Uncertainty Analysis of Ferroelectric Polydomain Structures

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Materials: Ferroelectrics

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

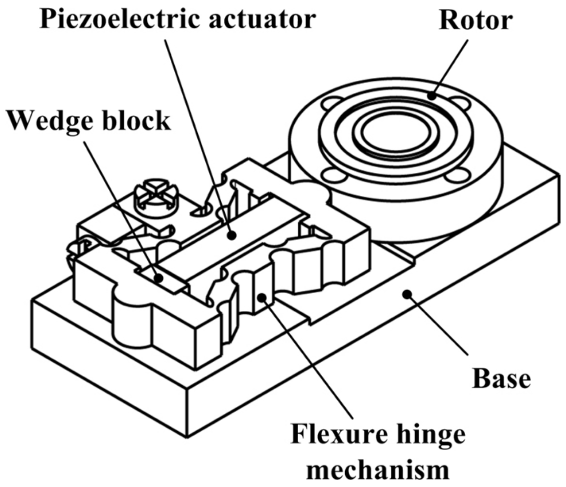


Figure: Schematic of nanoposition stage[1].

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.

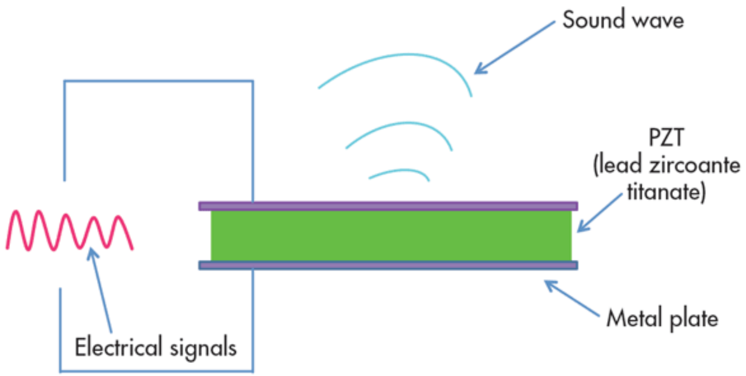


Figure: Schematic of piezoelectric in sonar transducer[2].

1. Li, Jianping, et al. "Design and experimental tests of a dual-servo piezoelectric nanopositioning stage for rotary motion." *Review of Scientific Instruments* 86.4 (2015): 045002.
2. http://www.electronicdesign.com/power/what-piezoelectric-effect

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].

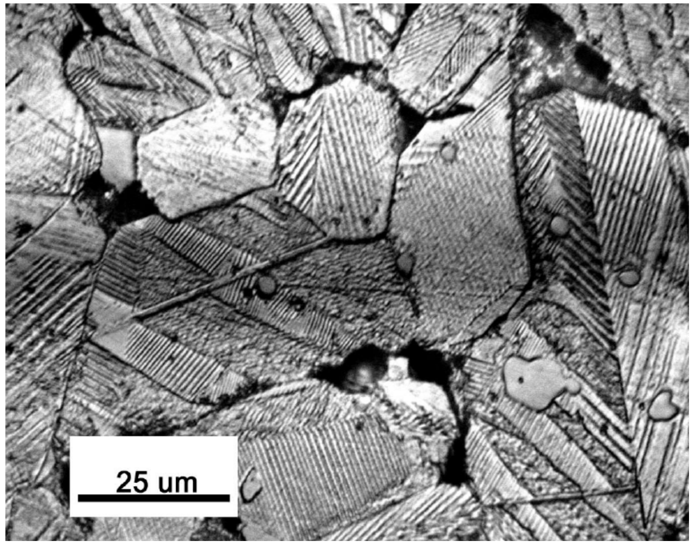


Figure: Domain structures in Barium Titanate[3].

