Uncertainty Analysis of Ferroelectric Polydomain Structures

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Materials: Ferroelectrics

- **Applications:**
  - Energy harvesting
  - Structural health monitoring
  - Flow control
  - Ultrasound
  - Robotics
  - Sonar
  - Nanopositioning

**Figure:** Schematic of nanoposition stage

**Figure:** Piezoelectric ceramics are mechanically deformed when in the presence of an electric field. The reverse mechanism is also true, in that an electrical response is generated if a mechanical load is applied.

Polydomain Structures

• Atomic structure broken up into domains
  • Domains – regions of uniform polarization

• Domains divided by walls
  • Most active material behavior occurs along domain wall
  • Extending work done by Cao & Cross\(^1\) and Meyer & Vanderbilt\(^2\).

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Polydomain Structures

180° Domain Wall

Figure: 180° domain wall – two distinct polarization regions. On the left (blue) we have polarization in the negative $x_3$ direction and on the right (red) the polarization is in the positive $x_3$ direction. The polarization switches by 180° as you pass through the domain wall.

90° Domain Wall

Figure: 90° domain wall – two distinct polarization regions. On the left (blue) we have polarization with components in the positive $x_1$-direction and negative $x_2$-direction. On the right (red) the polarization is in the positive $x_1$ - and $x_2$-direction. The polarization switches by 90° as you pass through the domain wall.
Continuum Model

• Free energy density

\[ u(P_i, P_{i,j}, \varepsilon_{ij}) = u_M(\varepsilon_{ij}) + u_L(P_i) + u_C(P_i, \varepsilon_{ij}) + u_G(P_{i,j}) \]

• Components

- \( u_M \) - elastic energy
- \( u_L \) - Landau energy
- \( u_C \) - electrostrictive energy
- \( u_G \) - polarization gradient energy

- \( P_i \) - polarization in \( i^{th} \) direction
- \( P_{i,j} \) - polarization gradient
- \( \varepsilon_{ij} \) - strain
Continuum Model:
Monodomain Structures

Energy: \( u(P_i, \varepsilon_{ij}) = u_M(\varepsilon_{ij}) + u_L(P_i) + u_C(P_i, \varepsilon_{ij}) \)

Stress: \( \sigma_{ij} = \left( \frac{\partial u}{\partial \varepsilon_{ij}} \right) \)

\[ u_L(P_i) = \alpha_1 (P_1^2 + P_2^2 + P_3^2) + \alpha_{11} (P_1^2 + P_2^2 + P_3^2)^2 \]
\[ + \alpha_{12} (P_1^2 P_2^2 + P_2^2 P_3^2 + P_1^2 P_3^2) + \ldots \]

\[ u_C = -q_{11} (\varepsilon_{11} P_1^2 + \varepsilon_{22} P_2^2 + \varepsilon_{33} P_3^2) \]
\[ -q_{12} [\varepsilon_{11} (P_2^2 + P_3^2) + \varepsilon_{22} (P_1^2 + P_3^2) + \varepsilon_{33} (P_1^2 + P_2^2)] \]
\[ -q_{44} (\varepsilon_{12} P_1 P_2 + \varepsilon_{13} P_1 P_3 + \varepsilon_{23} P_2 P_3) \]
Uncertainty Quantification: Bayesian Statistical Analysis

• Statistical Model: \( M^{data}(i) = M(i; \theta) + \varepsilon_i, \quad i = 1, \ldots, N \)

• Bayes’ Relation

\[
\pi(\theta|M^{data}) = \frac{p(M|\theta)\pi_0(\theta)}{\int_{\mathbb{R}^p} p(M|\theta)\pi_0(\theta)d\theta}
\]

• Posterior Density: \( \pi(\theta|M^{data}) \)

• Prior Density: \( \pi_0(\theta) \)

• Likelihood Function: \( p(M|\theta) = e^{-\sum_{i=1}^{n}[M^{data}(i) - M(i; \theta)]^2/(2\sigma^2)} \)
  - Assume observation errors are independent and identically distributed (iid): \( \varepsilon_i \sim N(0, \sigma^2) \).
Uncertainty Quantification: Monodomain Structures

• Posterior densities: $\pi(\theta|M^{data})$

• Pairwise correlation:

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Uncertainty Propagation: Monodomain Structures

- Energy density: $u$

**Figure:** (Left) Uncertainty propagation through energy model and (Right) uncertainty in normal stress in the $x_1$ direction.
Continuum Model: Polydomain Structures

• Governing equations

Ginzburg-Landau: \( \frac{d}{dx_j} \left( \frac{\partial u}{\partial P_{i,j}} \right) - \frac{\partial u}{\partial P_i} = 0 \)

