\int_{\mathcal{V}} (E_i + \phi_i) \delta P_1 d\mathcal{V} + \int_{\partial \mathcal{V}} \left( -\epsilon_0 \phi_i + P_1 \right) \delta \phi_i d\mathcal{V} = \\
= \int_{\mathcal{V}} b_i \delta u_i d\mathcal{V} + \int_{\partial \mathcal{V}_Q} \tilde{Q}_i \delta u_i d\mathcal{V} + \int_{\partial \mathcal{V}_R} \tilde{R}_i n_k \delta \alpha_{ik} dS + \sum_\beta \int_{C_T^\beta} \tilde{T}_i \delta u_i dS - \\
\int_{\partial \mathcal{V}_\omega} \left( q_i \delta \phi d\mathcal{V} - \int \tilde{\omega} \delta \phi dS \right),
\end{align*}
\]

where \( \kappa_{ijk} = \alpha_{j,k,i}, \sigma_{ij}^{(0)} = \frac{\partial \tilde{V}_i}{\partial u_{(i,j)}}, \bar{\mu}_{ij} = \frac{\partial \tilde{V}_i}{\partial \bar{\mu}_{ij}}, E_i = \frac{\partial \tilde{V}_i}{\partial P_1}, \bar{m}_{ij} = n_k \bar{\mu}_{kij}, \) and \( \bar{m}_i^t = \bar{m}_{ij} - \bar{m}_{ik} n_k n_j, \) with \( \delta \mathbf{u} = \mathbf{0} \) on \( \partial \mathcal{V}_u \) and \( C_u^\beta, \delta \mathbf{\alpha} \cdot \mathbf{n} = \mathbf{0} \) on \( \partial \mathcal{V}_d, \) and \( \delta \phi = 0 \) on \( \partial \mathcal{V}_\phi. \)

The finite element solutions are based on Eqn(5.29). We develop the 9-node isoparametric plane-strain element (II-87) shown in Fig.5.1. The quantities \( (u_1, u_2, \alpha_{11}, \alpha_{21}, \alpha_{22}, \phi) \) are used as degrees of freedom at all nodes; the quantities \( (\tilde{\sigma}_{11}^{(2)}, \tilde{\sigma}_{22}^{(2)}, \tilde{\sigma}_{12}^{(2)}, \tilde{\sigma}_{21}^{(2)}, P_1, P_2) \) are
additional degrees of freedom at the corner nodes. A bi-quadratic Lagrangian interpolation for \( (u_1, u_2, \alpha_{11}, \alpha_{22}, \alpha_{21}, \alpha_{12}, \phi) \) and a bi-linear interpolation for \( (\tilde{\sigma}_{11}^{(2)}, \tilde{\sigma}_{22}^{(2)}, \tilde{\sigma}_{12}^{(2)}, \tilde{\sigma}_{21}^{(2)}, P_1, P_2) \) are used in the isoparametric plane. The resulting global interpolation for all nodal quantities is continuous in a finite element mesh.

The element described above is implemented into the ABAQUS general purpose finite element program, under the framework of Hibbitt (1984). This code provides a general interface so that a particular new element can be introduced as a “user subroutine” (UEL).

The formulation described by the functional (5.16) is valid for materials with energy function of a general form, including those with non-linear constitutive laws. Here we focus attention on linear materials with a general energy function \( \tilde{W}_L \) of the form

\[
\tilde{W}_L (\varepsilon, \kappa, \mathbf{P}) = \frac{1}{2} C_{ijkl} \varepsilon_{ij} \varepsilon_{kl} + \frac{1}{2} \tilde{A}_{ijklm} \varepsilon_{ij} \varepsilon_{kl} + \frac{1}{2} a_{ij} P_i P_j + d_{ijk} \varepsilon_{ij} P_k + \tilde{f}_{ijkm} \varepsilon_{ij} P_m, \tag{5.30}
\]

where \( C \) is the fourth-order elasticity tensor, and \( (\tilde{A}_{ijklm}, a_{ij}, d_{ijk}, \tilde{f}_{ijkm}) \) are constitutive tensors. In the problems solved we use isotropic materials with an energy function \( \tilde{W}_L \) of the form

\[
\tilde{W}_L (\varepsilon, \kappa, \mathbf{P}) = \frac{1}{2} \lambda \varepsilon_{ii} \varepsilon_{jj} + \mu \varepsilon_{ij} \varepsilon_{ij} + \frac{1}{2} \ell^2 \left[ \lambda \tilde{\kappa}_{ijj} \tilde{\kappa}_{jjk} + \mu \left( \tilde{\kappa}_{ijk} \tilde{\kappa}_{jik} + \tilde{\kappa}_{kji} \tilde{\kappa}_{kji} \right) \right] + \frac{1}{2} a P_i P_i + \left[ \tilde{f}_1 \tilde{\kappa}_{ii} + \tilde{f}_2 (\tilde{\kappa}_{iji} + \tilde{\kappa}_{jii}) \right] P_j, \tag{5.31}
\]

where \((\lambda, \mu)\) are the usual Lamé parameters, \( \ell \) is an internal “material length”, \( a \) is reciprocal susceptibility constant, which is related to the permittivity of the dielectric \( \epsilon \) by
\[
\epsilon = \epsilon_0 + a^{-1}.
\]
Constants \( \tilde{f}_1, \tilde{f}_2 \) are the two flexoelectric constants and we often refer to \( \tilde{f} = \tilde{f}_1 + 2\tilde{f}_2 \) as the volumetric flexoelectric constant. Note that the third-order piezoelectric tensor \( d_{ijk} \) vanishes for materials with centrosymmetry, e.g. isotropic or cubic materials.

The corresponding constitutive equations are

\[
\sigma^{(0)}_{ij} = \frac{\partial \tilde{W}_L}{\partial \epsilon_{ij}} = 2\mu \epsilon_{ij} + \lambda \epsilon_{kk} \delta_{ij},
\]

(5.32)

\[
\tilde{\mu}_{ijk} = \frac{\partial \tilde{W}_L}{\partial \tilde{\kappa}_{ijk}} = \frac{\ell^2}{2} \left[ \lambda \left( \tilde{\kappa}_{nn} \delta_{jk} + \tilde{\kappa}_{jnn} \delta_{ik} \right) + \mu \left( 2 \tilde{\kappa}_{ijk} + \tilde{\kappa}_{kji} + \tilde{\kappa}_{kij} \right) \right] + \tilde{f}_1 \delta_{ij} P_k + \tilde{f}_2 \left( \delta_{ik} P_j + \delta_{jk} P_i \right),
\]

(5.33)

\[
E_i = \frac{\partial \tilde{W}_L}{\partial P_i} = a P_i + \tilde{f}_1 \tilde{\kappa}_{jji} + \tilde{f}_2 \left( \tilde{\kappa}_{ijj} + \tilde{\kappa}_{jij} \right),
\]

(5.34)

where \( \delta_{ij} \) is the Kronecker delta.

Compared with the energy density we used in the preceding chapters, \( \hat{W}_L \), first when \( \mathbf{P} = \mathbf{0} \) the energy function can be written also in the well known form as in Amanatidou & Aravas (2002).

\[
\hat{W}_L (\epsilon, \kappa, \mathbf{0}) = \hat{W}_L (\epsilon, \kappa) = \frac{1}{2} \lambda \epsilon_{ii} \epsilon_{jj} + \mu \epsilon_{ij} \epsilon_{ij} + \frac{1}{2} \left( \lambda \epsilon_{ijj} \epsilon_{kkk} + 2 \mu \epsilon_{ijk} \epsilon_{kk} \right),
\]

(5.35)

with \( \hat{\kappa}_{ijk} = \epsilon_{jk,i} \), which leads to

\[
\sigma^{(0)}_{ij} - \hat{\mu}_{kij,k} = 2\mu \epsilon_{ij} + \lambda \epsilon_{kk} \delta_{ij} - \ell^2 \nabla^2 \left( 2\mu \epsilon_{ij} + \lambda \epsilon_{kk} \delta_{ij} \right),
\]

(5.36)

where \( \hat{\mu}_{ijk} = \frac{\partial \hat{W}_L}{\partial \hat{\kappa}_{ijk}} = \ell^2 \sigma_{jk,i} \). The expression above for \( \sigma^{(0)}_{ij} - \hat{\mu}_{kij,k} \) is formally similar to the expression used by Aifantis (1992) and Altan & Aifantis (1992) in their version of an isotropic gradient elasticity theory. On the other hand, since the flexoelectric tensor \( \tilde{f} \) and \( \tilde{f} \) are also different, but only different by a linear transformation in the isotropic case:

\[
\tilde{f}_1 = f_2, \quad \tilde{f}_2 = \frac{f_1 + f_2}{2}
\]

(5.37)
5.6 Applications

5.6.1 Code validation

The element I9-87 passes the patch test of bi-quadratic displacement field under pure gradient elasticity (all electric nodal degrees of freedom suppressed, i.e. $\phi = 0, P_i = 0$) and bi-linear potential field for pure electrostatics (all displacement and stress nodal degrees of freedom suppressed, i.e., $u_i = 0, \alpha_{ij} = 0, \tilde{\sigma}_{ij}^{(2)} = 0$). Note that a bi-quadratic potential or a bi-quadratic displacement field generates a quadratic polarization, which cannot be captured by the bi-linear interpolation used in the element. Therefore, in the case of the coupled electro-mechanical problem, this element passes the patch test for bi-linear displacement and potential fields. In addition to the patch-test, the element was validated by comparing the finite element solution to the analytical solution of a flexoelectric tube under pressure with a potential difference between the inner and outer surfaces (Fig. 5.2a).