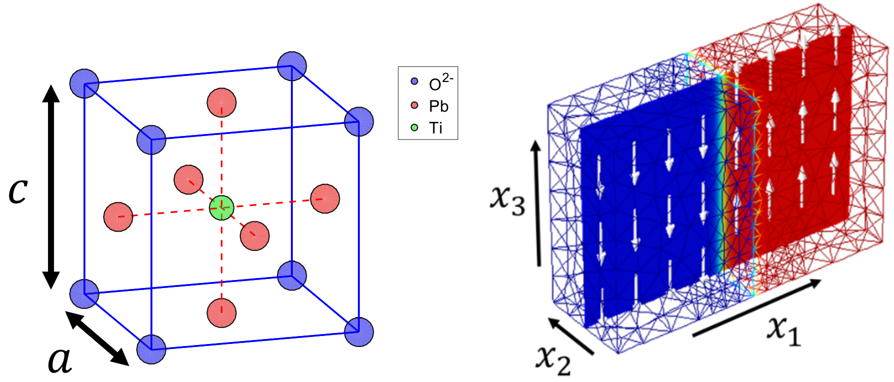


Figure: (Left) Unit cell width is approximately 4 angstroms. (Right) Domains separated by walls that are approximately 5 angstroms wide.

1. Cao, W., and Cross, L.E. "Theory of Tetragonal Twin Structures in Ferroelectric Perovskites with a First-Order Phase Transition." *Physical Review B* 44.1 (1991)
2. Meyer, B., and Vanderbilt, D. "*Ab initio* study of ferroelectric domain walls in $PbTiO_3$". Physical Review B, 65(10):104111, 2002.
3. Liang, D., Stone, D., and Lakes, R. "Softening of bulk modulus and negative Poisson ratio in barium titanate ceramic near the Curie point." *Philosophical Magazine Letters* 90.1 (2010): 23-33.

Polydomain Structures

180° Domain Wall

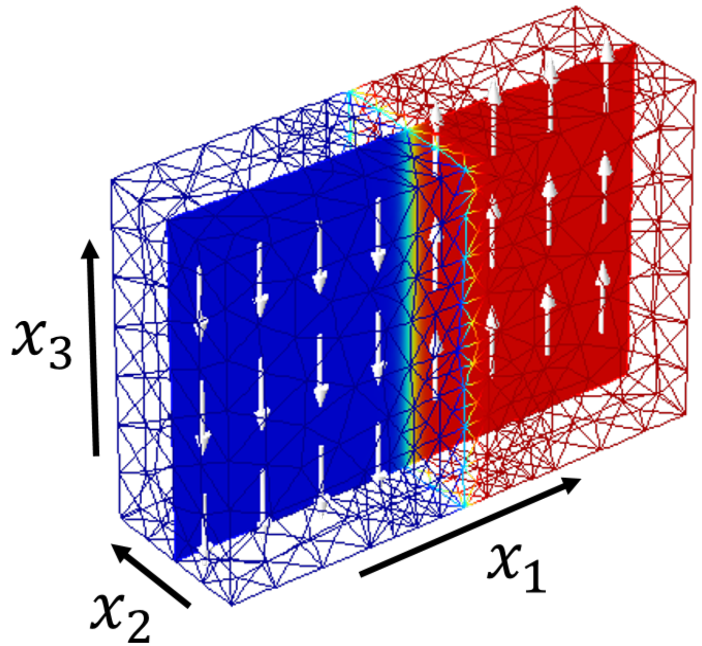


Figure: 180° domain wall – two distinct polarization regions. On the left (blue) we have polarization in the negative x_3 direction and on the right (red) the polarization is in the positive x_3 direction. The polarization switches by 180° as you pass through the domain wall.