Momentum: \( \sigma_{i,j,j} = \frac{d}{dx_j} \left( \frac{\partial u}{\partial \varepsilon_{i,j}} \right) = 0 \)

• Gradient energy

\[
    u_G = \frac{g_{11}}{2} \left( P_{1,1}^2 + P_{2,2}^2 + P_{3,3}^2 \right) + g_{12} \left( P_{1,1} P_{2,2} + P_{1,1} P_{3,3} + P_{2,2} P_{3,3} \right) \\
    + \frac{g_{44}}{2} \left[ \left( P_{1,2} + P_{2,1} \right)^2 + \left( P_{1,3} + P_{3,1} \right)^2 + \left( P_{2,3} + P_{3,2} \right)^2 \right]
\]
Continuum Model: 180° Domain Wall

• Assume:

\[ P_1 = P_2 = 0, P_3 \neq 0, \varepsilon_{ij} = 0 \ (i \neq j), \text{ and only spatial variation is in } x_1\text{-direction} \]

• Ginzburg-Landau:

\[
\frac{\partial}{\partial x_1} \left( \frac{\partial u}{\partial P_{3,1}} \right) - \frac{\partial u}{\partial P_3} = 0 \rightarrow 2\alpha_1^+ P_3 + 4\alpha_{11} P_3^3 + 6\alpha_{111} P_3^5 = g_{44} P_{3,11}
\]

where \( \alpha_1^+ = \alpha_1 - q_{11} \varepsilon_{33} - q_{12} (\varepsilon_{11} + \varepsilon_{22}) \)

• Momentum:

\[
\sigma_{11,1} = \frac{\partial}{\partial x_1} \left( \frac{\partial u}{\partial \varepsilon_{11}} \right) = c_{11} \varepsilon_{11,1} - 2q_{12} P_3 P_{3,1} = 0
\]

• Numerically solve for \( P_3 \) and \( \varepsilon_{11} \)

Figure: 180° domain wall numerical solution for polarization and strain. Numerical solution converges to steady state solution.
Model Comparison: 180° Domain Wall

- Finite difference (FD)
  - Simplified model
- Finite element analysis (FEA)
  - More degrees of freedom
- Good model agreement between FD and FEA
  - Compare quantities of interest

Figure: 180° domain wall energy along $x_1$-axis. (Top Right) Polarization switches from negative to positive within the nanoscale domain wall region. Compared solution found using FEA and FD: (Bottom Left) Landau energy density and (Bottom Right) total energy density.
Polydomain Structures: 180° Domain Wall

• Domain wall energy

\[ E_{180°} = \int_{-\infty}^{\infty} (u - u_0) \, dx_1 \]

• From literature

\[ E_{180°} = 132 \text{ mJ/m}^2 \]


Figure: Excess energy density through 180° domain wall energy along \( x_1 \)-axis. Uncertainty from continuum model parameters propagated through to generate 50% - 99% credible intervals.
Continuum Model: 90° Domain Wall

• Easier to work in rotated coordinate system:
  • Rotate 45° degrees around the $x_3$ axis – $(x_S, x_r, x_3)$

• Ginzburg-Landau:

$$\frac{\partial}{\partial x_s} \left( \frac{\partial u}{\partial P_s} \right) - \frac{\partial u}{\partial P_s} = 0 \quad \Rightarrow \quad G_{ss} P_{s,ss} = \beta_1 P_s + \beta_2 P_s^3 + \beta_3 P_s^5 + \beta_4 P_s^2 P_r^2 + \beta_5 P_s P_r^4 + \beta_6 P_s^3 P_r^2$$

$$\frac{\partial}{\partial x_s} \left( \frac{\partial u}{\partial P_r} \right) - \frac{\partial u}{\partial P_r} = 0 \quad \Rightarrow \quad G_{rs} P_{r,ss} = \gamma_1 P_r + \gamma_2 P_r^3 + \gamma_3 P_r^5 + \gamma_4 P_s^2 P_r + \gamma_5 P_s^4 P_r + \gamma P_s^2 P_r^3$$

where $\beta_i, \gamma_i = f(\alpha_1, \alpha_{11}, \ldots, q_{11}, \ldots, c_{11}, \ldots, g_{11}, \ldots)$
Conclusions & Future Work: Quantum-Informed Continuum Modeling

• 180°
  • Developed numerical approximation and verified with finite element solution
  • Quantified uncertainty associated with exchange parameter

• 90°
  • Developed numerical approximation
  • Ongoing effort to verify with finite element analysis
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