Figure 5.2: (a) A cylindrical flexoelectric tube with inner and outer radius $r_i$ and $r_o$ respectively, is loaded under pressure $p_i$ and $p_o$, and a voltage difference $V$ across the two surfaces. (b) Finite element mesh used in the calculations (40 elements radially, 20 elements circumferentially).

The tube is loaded by internal and external pressures $p_i$ and $p_o$, and a voltage difference $V$ is applied across the inner and outer surfaces. The corresponding boundary conditions
are

\[ \hat{Q}_r = -p_i, \quad \hat{R}_r = 0, \quad \phi = V; \quad \text{at} \quad r = r_i, \quad (5.38) \]
\[ \hat{Q}_r = -p_o, \quad \hat{R}_r = 0, \quad \phi = 0; \quad \text{at} \quad r = r_o. \quad (5.39) \]

This problem is of interest for studies of flexoelectric cylindrical capacitors, stress concentration, and defects in flexoelectric materials. The analytical solution of this problem has been given in Chapter 2.6.3 and can be written in the form

\[ u_r(r) = A r + B r + C K_1 \left( \frac{r}{\ell_0} \right) + D I_1 \left( \frac{r}{\ell_0} \right), \quad (5.40) \]
\[ \phi(r) = G + H \ln r - \frac{\tilde{f}}{a \epsilon} \left( \frac{\partial u_r}{\partial r} + \frac{u}{r} \right), \quad (5.41) \]

where \((A, B, C, D, G, H)\) are constants determined from the boundary conditions, \(\tilde{f} = \tilde{f}_1 + 2\tilde{f}_2\), \(a \epsilon = 1 + a \epsilon_0\), \(I_1(x)\) and \(K_1(x)\) the first order modified Bessel functions of the first and second kind respectively, and

\[ \ell_0^2 = \ell^2 - \frac{\epsilon_0 \tilde{f}^2}{a \epsilon (\lambda + 2 \mu)}, \quad (5.42) \]

which is the characteristic length scale of this flexoelectric problem.

Calculations are carried out for the following non-dimensional parameters

\[ \left\{ \nu, \frac{\ell}{r_i}, \frac{r_o}{r_i}, a \epsilon_0, \frac{\tilde{f}}{r_i \sqrt{a E}} \right\} = \left\{ 0.3, \frac{1}{3}, 10, 0.18, 0.53 \right\} \quad (5.43) \]

where \(E\) is the Young’s modulus and \(\nu\) the Poisson’s ratio with which we can recover the Lamé parameters. In view of the axial symmetry, the problem is mathematically one-dimensional, since the solution depends only on the radial coordinate \(r\). In the finite element calculations, one quarter of the cross section was analyzed and appropriate symmetry conditions were enforced. Figure 5.2b shows the 40-by-20 finite element mesh used in the calculations.

Figure 5.3(b) shows a comparison of the numerical and analytical solutions for the SGE (\(\tilde{f}_1 = \tilde{f}_2 = 0\)) and the flexoelectric (coupled) problems. In both cases the numerical solutions agree very well with the corresponding analytical solutions. For a mixed formulation, the “Lagrange multiplier” fields are of interest due to potential instability. Therefore, a com-
Figure 5.3: Comparison of finite element and analytical solutions: (a) displacement \( u_r \), and (b) \( \tilde{\sigma}_{rr}^{(2)} \) and \( \tilde{\sigma}_{\theta\theta}^{(2)} \), for the tube problem in Fig. 5.2.

Comparison of components of \( \tilde{\sigma}^{(2)} \) with the analytical solution is also made in Figure 5.3b. The finite element solution exhibits good agreement and stability.

Figure 5.4 shows the variation of the electric potential \( \phi \) and the polarization \( P_r \) as determined from the finite element solution together with the analytical solution; again there is excellent agreement between the numerical and analytical solutions.

Figure 5.4: Radial variation of the electric potential \( \phi \) (a) and the polarization \( P_r \) (b), for the tube problem in Fig. 5.2.
5.6.2 Elliptical hole in a plate

We consider the problem of a cylindrical elliptical hole in a plane strain tension field and a uniform electric field (Fig.5.5). The major axis of the ellipse is in the horizontal $x_1$-direction and the tension field $\sigma^\infty$ and the electrical field are applied in the vertical $x_2$-direction. The electric field is created by the opposite surface charges $\pm \omega^\infty$ at infinity, as shown in Fig.5.5. The ratio of major to minor semi-axes of the ellipse is $r_a/r_b = 2$. The surface of the hole is assumed to be traction- and charge-free.

\begin{align*}
\bar{Q}_1 &= 0, \quad \bar{Q}_2 = \pm \sigma^\infty, \quad \bar{R}_1 = 0, \quad \bar{R}_2 = \pm \frac{\bar{f}}{a \epsilon} \omega^\infty, \quad D_2 = \omega^\infty \quad \text{as} \quad x_2 \to \pm \infty, \quad (5.44) \\
\bar{Q} &= 0, \quad \bar{R}_1 = 0, \quad \bar{R}_2 = \pm \frac{\bar{f}_1}{a \epsilon} \omega^\infty, \quad D_1 = 0 \quad \text{as} \quad x_1 \to \pm \infty, \quad (5.45) \\
\bar{Q} &= 0, \quad \bar{R} = 0, \quad \mathbf{D} \cdot \mathbf{n} = 0 \quad \text{on} \quad \left(\frac{x_1}{r_a}\right)^2 + \left(\frac{x_2}{r_b}\right)^2 = 1, \quad (5.46)
\end{align*}

where $\bar{f} = \bar{f}_1 + 2\bar{f}_2$ and $a \epsilon = 1 + a \epsilon_0$. The boundary conditions listed above are consistent with uniform stress and electric fields at infinity.

A square plate with dimensions $2w \times 2w$, with $w = 10r_a$, is used in the finite element calculations; because of symmetry, one half of the plate is analyzed and the appropriate symmetry conditions are imposed (Fig.5.5b). The side $w$ is substantially larger than $r_a$ and...
the solution of this finite-size plate problem is expected to be close to the infinite domain problem. The calculations are carried out for

\[
\left\{ \nu, \frac{b}{r_a}, \frac{w}{r_a}, \frac{\tilde{f}_1}{r_a \sqrt{a E}}, \frac{\tilde{f}}{r_a \sqrt{a E}} \right\} = \left\{ 0.30, \frac{1}{3}, \frac{1}{2}, 10, 0.0018, 0.13, 0.24 \right\}.
\] (5.47)

Figure 5.6 shows the variation of the normal strain \(\varepsilon_{22}\) and the polarization \(P_2\) along the \(x_1\)-axis ahead of the elliptical hole. A concentration of strain and polarization appears at the “tip” of the hole over a distance approximately equal to the size \(r_a\) of the major semi-axis.

Figure 5.6(a) shows also the corresponding results of strain-gradient elasticity without any flexoelectric coupling, i.e., for \(\tilde{f}_1 = \tilde{f}_2 = 0\). Figure 5.6(b) shows the polarization \(P_2\) ahead of the hole as determined by pure electrostatics as well. For the values of the parameters used in the calculations, it appears that the flexoelectric effects have minimal influence on deformation field along \(x_1\) axis but greater influence on the polarization field.