90° Domain Wall

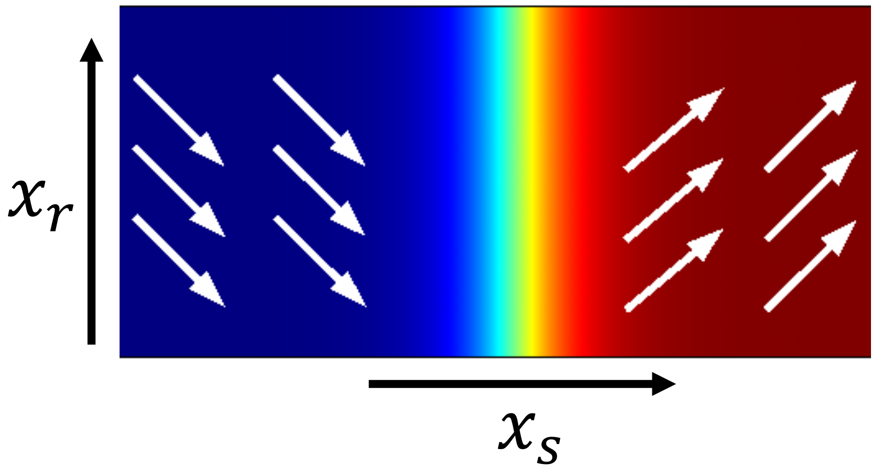


Figure: 90° domain wall – two distinct polarization regions. On the left (blue) we have polarization with components in the positive x_1-direction and negative x_2-direction. On the right (red) the polarization is in the positive x_1- and x_2-direction. The polarization switches by 90° as you pass through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

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

$$u_L(P_i) = \alpha_1(P_1^2 + P_2^2 + P_3^2) + \alpha_{11}(P_1^2 + P_2^2 + P_3^2)^2$$
$$+ \alpha_{12}(P_1^2 P_2^2 + P_2^2 P_3^2 + P_1^2 P_3^2) + \cdots$$

$$u_C = -q_{11}(\varepsilon_{11}P_1^2 + \varepsilon_{22}P_2^2 + \varepsilon_{33}P_3^2)$$
$$-q_{12}[\varepsilon_{11}(P_2^2 + P_3^2) + \varepsilon_{22}(P_1^2 + P_3^2) + \varepsilon_{33}(P_1^2 + P_2^2)]$$
$$-q_{44}(\varepsilon_{12}P_1P_2 + \varepsilon_{13}P_1P_3 + \varepsilon_{23}P_2P_3)$$

Uncertainty Quantification: Bayesian Statistical Analysis

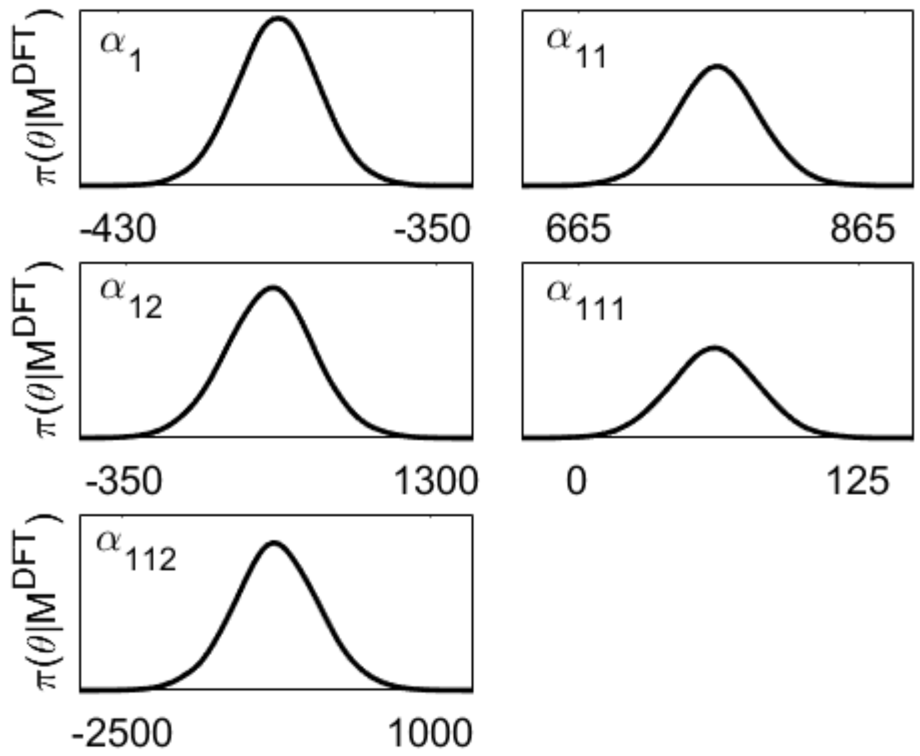
- Statistical Model: $M^{data}(i) = M(i;\theta) + \varepsilon_i, \quad i = 1, \dots, N$
- Bayes' Relation