![Figure 5.6](image)

Figure 5.6: Variation of normal strain \(\varepsilon_{22}\) (a) and polarization \(P_2\) (b) along \(x_1\)-axis, for a plate with an elliptical hole as depicted in Fig.5.5

Figure 5.7 shows contour plots of the normal strain \(\varepsilon_{22}\) and polarization \(P_2\) in the plate. Due to the flexoelectric coupling, the profiles are not symmetric with respect to \(x_1\)-axis, in spite of the centrosymmetric geometry. It is also interesting to note that this effect which breaks the symmetry of polarization field only depends on how the material is “poled”, not “material anisotropy” because our constitutive equations are isotropic. If we flip the electric field, then the net polarization is rotated by 180 degrees. This is similar to poling of certain
piezoelectrics as in Abdollahi & Arias (2015). In our simplified material model this effect is reversible; in real materials, however, the stress and electric fields might cause elliptical (or other) defects to move or migrate (evolution of microstructure) in an irreversible manner and even create residual polarization.

Figure 5.7: Contour plots of (a) $\varepsilon_{22}$ and (b) $P_2$ for a plate with an elliptical hole as depicted in Fig. 5.5. Loads are prescribed as: $\sigma^\infty/E = 1/200$ and $\omega^\infty/(\sqrt{a^{-1}E}) = 3.2 \times 10^{-3}$.

5.6.3 Stationary crack

We consider the plane strain problem of an edge-cracked panel (ECP) loaded with a uniformly distributed load as shown in Fig.5.8(a) or by a uniform far field electric load, resulting in surface charge, as in Fig.5.8(b). The crack faces are assumed to be traction- and charge-free. This is an insulating crack which is an ideal model where the crack faces are charge free (also called the impermeable condition).

In the following we use the finite element solution to determine the coefficients that enter the asymptotic solution (“stress intensity factors”). The panel that we studied here is a block with total width $w$ and total height of $2h$. The edge crack is placed at the left half of the specimen (starting from origin), with a length of $w/2$, as shown in Fig.5.8.

Relevant non-dimensional parameters are:

$$\bar{q} = \left\{ \nu, \frac{a \varepsilon_0}{w}, \frac{h}{w}, \alpha = \frac{\bar{f}_1}{\ell \sqrt{\alpha}} \right\}, \beta = \frac{\bar{f}}{\ell \sqrt{\alpha}} = \left\{ 0.0, 0.0018, \frac{1}{20}, \frac{1}{2}, 0.56, 0.56 \right\}$$ (5.48)
Figure 5.8: (a) Mode I insulating crack loaded by uniform distributed load at infinity. (b) Pure Mode D crack loaded by a far field electrical load (surface charge induced by external electric field).

First, consider a Mode I insulating crack loaded by a mechanical load $T$. The boundary conditions for this problem are (Fig.5.8a)

\[ \tilde{Q}_1 = 0, \quad \tilde{Q}_2 = \pm T, \quad \tilde{R} = 0, \quad D_2 = 0 \quad \text{at} \quad x_2 = \pm h, \quad (5.49) \]
\[ \tilde{Q} = 0, \quad \tilde{R} = 0, \quad D_1 = 0 \quad \text{at} \quad x_1 = \pm w/2, \quad (5.50) \]
\[ \tilde{Q} = 0, \quad \tilde{R} = 0, \quad D_2 = 0 \quad \text{on} \quad x_2 = \pm 0, \quad x_1 < 0. \quad (5.51) \]

The asymptotic crack-tip fields in a flexoelectric solid

These crack-tip fields are different from the corresponding fields in LEFM and LPFM as shown in Chapter 4. In particular, the leading term in the asymptotic expansion of the crack-tip displacement field is $r^{3/2}$, $r$ being the radial distance from the crack-tip.

We consider the crack-tip intensities based on Eqn(4.21):

\[ C_{11} = \lim_{r \to 0} \frac{w_2(r, \pi)}{\sqrt{r^3/\ell}} \quad \text{and} \quad C_{12} = -\lim_{r \to 0} \frac{\Omega_3(r, \pi)}{\sqrt{r/\ell}}. \quad (5.52) \]

where $\Omega_3(r, \theta) = (u_{2,1} - u_{1,2})/2$ is the out of plane component of rotation vector $\Omega$. Here, we propose normalizing the solution in the following fashion, similar to that of Aravas &
Giannakopoulos (2009),

\[ u = \frac{wT}{E} \tilde{u}(\tilde{q}), \quad \omega_3 = \frac{T}{E} \tilde{\omega}_3(\tilde{q}), \quad P = \frac{T}{\sqrt{\nu E}} \tilde{P}(\tilde{q}), \quad (5.53) \]

where \( \tilde{\cdot} \) denotes quantities that are non-dimensionalized. We know that in the asymptotic theory the intensity factors \( (C_{11}, C_{12}) \) are dimensionless quantities, therefore, these intensity factors should be proportional to the parameter \( T/E \)

\[ C_{11} = \frac{T}{E} \tilde{C}_{11}(\tilde{q}) \quad \text{and} \quad C_{12} = \frac{T}{E} \tilde{C}_{12}(\tilde{q}). \quad (5.54) \]

As a result, the above intensity factors can be normalized as

\[ \tilde{C}_{11} = \lim_{r \to 0} \frac{u_2(r, \pi)/\left(T\ell/E\right)}{\left(r/\ell\right)^{3/2}} \quad \text{and} \quad \tilde{C}_{12} = -\lim_{r \to 0} \frac{\Omega_3(r, \pi)/\left(T/E\right)}{\sqrt{r/\ell}}. \quad (5.55) \]

Considering the limits of Eqn(5.52) of the numerical solution we conclude that for the particular geometry and material analyzed we have

\[ \tilde{C}_{11} = 11.20 \quad \text{and} \quad \tilde{C}_{12} = 14.12. \quad (5.56) \]

Figure 5.9 shows the radial variation of the finite element solution for \( (u_2, \Omega_3) \) on the crack face \( (\theta = \pi) \) together with the prediction of the asymptotic solution. The leading term provides an accurate description of the displacement and rotation fields on \( \theta = \pi \) in the range \( 0 < r < \ell/10 \). Within this range (except for elements very close to the tip), the asymptotic solution of Chapter 4 captures the leading order of the singularity correctly. Further away, higher-order terms become significant and the finite element solution deviates from the asymptotic solution.

With these intensity factors \( C_{11} \) and \( C_{12} \) on hand, according to the result in Chapter 4, we can easily determine the crack tip polarization field as follows

\[ \frac{P_r(r, \theta)}{\sqrt{\mu \epsilon}} = \frac{\alpha (3C_{11} - 2C_{12})}{8(1 - \alpha^2)} \left( \cos \frac{\theta}{2} + 3 \cos \frac{3\theta}{2} \right) \sqrt{\frac{\ell}{r}}. \quad (5.57) \]

We used the above equation to predict the polarization field along \( \theta = 0 \). We see that the region of “C-dominance” (in analogy to K-dominance in LEFM), which is the region where...
Figure 5.9: Log-log plot of (a) $u_2(r, \pi)$ and (b) $\Omega_3(r, \pi)$ for a Mode I insulating crack.

the asymptotic field dominates other terms, is around $1/10$ of the characteristic length scale of the problem. Within that range, we plot the angular distribution of the polarization at $r = \ell/10$, $\ell/15$, $\ell/20$, respectively, and compare that to the analytic predictions in Fig.5.10. We find that the closer the points are to the crack tip, the better FEM agrees with the asymptotic solution except when we are very close to the crack face. This difference is also observed in Aravas & Giannakopoulos (2009) and it tends to shrink as $r$ becomes smaller.

Figure 5.10: Predicted polarization field compared to finite element calculation for Mode I insulating crack. (a) is the radial profile and (b) is the angular profile. The closer to the crack tip, the better the calculation agrees with the theory.

86
Another type of crack that utilizes the impermeable condition is the Mode D crack. As shown in Fig.5.8, in Mode D no mechanical loading \( \tilde{Q} \) is applied but there is an electric field perpendicular to the crack faces such that a charge equal but opposite in sign is induced on the top and bottom surfaces. Thus, the boundary conditions for a Mode D crack are

\[
\begin{align*}
\tilde{Q} &= 0, \quad \tilde{R}_1 = 0, \quad \tilde{R}_2 = \pm \frac{\tilde{f}}{a \epsilon} \omega_0, \quad D_2 = \omega_0 \quad \text{at} \quad x_2 = \pm h, \quad (5.58) \\
\tilde{Q} &= 0, \quad \tilde{R}_1 = 0, \quad \tilde{R}_2 = \pm \frac{\tilde{f}_1}{a \epsilon} \omega_0, \quad D_1 = 0 \quad \text{at} \quad x_1 = \pm w/2, \quad (5.59) \\
\tilde{Q} &= 0, \quad \tilde{R} = 0, \quad D_2 = 0 \quad \text{on} \quad x_2 = 0, \ x_1 < 0. \quad (5.60)
\end{align*}
\]

Again, here the conditions put on \( \tilde{R} \) impose uniform stress and electric field at far field.