$$\pi\left(\theta \middle| M^{data}\right) = \frac{p(M|\theta)\pi_0(\theta)}{\int_{\mathbb{R}_p} p(M|\theta)\,\pi_0(\theta)d\theta}$$

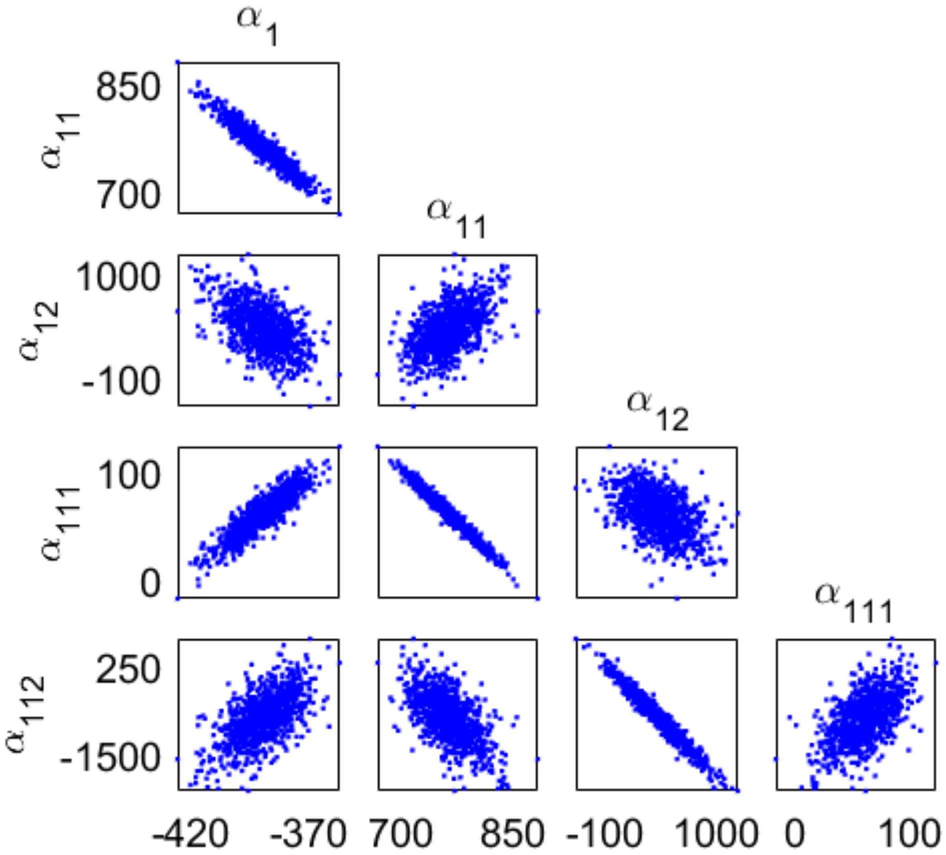
- Posterior Density: $\pi\left(\theta \middle| M^{data}\right)$
- Prior Density: $\pi_0(\theta)$
- Likelihood Function: $p(M|\theta) = e^{-\sum_{i=1}^{n}\left[M^{data}(i) - M(i;\theta)\right]^2/(2\sigma^2)}$
  - Assume observation errors are independent and identically distributed (iid): $\varepsilon_i \sim N(0,\sigma^2)$.

Uncertainty Quantification: Monodomain Structures

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



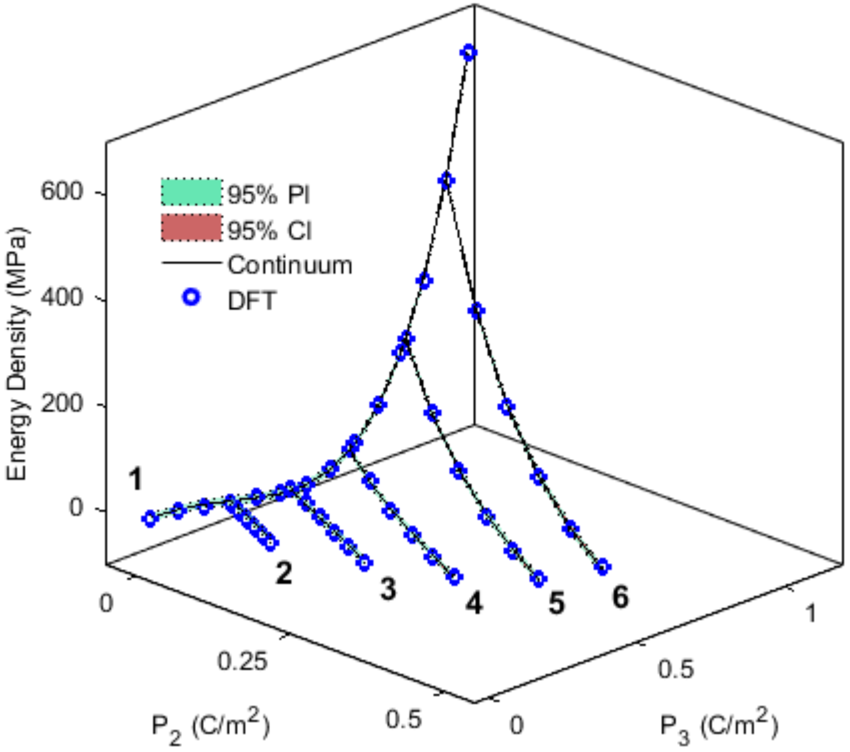
- Pairwise correlation:



Uncertainty Propagation: Monodomain Structures

- Energy density: u

Stress: σ_{11}



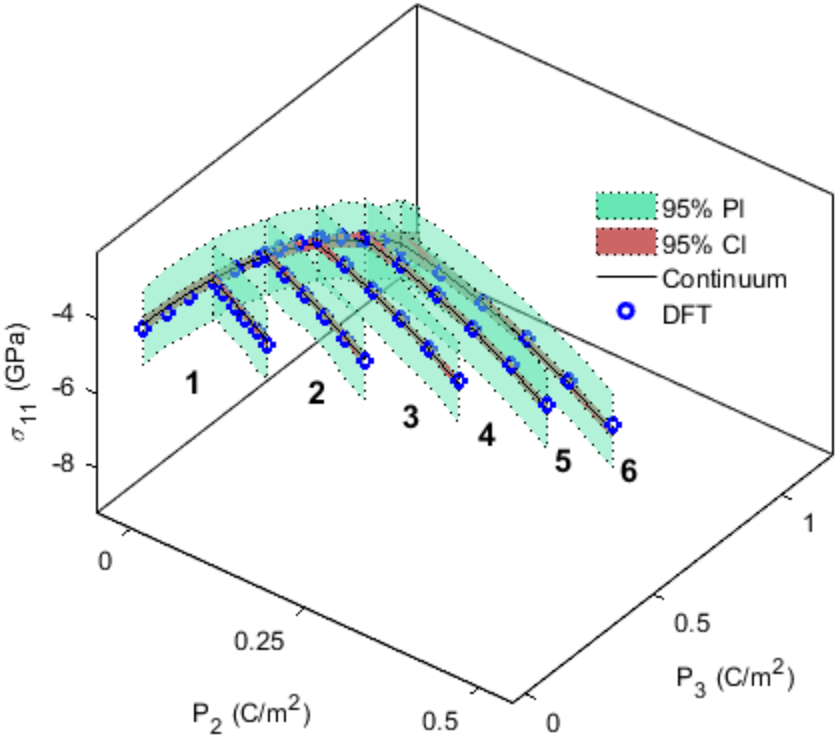


Figure: (Left) Uncertainty propagation through energy model and (Right) uncertainty in normal stress in the x_1 direction.