There is an electric intensity factor for this type of crack which is given by

\[
K_D = \lim_{r \to 0} \sqrt{2 \pi r} D_2(r, 0). \quad (5.61)
\]

Once we have this, the corresponding asymptotic deformation field can be easily determined. For example, the first two leading order asymptotics of rotation vector \( \Omega_3 \) can be calculated as in Chapter 4

\[
\Omega_3(r, \theta) = D + C_{22} \sqrt{\frac{\pi}{\ell}} \cos \frac{\theta}{2}, \quad C_{22} = \frac{K_D}{\sqrt{2 \pi \mu \epsilon \ell}} \left[2 \alpha (1 - \nu) - \beta (1 - 2 \nu)\right]. \quad (5.62)
\]

where \( D \) is a constant. We used the above equation to predict the rotation field around a Mode D crack and obtained excellent agreement between FEM and the analytic solution given in Chapter 4, as shown in Fig.5.11.

The above two exercises validate the asymptotic theory developed in Chapter 4 and give us the range of lengths over which this asymptotic solution is valid. We note that strain becomes non-singular around the crack tip, but the polarization field is singular like \( r^{-1/2} \). The region of dominance is quite small since the gradient characteristic length scale is usually in the range of tens to hundreds of nanometers as pointed out by Nowacki (2006). However, the energy release rate is affected by these asymptotic fields, which in turn determines the conditions for crack propagation.
Figure 5.11: Predicted rotation $\Omega_3$ compared with finite element calculation (Mode D crack), in (a) radial and (b) angular direction. Note that $\omega_0$ is the surface charge density at bottom.

### 5.6.4 Periodic structures

Recently, new material processing techniques have been used to produce solids with periodic structures to create meta-materials for improved or desired functionality. For instance, Piccione & Gianola (2015) fabricated nanomeshes, a periodic array of squares with a circular hole inside exhibit higher thermoelectric responses than that of crystal silicon. An example of such a structure is sketched in Fig.5.12.

Figure 5.12: Periodic structure with a repeating unit cell $ABCD$.

In order to determine the macroscopic electromechanical response of this periodic structure, we study the behavior of the unit cell $ABCD$ using appropriate periodic boundary conditions as described in the following.
Let $\bar{F}$ be the macroscopic deformation field in the periodic structure. The presence of the hole in the unit cell perturbs the displacement filed locally in the unit cell. In fact, the displacement field $u(x)$ in the unit cell can be written in the form

$$u_i(x) = (\bar{F}_{ij} - \delta_{ij}) x_j + u^*_i(x),$$

where $u^*(x)$ is a periodic function with zero mean deformation gradient on the unit cell.

We denote the quantities on sides $AB$, $BC$, $CD$ and $DA$ with superscript $l$, $b$, $r$ and $u$, respectively. Then periodicity requires

$$u^*_u = u^*_b, \quad u^*_l = u^*_r.$$  \hspace{1cm} (5.64)

Hence, the total displacement field satisfies the conditions

$$u^*_i - u^*_i = (\bar{F}_{ij} - \delta_{ij}) (x^*_j - x^*_j) \quad \text{and} \quad u^*_i - u^*_i = (\bar{F}_{ij} - \delta_{ij}) (x^*_j - x^*_j).$$

Let $L$ be the length of the sides of the square unit cell. Then

$$x^*_j - x^*_j = \delta_{j2} L, \quad x^*_j - x^*_j = \delta_{j1} L,$$

so that

$$u^*_i - u^*_i = (\bar{F}_{i2} - \delta_{i2}) L \quad \text{and} \quad u^*_i - u^*_i = (\bar{F}_{i1} - \delta_{i1}) L.$$  \hspace{1cm} (5.67)

Similarly, for the electric field, we have

$$\phi^{u,r} - \phi^{b,l} = \bar{E}_j \left( x^{u,r}_j - x^{b,l}_j \right),$$

where $\bar{E}$ is the macroscopic electric field. The macroscopic fields $\bar{F}$ and $\bar{E}$ are the fields that develop in the structure when there are no microscopic holes.

We use the finite element method to study the response of the square unit cell when subject to mechanical and electrical loads. Since the displacement gradients $\alpha_{ij} = u_{i,j}$ are treated as independent degrees of freedom in the finite element formulation, similar
periodicity conditions are imposed on $\alpha$ in the numerical solution:

$$\alpha^u - \alpha^b = \alpha^r - \alpha^l = \bar{F} - \delta.$$  \hfill (5.69)

The periodicity conditions are imposed in ABAQUS through a “user MPC” subroutine.

In the following we present results for the case in which the macroscopic loads on the unit cell are a normal strain $\bar{\varepsilon}_{22}$ in the $x_2$–direction and electric field $\bar{E}_2$, also in the $x_2$–direction, which is created by opposite charges $\pm \bar{\omega}$ at on the top and bottom surfaces of the unit cell. Calculations are carried out for the following parameters

$$\{\nu, \ a \varepsilon_0, \ \frac{\ell}{L}, \ \frac{\ell}{R}\} = \left\{0.30, \ 0.0018, \ \frac{1}{12}, \ \frac{1}{3}\right\}$$  \hfill (5.70)

and various values of $\tilde{f}_1 = \tilde{f}_1/(R/\sqrt{a \mu})$ and $\tilde{f}_2 = \tilde{f}_2/(R/\sqrt{a \mu})$. Here $R$ is the radius of the hole and $L$ the length of the sides of the unit cell. This creates a meta-material with defect volume fraction of $\pi/16 \approx 19.6\%$.

![Graph](image.png)

Figure 5.13: Variation of the opening normal strain $\varepsilon_{22}$ (a) and polarization $P_2$ (b) along the $x_1$–axis ahead of the void due to a macroscopic strain $\bar{\varepsilon}_{22}$ and an electric field $\bar{E}_2$ in the $x_2$–direction, unit-cell under tension.

Figure 5.13 shows the variation of the normal strain $\varepsilon_{22}$ and the polarization $P_2$ along the $x_1$–axis ahead of the hole. Figure 5.13 shows also the corresponding solutions of SGE and electrostatics. The strain distribution $\varepsilon_{22}$ appears to be insensitive to the values of the flexoelectric constants, whereas the polarization changes significantly when these constants

90
are varied.

We consider next the problem in which the macroscopic loads on the unit cell are a shear strain $\bar{\varepsilon}_{12}$ in the $x_2$-direction and electric field $\bar{E}_2$ created by opposite charges $\pm \bar{\omega}$ at on the top and bottom surfaces of the unit cell. Now the problem is expected to be anti-symmetric about the $x_1$-axis, and due to the flexoelectric coupling, some interesting effects are observed.

![Graph](image)

**Figure 5.14:** Variation of shear strain $\varepsilon_{12}$ (a) and polarization $P_1$ (b) along the $x_2$-axis above of the void due to a macroscopic strain $\bar{\varepsilon}_{12}$ and an electric field $\bar{E}_2$ in the $x_2$-direction, unit-cell under shear.

Figure 5.14 shows the variation of the shear strain $\varepsilon_{12}$ and the polarization $P_1$ along the $x_2$-axis above the hole. Figure 5.14 shows also the corresponding solutions of SGE and electrostatics. The strain profile of $\varepsilon_{12}$ is affected by flexoelectricity and the relative effect is related to the magnitude of the flexoelectric constant. The effect is highly localized around the hole or meta defect whereas the overall profile of $\varepsilon_{12}$ is relatively flat and small gradient is developed, at least along this axis. More interestingly, due to the coupling of strain gradient and polarization, extra polarization along $x_1$ direction is produced. In other words, flexoelectricity rotates the polarization field towards $x_1$-axis. Other polarization rotation phenomena can also be found in the works of Catalan et al. (2011), Lu et al. (2012); they are realized in ferroelectric thin films and are believed to have applicability in memory devices. Here, however, we have demonstrated flexoelectric rotation of polarization in periodic meta-structures.
The analyses of the periodic meta-structure and the elliptical hole problems suggest an alternative way of studying flexoelectricity. Recall that due to Timoshenko & Goodier (1969), the classical solution of a circular hole in an infinite elastic body (under uniaxial tension) predicts a stress concentration factor of 3 and that strain/stress decays to the far field level $\bar{\epsilon}$ as $(r/R)^{-2}$. Therefore, a good estimate of strain gradient around the hole, where $r \sim R$, can be calculated through

$$|\tilde{\kappa}| \simeq \eta \bar{\epsilon}$$

where $\eta$ is the concentration factor. Therefore, these periodic structures can generate considerably large strain gradient, when the holes are small. Reducing the size of the hole produces greater strain gradient without increased deformation, which sometimes causes inelastic behavior of the material. Indeed, periodic nano-scale or even atomistic scale holes have already been observed to alter the electromechanical behaviors of certain 2D materials Zelisko et al. (2014). However, holes of these scales are difficult to make; experimental observations are possible only due to certain inherent atomic structures. On the other hand, for meta-materials, the size of the hole can be in the range of hundreds of nanometers as in Piccione & Gianola (2015), which, by the above analysis, can also produce large gradients. For these structures, we can design the arrangement, size and spacing so as to meet different needs. Combining precise mechanical and electrical probes, it is possible to demonstrate how flexoelectricity can be used to alter material properties in larger and realizable scales as well.