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

- 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:

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

- Ginzburg-Landau:

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

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

- Momentum:

$$\sigma_{11,1} = \frac{\partial}{\partial x_1}\left(\frac{\partial u}{\partial \varepsilon_{11}}\right) = c_{11}\varepsilon_{11,1} - 2q_{12}P_3P_{3,1} = 0$$

- Numerically solve for P_3 and ε_{11}

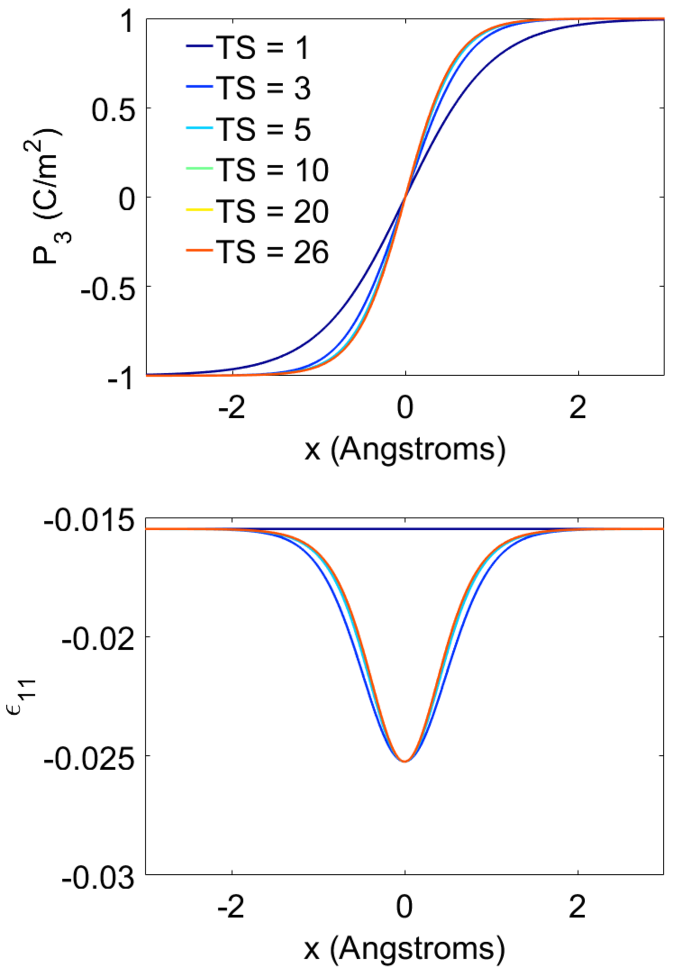


Figure: 180° domain wall numerical solution for polarization and strain. Numerical solution converges to steady state solution.