Moreover, this periodic structure can be a new source where we can measure flexoelectric constants. So far, the most reliable means to measure them is through beam bending experiments. These, however, cannot determine all components of the flexoelectric tensor (even the simplest isotropic one) as pointed out by Zubko et al. (2007). Therefore, alternative measurement techniques are required. The truncated pyramid structure is one such technique, but due to non-trivial deformation concentration around the edges, this method can hardly measure the correct flexoelectric constant. Besides, recent study of Hong & Vanderbilt (2013) predicted that some materials (such as, silicon) have finite volumetric flexoelectric constant $\tilde{f}$, but vanishing or very small bending flexoelectric constants. The
beam bending experiments are of little use for such materials, but the periodic structure studied here could be an ideal set up to overcome these difficulties. It gives a large gradient, but within a smooth profile (without singular fields due to sharp edges). The magnitude of the gradients can be easily controlled by altering loading or geometry (without exceeding the elastic limit). Both $\tilde{f}$ and $\tilde{f}_1$ (isotropic case) appear in the solutions, so we can determine them by appropriate measurements.

5.7 Concluding remarks

In this chapter, we have formulated a variational form that is completely consistent with the continuum theory of flexoelectricity. The form utilizes a mixed formulation and circumvents the difficulties of modeling gradient effects in flexoelectric solids by introducing extra degrees of freedom. This variational form is general and can incorporate the piezoelectric effect as well. A new element is developed for adapting the variational form to finite element calculation. The known analytic solution of a pressurized tube is employed as a benchmark problem for validation. Then the method is used to study three types of problems which are beyond current analytic capability. Asymptotic theories of cracks are confirmed and a more precise description of the fracture landscape is accomplished. Single hole in an infinite medium as well as periodic meta-structures illustrate the non-trivial coupling of electric loading and deformation. They also offer further inspiration for alternative means of measuring and utilizing flexoelectricity.
Chapter 6

Closure

This dissertation investigated continuum and computational modeling techniques for flexoelectric solids. Governing equations were derived by a generalized Toupin’s variational principle and then used for analyzing interesting boundary value problems. They were also employed to study defects, where strong gradients are known to exist. A “mixed” finite element scheme was formulated based on the continuum theory. This computational tool gave insights into problems in more complicated geometries.

We began the investigation by a review of classical continuum theories on electromechanics. The governing differential equations of the classical theory follow as a result of Toupin’s variational principle. By adding strain gradients, this principle was generalized to study flexoelectricity. It was recognized that higher-order stresses give extra contributions to the physical stresses, in the bulk, as well as, on the boundary. A reciprocal theorem was proved for linear flexoelectricity. We then restricted ourselves to an isotropic flexoelectric material and derived Navier type governing equations. The flexoelectric effect raised the order of the governing differential equations and altered the effective length scales in the equations. Based on the formulation, it was realized that gradient elasticity is an essential part of flexoelectricity, and it gives upper bounds on the flexoelectric coupling constants.

Using the above theory, we then looked into four different boundary value problems that are closely related to experiments. We first studied the problem of beam bending, which is one of the most common ways of utilizing flexoelectricity. We pointed out that the measurements using this approach gave the bending flexoelectric constant, a linear
combination of transverse and longitudinal flexoelectric constant. We showed that applying an electric voltage across the beam thickness resulted in bending moments. In addition, a size-dependent flexoelectric stiffening between short circuited and open circuited beam followed from our analysis. We then considered a circular shaft under torsion and found that it does not create any flexoelectric coupling effect, if it is made of isotropic or cubic material. Our analysis of a pressurized cylinder shed light on how to control stress concentration in flexoelectric materials. We found that flexoelectricity causes an azimuthal polarization in cylinders under shear.

The theory was used to examine the interplay of flexoelectricity with defects. This interplay is intriguing because defects create strong gradients, and hence magnify the flexoelectric coupling effect. Our analysis revealed that the presence of a non-charged point defect in a flexoelectric solids creates a Yukawa type of electric potential field around it through flexoelectric coupling. This electric potential decays exponentially in the far field and can only be observed when defect size is in the same range as the flexoelectric length scale. When it comes to dislocations, we learned that screw dislocations in isotropic or cubic flexoelectric solids do not polarize (in agreement with experiments), but edge dislocations do. We calculated the polarized charges and electric field due to an edge dislocation. Our estimates agreed with experiments in alkali salts and ice.

For cracks, we showed that the leading order of the asymptotic field in flexoelectric solids is altered due to gradient effects. Also, gradient effects result in additional intensity factors to characterize the full fracture behavior of the solids. We found that the crack opening profile changes to a cusp-like shape, rather than the parabolic shape in linear fracture mechanics. A path independent J integral can still be calculated, but in a slightly different manner. These integrals show that, similar to piezoelectric solids, flexoelectric coupling reduces the energy release rate so that more energy must be supplied in order for a crack to grow.

To deal with more complicated geometries, we designed a finite element scheme that is consistent with the continuum theory. The scheme utilizes a “mixed” formulation and treats displacement and displacement gradient as separate variables, but their relation is enforced in an integral sense. A completely equivalent Type I gradient elasticity is used in the formulation. Effects of higher-order stresses are introduced by some virtual stresses
conjugate to strain gradients. Based on Toupin’s variational principle, we derive a weak form for this “mixed” formulation. A special 9-node element is designed to implement the formulation. The finite element code is then written for isotropic flexoelectric solids and validated through patch test and benchmark problems.

This computational tool helps us dig into three types of complicated structures. First, we studied an elliptical hole in a plate. In that problem, we observed that net flexoelectric polarization can be induced by mixing electrical and mechanical loads. This could help us understand the flexoelectric polarization associated with the evolution of micro-voids in solids. Then we studied an edge crack panel and compared our finite element result with that of the asymptotic analysis described above. We found that the singularity predicted by the asymptotic theory is correct, but the theory is valid only very close to the crack tip. Our finite element analysis also helped visualize the changes in symmetry properties of fields around the crack tip due to mixing modes—another prediction from the asymptotic theory.

Last, a structure with periodic holes in it was studied. Periodic boundary conditions were imposed to compute an average response of this solid. Materials with large flexoelectric coupling constants can generate large polarization in these structures without perturbing the deformation significantly. We showed that flexoelectric rotation is also possible by applying shear to the structure. This meta-defect structure has potential as an alternative for measuring and utilizing flexoelectricity.

In spite of all this work the theoretical development of this subject is far from complete. Our work relied on the small deformation assumption, but finite deformation kinematics will generalize the applicability of the theory to soft materials. Another aspect that is not discussed in this work is dynamics. How does flexoelectricity affect wave propagation? Can we examine wave propagation in structures with periodic cells? Can we look at dynamic crack growth in these solids? An intriguing possibility is that dynamically moving cracks in flexoelectric solids can give rise to electro-magnetic radiation due to time varying electric fields. Can we study such phenomena? Also of interest are problems in which flexoelectricity affects the stability of structures, e.g., buckling of ribbons and plates.

In conclusion, we have studied flexoelectricity starting from fundamental variational principles and derived consistent governing equations and proper boundary conditions. We have solved important problems analytically to compare with experiments and motivate
application. We have studied defects and their interplay with flexoelectricity in this fashion. Our studies on cracks give insights into the fracture behavior of flexoelectric solids. We have developed a finite element method that is consistent with the flexoelectric continuum theory using a “mixed” formulation. We have applied it to certain problems of interest and predicted the effective behavior of complicated structures.
Appendix A

Appendix of Chapter 2

A.1 Example of reciprocity

We will use our solution to the flexoelectric beam to demonstrate the reciprocal theorem. Consider two problems (see figure A.1) for two clamped-clamped beams with exactly same geometries (thickness $2h$, width $w$ and length $L$). In the original problem, a force $Q$ is exerted at $x_1 = L_1$; in the reciprocal problem, a constant voltage $V$ is prescribed across the beam from $L_2$ to $L$. We model this voltage as a step function and neglect edge effects. The deflection profile of the beam is $u_2(x_1)$. The variables in the original problem will have upper index 1 and those in the reciprocal problem will have upper index 2.