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

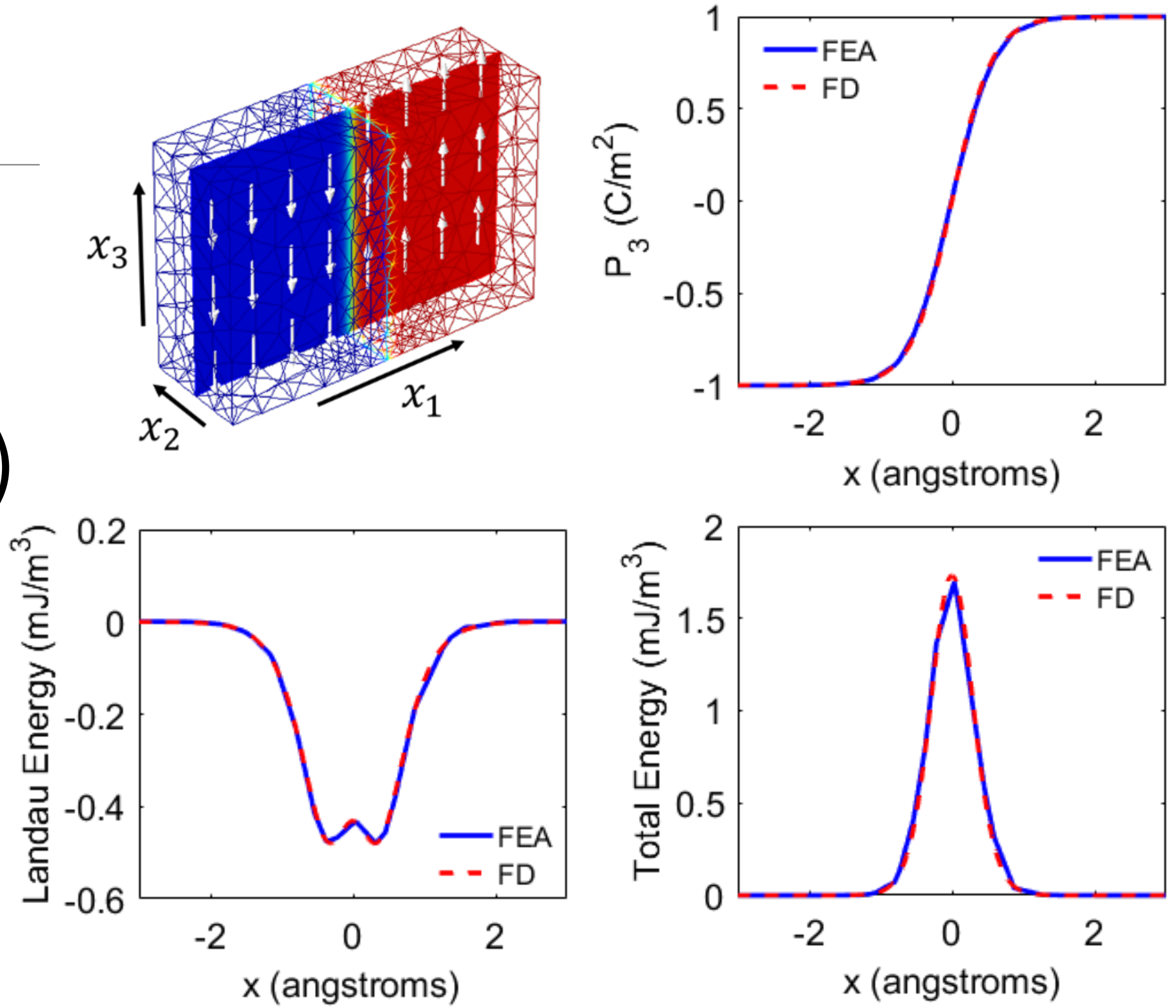


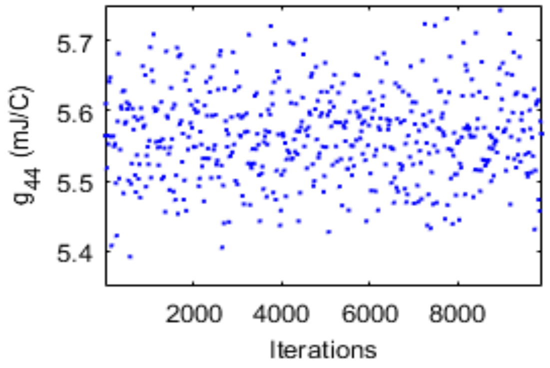
Figure: 180° domain wall energy along x_1-axis. (Top Right) Polarization switches from negative to positive within the nanoscale domain wall region. Compared solution found using FEA and FD: (Bottom Left) Landau energy density and (Bottom Right) total energy density.