We will start with the reciprocal problem. Since there is no distributed load along the beam, Eqn(2.59) and (2.58) give:

$$\kappa^{(2)} = \frac{d^2 u_2^{(2)}}{dx_1^2} = \frac{\hat{f}_b A}{aG_E} E_2 H(x_1 - L_2) = \frac{E_2}{V_b} H(x_1 - L_2)$$

\hspace{2cm} (A.1)

Figure A.1: In (a), a point load $Q$ is applied, while in (b) there is a potential difference $V$ between the upper and lower surface over a portion of the beam.
where \( V_b = a G_E / (J_f A) \) is introduced to avoid redundant repetition of constants and \( H(.) \) is the unit step function. We will use the Macaulay bracket \( \langle . \rangle^n \) to denote the \( n \)th antiderivative of \( H(.) \). By applying the clamped boundary conditions at the two ends, the deflection profile in the reciprocal problem can be calculated:

\[
 u_2^{(2)}(x_1) = -\frac{E}{V_b} \left[ -\frac{1}{2}(x_1 - L_2)^2 + L_2(L - L_2)\frac{x_1^3}{L^3} + (L - L_2)(L - 3L_2)\frac{x_1^2}{2L^2} \right]
\]

(A.2)

Using this we are able to determine \( W^{(12)} \):

\[
 W^{(12)} = Q u_2^{(2)}(L_1) = \frac{QV}{4hV_b} \left[ -(L_1 - L_2)^2 + 2L_2(L - L_2)\frac{L_1^3}{L^3} + (L - L_2)(L - 3L_2)\frac{L_1^2}{L^2} \right]
\]

(A.3)

For the original problem the deflection and electric displacement are given by:

\[
 u_2^{(1)}(x_1) = \frac{Q}{6G_E} \left[ -(L - L_1)^2(L + 2L_1)\frac{x_1^3}{L^3} + 3(L - L_1)^2L_1\frac{x_1^2}{L^2} + (x_1 - L_1)^3 \right],
\]

(A.4)

\[
 D_2^{(1)}(x_1) = \frac{\hat{f}_b}{A V_b} = \frac{Q}{A V_b} \left[ -(L - L_1)^2(L + 2L_1)\frac{x_1}{L^3} + (L - L_1)^2L_1\frac{x_1}{L^2} + (x_1 - L_1) \right]
\]

(A.5)

Hence, we are able to calculate \( W^{(21)} \) as:

\[
 W^{(21)} = -w \int_{L_2}^{L} D_2^{(1)} V dx_1 = \frac{QV}{4hV_b} \left[ \frac{L_2(L - L_1)^2}{L^3} (2L_1L - 2L_2L_1 - LL_2) + (L_2 - L_1)^2 \right]
\]

(A.6)

Note that \( (L_1 - L_2)^2 + (L_2 - L_1)^2 = (L_1 - L_2)^2 \), so \( W^{(12)} = W^{(21)} \).

### A.2 Solution to a bimorph system

In this appendix we consider a simple model of a bimorph that is frequently used in experiments on pizoe- and flexoelectric solids. These have been analyzed computationally in Abdollahi & Arias (2015). Here we will formulate an analytical model to emphasize how flexoelectricity alters the electromechanical response and why we must include gradient elastic terms in the energy. We will formulate the solution using the electric field \( E_i \) instead of the polarization. The energy storage function of a solid with electromechanical coupling is \( W = W(\varepsilon_{ij}, D_j) \). Hence, to formulate the problem using electric field and strain, we must
Figure A.2: Two different arrangements of the bimorph piezoelectric beams with flexoelectric effects. a) series b) parallel. Beams can be designed to be tail-to-tail (TT) and head-to-head (HH) in terms of poling direction. From Abdollahi & Arias (2015). Copyright 2015, American Society of Mechanical Engineers.

do a Legendre transformation:

\[
\mathcal{H}(\varepsilon_{ij}, E_i) = \mathcal{W}(\varepsilon_{ij}, D_i) - D_i E_i
\]  

(A.7)

where \( \mathcal{H} \) is the enthalpy in this formulation. Since we want to include the flexoelectric effect we must include the strain gradient. The enthalpy up to quadratic order is

\[
\mathcal{H} = \frac{1}{2} C_{ijkl} \varepsilon_{ij} \varepsilon_{kl} + \frac{1}{2} \hat{A}_{ijklmn} \varepsilon_{jk, i} \varepsilon_{mn, l} - \frac{1}{2} \varepsilon_{ij} E_i E_j - e_{ijk} \varepsilon_{ij} E_k - \hat{f}_{ijkl} \varepsilon_{jk, i} E_l,
\]

(A.8)

where \( C \) is the elasticity tensor and \( (\hat{A}_{ijklmn}, e_{ijk}, \hat{f}_{ijkl}, \epsilon_{ij}) \) are relevant material tensors. Abdollahi & Arias (2015) set \( A_{ijklmn} = 0 \) and consider two beams stuck together with different or same poling directions (a bimorph) and analyze it using the finite element method. The set-up of the bimorph system is sketched in Fig.A.2. Note that the \( \hat{f} \) in this analysis is different from that in the preceding chapters in dimension.

The coordinates are the same as those in Chapter 2.6.1, except that now our beam is in the \( \mathbf{e}_1 - \mathbf{e}_3 \) plane. So, for the bimorph system (TT series arrangement), the strain profile can be written as

\[
\varepsilon_{11} = \begin{cases} 
-\kappa x_3^u, & 0 < x_3^u < h, \\
\kappa (h - x_3^l), & 0 < x_3^l < h 
\end{cases}
\]

(A.9)
where $\kappa$ is the curvature and superscripts $u$ and $l$ denote upper layer and lower layer, respectively. This result is due to Smits et al. (1991). The electric field $E_3$ is assumed to be constant along $x_3$ direction. Note that we choose the $x_3$ axis to be aligned with the poling direction, which is a convention in problems in piezoelectricity. Assuming $h$ to have the same properties as in Chapter 2.6.1, the free energy density of the upper layer $H^u$ can be written as

$$H^u = \frac{1}{2} E(-\kappa x_3^u)^2 + \frac{1}{2} E\ell^2(-\kappa)^2 - d_0 \kappa E_3 x_3^u + \hat{f}_b \kappa - \frac{1}{2} \epsilon^s E_3^2$$ (A.10)

where $\hat{f}_b$ is the effective bending flexoelectric coupling constant as in Chapter 2.6.1 and $\epsilon^s = \epsilon_{33}^s$ is the clamped permittivity constant (short circuited mode), which is smaller than the free permittivity constant (open circuited mode) and their difference is proportional to $d_0^2/E$ as in Smits et al. (1991). Here, $d_0 = -d_{31}$, the appropriate piezoelectric constant. For the lower layer

$$H^l = \frac{1}{2} E[\kappa(h-x_3^l)]^2 + \frac{1}{2} E\ell^2(-\kappa)^2 - d_0 \kappa E_3(h-x_3^l) + \hat{f}_b \kappa - \frac{1}{2} \epsilon^s E_3^2$$ (A.11)

Now, integrating from bottom to the top

$$H_b = w \left( \int_0^h H^u dx_3^u + \int_0^h H^l dx_3^l \right)$$ (A.12)

$$= \left( \frac{1}{3} + \frac{\ell^2}{h^2} \right) Ewh^3 \kappa^2 - \left( d_0 - 2 \frac{\hat{f}_b}{h} \right) wh^2 \kappa E_3 - \epsilon^s whE_3^2$$

where $H_b$ is the free energy density per unit length of the bimorph. The bending moment can be written as:

$$M(x_1) = \left( 1 + \frac{3\ell^2}{h^2} \right) EI \kappa - \left( d_0 - \frac{2\hat{f}_b}{h} \right) whE_3$$ (A.13)

$$Q^e(x_1) = \left( d_0 - \frac{2\hat{f}_b}{h} \right) wh \kappa + 2\epsilon^s whE_3$$ (A.14)

where $I = \frac{2}{3} wh^3$ is the moment of inertia of the bimorph and $Q^e$ is the charge density on the boundary. By observation, the effective Young’s modulus is given by:

$$E^e = E \left( 1 + \frac{3\ell^2}{h^2} \right).$$ (A.15)
and the effective piezoelectric constant:

\[ d_0^e = d_0 - 2\hat{f}_b = d_0\left(1 - \frac{2h_0}{h}\right) \]  \hspace{1cm} (A.16)

where \( h_0 = \hat{f}_b/d_0 \). Clearly, flexoelectricity, in this case, can work for or against the piezoelectric effect, depending on the sign of \( \hat{f} \). When they work against each other, in small size specimens, the direction of effective behavior can be reversed compared to the original piezoelectric bimorph. This is also observed in Abdollahi & Arias (2015).

On the other hand, there is another effect that is associated with the dielectric permittivity. This can be observed by an open circuit bending. Suppose a force \( F \) per width is applied at the end of the beam and the beam is in open circuit, so that we can measure the voltage difference \( V \):

\[ \frac{2}{3}E^e h^3 \kappa - d_0^e h^2 E_3 = F(L - x_1), \]  \hspace{1cm} (A.17)

\[ 2\epsilon^e h\kappa + d_0^e h^2 E_3 = 0. \]  \hspace{1cm} (A.18)

Solving the above equations with the relation \( E_3 = V/2h \) we have:

\[ V = \frac{3d_0^e FL}{4\epsilon^{se} E^e h}, \]  \hspace{1cm} (A.19)

where the effective free permittivity constant is modified as:

\[ \epsilon^{se} = \epsilon^e + \frac{3(d_0^e)^2}{4E^e}. \]  \hspace{1cm} (A.20)

There is an enhancement in the permittivity. Since both \( d_0^e \) and \( E^e \) are functions of \( h \), and will be dominated by the 1/h term at small scales, the enhancement will approach a constant in the small scale limit. This observation is different than that of Abdollahi & Arias (2015).

In their calculations, gradient elasticity is omitted (\( \ell = 0 \)) resulting in a constant \( E \) at small scale. Therefore, they reported a blowing up in the enhancement of \( \epsilon^e \) at small scales. This shows why we need to include gradient elasticity in the study of flexoelectric systems.

Equation (A.19) clearly shows that due to flexoelectricity, the response of a beam is size dependent. Since \( d_0^e \), \( \epsilon^{se} \) and \( a \) are all dominated by the 1/h term and the aspect ratio \( L/h \)
is kept constant, we know that $V$ will first increase, and then decrease as the stiffening of $\epsilon^s$ and $E^s$ takes over at small scales.
Appendix B

Appendix to Chapter 4

B.1 Conventional intensity factors

Mode III cracks in flexoelectric solids are very similar to those in SGE and they inherit the same intensity factors Zhang et al. (1998). We will focus here on the planar cracks. Due to strain gradient and electrostatics we now have more intensity factors to calculate. Unfortunately, if we use the conventional intensity factors $K_I, K_{II}, K_{IV}$ and $K_E$ then the expressions for the energy release rate become too cumbersome. We could use the definitions for intensity factors as in Aravas & Giannakopoulos (2009), but $C_{ij}$, $i,j = 1,2$ and $K_4^{I,II}$ give us a more compact way of presenting the major results. In the following we will connect these constants to the conventional intensity factors.

For stresses, we follow Aravas (2011) and write

$$\sigma_{ij} = \tau_{ij} - \frac{2}{3} \mu_{ijk,k} - \frac{1}{3} \hat{\mu}_{kij,k}$$  \hspace{1cm} (B.1)

The stress defined in this manner is called the true stress Mindlin & Eshel (1968) and is consistent with couple-stress theory. Now, for the conventional $K_I$ intensity we need $\sigma_{22}$ at
\[ \theta = 0 \text{ in Mode I. The dominant term for } \sigma_{22} \text{ is} \]

\[
\sigma_{22}(r, 0) = -\frac{\mu (r/l)^{\frac{3}{2}}}{12(1-\nu)(1-\alpha^2)} \left\{ 3C_{11}(1+\alpha\beta-3\alpha^2)(1-\nu) + 2C_{12} \left[ \alpha(\beta+2\alpha)(1-\nu) + \nu(1-\alpha^2) \right] + 2K_4^1(1-\alpha^2) \left[ \beta(1-2\nu) - \alpha(1-\nu) \right] \right\}
\]  

(B.2)

The \( K_1 \) intensity factor is defined as

\[
K_1 = \lim_{r \to 0} \sqrt{2\pi r} \sigma_{22}(r, 0) \to \infty.
\]  

(B.3)

We have found that the conventional definition of \( K_1 \) is not useful here just as in SGE Aravas & Giannakopoulos (2009). The reason for this is that the stress is singular as \( r^{-3/2} \) due to strain gradient effects. Hence, we define

\[
K_{1D} = \lim_{r \to 0} \sqrt{\frac{2\pi r^3}{l^2}} \sigma_{22}(r, 0) = -\frac{\mu \sqrt{2\pi l}}{12(1-\nu)(1-\alpha^2)} \left\{ 3C_{11}(1+\alpha\beta-3\alpha^2)(1-\nu) + 2C_{12} \left[ \alpha(\beta+2\alpha)(1-\nu) + \nu(1-\alpha^2) \right] + 2K_4^1(1-\alpha^2) \left[ \beta(1-2\nu) - \alpha(1-\nu) \right] \right\}
\]  

(B.4)

where \( K_4^1 \) is related to \( K_E \) in the following fashion:

\[
K_E = \lim_{r \to 0} \sqrt{\frac{2\pi r^3}{l^2}} E_1(r, 0) = \sqrt{\frac{2\pi l}{\varepsilon}} \left[ \alpha C_{12} - K_4^1 + \frac{1-2\nu}{2-2\nu} \left( \beta^2 K_4^1 - \beta C_{12} \right) \right]
\]  

(B.5)

and to get insulating \( K_1 \), simply take \( K_4^1 = 0 \) and for conducting case, \( K_E = 0 \).

Similarly, we can work out the conducting case for the following \( K_{II} \) in mode II:

\[
K_{II} = \lim_{r \to 0} \sqrt{\frac{2\pi r^3}{l^2}} \sigma_{12}(r, 0).
\]  

(B.6)
We find that

\[
K_{II} = \frac{\mu \sqrt{2\pi l}}{12(1 - 2\nu) (2\alpha^2\nu - 3\alpha^2 + 1)} \left\{ 64\beta K_{II}^4 \alpha^2\nu - 24\beta K_{II}^4 \alpha^2 - 16\beta K_{II}^4 \nu + 16C_{22}\alpha^2\nu \right\} \quad (B.7)
\]

\[
- 56\alpha^3\nu K_{II}^4 + 10\alpha K_{II}^4 \nu + 20\alpha^3\nu^2 K_{II}^4 - 25C_{21} - 72\alpha^2\nu C_{21} + 36\alpha^2\nu^2 C_{21} + 8\beta K_{II}^4
\]

\[
- 32C_{21}\nu^2 + 39\alpha^3 K_{II}^4 - 13\alpha K_{II}^4 - 24\alpha^2 C_{22} - 32\beta K_{II}^4 \alpha^2\nu^2 + 27\alpha^2 C_{21} + 66C_{21}\nu + 8C_{22}\right\}.
\]

For the electric intensities

\[
K_{IV} = \lim_{r \to 0} \sqrt{2\pi r} D_2(r, 0) = \sqrt{2\pi \mu \epsilon l} K_{II}^4 \quad (B.8)
\]
Appendix C

Modeling Pyro-paraelectricity

When two crystalline materials are bonded together, due to lattice mismatch, strain relaxation takes place and creates a strong gradient of deformation if one of the materials is thin enough. In the paper Chin et al. (2015), we reported a pyro-paraelectric effect where we can make use of such gradients through flexoelectricity to create thermal-electric sensors. However, the model used in Chin et al. (2015) is a simplified version. Here, we present a more complete and consistent model.

The geometry is sketched in Fig.C.1, where the material in light gray with thickness of $h$ is of interest to us—a thin layer of Barium Strontium Titanate in its paraelectric phase. The darker gray part is the thicker platinum electrode used to measure the potential. There is another platinum electrode on the top, but in non-crystalline state. Therefore, the strain-gradient is not symmetric. Below the darker gray electrode, there sits the substrate which

![Figure C.1: Strain-relaxation takes place at the interface of two crystalline materials, due to the mismatch of their lattice constants. The interfacial strain is $\varepsilon_0$.](image)

107
is made of stiff and thick silicon oxide.