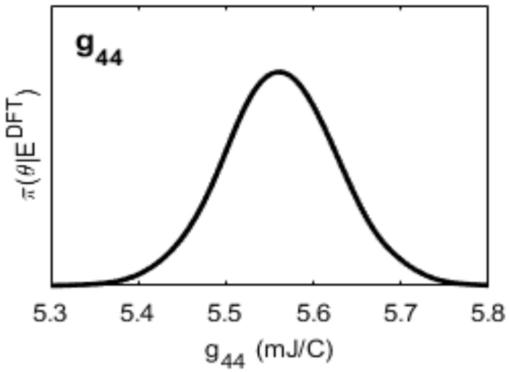
Polydomain Structures: 180° Domain Wall

- Domain wall energy

$$E_{180^\circ} = \int_{-\infty}^{\infty} (u - u_0)\, dx_1$$

- From literature[1]: $E_{180^\circ} = 132\ \mathrm{mJ/m^2}$





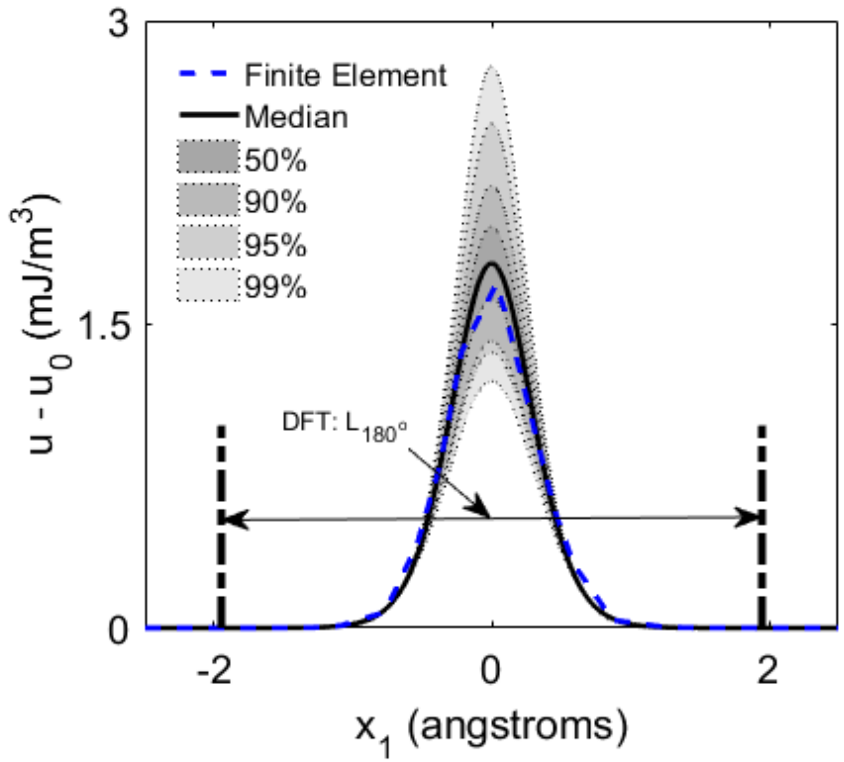
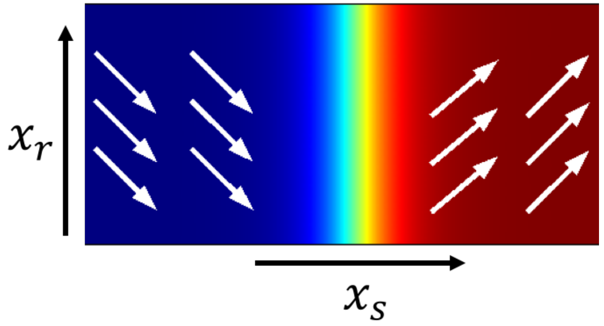


Figure: Excess energy density through 180° domain wall energy along x_1-axis. Uncertainty from continuum model parameters propagated through to generate 50% - 99% credible intervals.

1. Meyer, B., and Vanderbilt, D. "*Ab initio* study of ferroelectric domain walls in $PbTiO_3$". Physical Review B, 65(10):104111, 2002.

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:

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

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

where $\beta_i, \gamma_i = f(\alpha_1, \alpha_{11}, \dots, q_{11}, \dots, c_{11}, \dots, g_{11}, \dots)$

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

Acknowledgements

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