As the thickness is much smaller than the other dimensions, we will approximate this problem by formulating it as a 1D problem:

\[ u_1 = u_3 = 0, \quad u_2 = u_2(x_2), \quad \phi = \phi(x_2). \quad (C.1) \]

According to our theory in Chapter 2, the governing equations of this problem are:

\[
\frac{\partial^2 u_2}{\partial x_2^2} - \ell_0 \frac{\partial^4 u_2}{\partial x_2^4} = 0, \quad (C.2) \\
\frac{\partial^2 \phi}{\partial x_2^2} + \frac{\hat{f}}{a \epsilon} \frac{\partial^2 u_2}{\partial x_2^2} = 0, \quad (C.3)
\]

where \( \ell_0 \) is the volumetric flexoelectric coupling constant as in Chapter 2.6.3. The boundary conditions are:

\[ u_2 = 0, \quad \varepsilon_{22} = \varepsilon_0, \quad \phi = 0 \quad \text{at} \quad x_2 = 0, \quad (C.4) \]
\[ \dot{Q}_2 = 0, \quad \dot{R}_2 = 0, \quad \phi = 0 \quad \text{at} \quad x_2 = h. \]

The above boundary condition corresponds to a stress-free short circuited case. This is also the case in the experiments since the upper surface and lower surface are connected to measure the current flow. Solving the above boundary value problem gives the following strain field:

\[ \varepsilon_{22} = \varepsilon_0 \left[ \cosh \left( \frac{x_2}{\ell_0} \right) - \tanh \left( \frac{h}{\ell_0} \right) \sinh \left( \frac{x_2}{\ell_0} \right) \right]. \quad (C.5) \]

Note that the above reproduces the exact solution to elastic thin film strain relaxation in Nicola et al. (2005) if we exclude flexoelectricity. Now, the average strain, that is measured through X-ray diffraction, can be written as:

\[ \varepsilon_m = \frac{1}{h} \int_0^h \varepsilon_{22} dx_2 = \frac{\varepsilon_0}{h/\ell_0} \cdot \tanh \left( \frac{h}{\ell_0} \right) \quad (C.6) \]

Using this equation, \( \ell_0 \) can be determined from experimental data. The electric potential
can also be calculated:

\[ \phi = \hat{f} \varepsilon_0 \left[ 1 - \frac{x^2}{h} - \cosh \left( \frac{x^2}{l_0} \right) + \tanh \left( \frac{h}{l_0} \right) \sinh \left( \frac{x^2}{l_0} \right) \right]. \]  

(C.7)

So, the electric displacement is:

\[ D_2 = \frac{\hat{f} \varepsilon_0}{ah} = \frac{\mu^f \varepsilon_0}{h}, \]  

(C.8)

a constant through the film, which means that the surface charge on the top and bottom are equal but with opposite sign, just like a capacitor. So then, when subject to change of temperature, the current flow \( I_e \) measured by electrodes with an area of \( A \) can be written as:

\[ I_e = \frac{dQ_e}{dt} = \varepsilon_0 A \left( \frac{d\mu^f}{dT} \right) \frac{dT}{dt}. \]  

(C.9)

Since \( \mu^f \) is proportional to susceptibility, we know:

\[ \frac{d\mu^f}{dT} \propto \frac{d\chi}{dT}. \]  

(C.10)

The latter can be determined through measurements of the dielectric constants. As a result, when subject to temperature change, the sensor can produce current flow. This device will not be able to measure a constant temperature, but it is very sensitive to the change of temperature. The model used in Chin et al. (2015) is approximate, but it is accurate enough for the experiments.
Appendix D

Tensorial Components in Polar Coordinates

Here we present component forms of tensorial quantities, especially those that are derived in a differential manner. We follow the strain gradient elasticity (Type II formulation). First, the strain components can be given as:

\[ \varepsilon_{rr} = \frac{\partial u_r}{\partial r}, \quad (D.1) \]

\[ \varepsilon_{\theta\theta} = \frac{1}{r} \frac{\partial u_\theta}{\partial \theta} + \frac{u_r}{r}, \quad (D.2) \]

\[ \varepsilon_{r\theta} = \frac{1}{2} \left( \frac{1}{r} \frac{\partial u_r}{\partial \theta} + \frac{\partial u_\theta}{\partial r} - \frac{u_\theta}{r} \right), \quad (D.3) \]

from which volumetric strain \( \Theta \) can be calculated as:

\[ \Theta = \varepsilon_{rr} + \varepsilon_{\theta\theta} = \frac{\partial u_r}{\partial r} + \frac{u_r}{r} + \frac{1}{r} \frac{\partial u_\theta}{\partial \theta}. \quad (D.4) \]

Cauchy stress components can be given in the following fashion due to linear isotropic constitutive relations:

\[ \tau_{rr} = (\lambda + 2\mu)\varepsilon_{rr} + \lambda\varepsilon_{\theta\theta} \quad (D.5) \]

\[ \tau_{\theta\theta} = (\lambda + 2\mu)\varepsilon_{\theta\theta} + \lambda\varepsilon_{rr} \quad (D.6) \]

\[ \tau_{r\theta} = \tau_{\theta r} = 2\mu \varepsilon_{r\theta}. \quad (D.7) \]
Again due to constitutive relations, the higher order stresses are given by:

\[
\hat{\mu}_{rrr} = \ell^2 \hat{\tau}_{rrr} \frac{\partial}{\partial r} + \hat{f} P_r \tag{D.8}
\]

\[
\hat{\mu}_{\theta\theta} = \ell^2 \hat{\tau}_{\theta\theta} \frac{\partial}{\partial \theta} + \hat{f} P_r \tag{D.9}
\]

\[
\hat{\mu}_{\theta r} = \frac{\ell^2}{r} \left( \frac{\partial \tau_{rr}}{\partial \theta} - 2 \tau_{\theta r} \right) + \hat{f} P_\theta \tag{D.10}
\]

\[
\hat{\mu}_{\theta \theta} = \frac{\ell^2}{r} \left( \frac{\partial \tau_{\theta\theta}}{\partial \theta} + 2 \tau_{\theta \theta} \right) + \hat{f} P_\theta \tag{D.11}
\]

\[
\hat{\mu}_{rr\theta} = \hat{\mu}_{\theta r\theta} = \ell^2 \hat{\tau}_{rr\theta} \frac{\partial}{\partial r} + \hat{f} P_\theta \tag{D.12}
\]

\[
\hat{\mu}_{\theta\theta\theta} = \ell^2 \hat{\tau}_{\theta\theta\theta} \frac{\partial}{\partial \theta} + \hat{f} P_\theta \tag{D.13}
\]

For convenience we also compute \( p_{jk} = \hat{\mu}_{ijk,k} \):

\[
p_{rr} = \frac{\partial \hat{\mu}_{rrr}}{\partial r} + \frac{1}{r} \frac{\partial \hat{\mu}_{\theta\theta}}{\partial \theta} + \frac{\hat{\mu}_{rrr} - 2 \hat{\mu}_{\theta\theta}}{r} \tag{D.14}
\]

\[
p_{r\theta} = \frac{\partial \hat{\mu}_{rr\theta}}{\partial r} + \frac{1}{r} \frac{\partial \hat{\mu}_{\theta r\theta}}{\partial \theta} + \frac{\hat{\mu}_{rr\theta} + \hat{\mu}_{\theta r\theta} - \hat{\mu}_{\theta\theta\theta}}{r} \tag{D.15}
\]

\[
p_{\theta\theta} = \frac{\partial \hat{\mu}_{\theta\theta\theta}}{\partial r} + \frac{1}{r} \frac{\partial \hat{\mu}_{\theta r\theta}}{\partial \theta} + \frac{\hat{\mu}_{\theta\theta\theta} + 2 \hat{\mu}_{\theta r\theta}}{r} \tag{D.16}
\]

On the other hand, the electric field components are given as:

\[
E_r = -\frac{\partial \phi}{\partial r} \tag{D.17}
\]

\[
E_\theta = -\frac{1}{r} \frac{\partial \phi}{\partial \theta} \tag{D.18}
\]

The polarization field is then given by:

\[
P_r = \frac{1}{a} \left[ E_r - \hat{f}_2 \left( \nabla^2 u_r - \frac{u_r}{r^2} - \frac{2}{r^2} \frac{\partial u_\theta}{\partial \theta} \right) - (\hat{f}_1 + \hat{f}_2) \frac{\partial \Theta}{\partial r} \right], \tag{D.19}
\]

\[
P_\theta = \frac{1}{a} \left[ E_\theta - \hat{f}_2 \left( \nabla^2 u_\theta - \frac{u_\theta}{r^2} + \frac{2}{r^2} \frac{\partial u_r}{\partial \theta} \right) - (\hat{f}_1 + \hat{f}_2) \frac{\partial \Theta}{r \partial \theta} \right], \tag{D.20}
\]

where the Laplacian operator \( \nabla^2 \) takes the following form:

\[
\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2}. \tag{D.21}
\]
Bibliography


