Uncertainty Analysis of Continuum Phase Field Modeling in 180° Domain Wall Structures

Presenter: Paul Miles

Authors: Paul Miles[a], William Oates[a], Lider Leon[b], Ralph Smith[b]

[a]Department of Mechanical Engineering
Florida Center for Advanced Aero-Propulsion (FCAAP)
Florida A & M and Florida State University, Tallahassee, FL 32310

[b]Department of Mathematics
North Carolina State University, Raleigh, NC 27695

Outline

- Density Functional Theory (DFT)
- Monodomain
- Polydomain
- Conclusions & Future Work

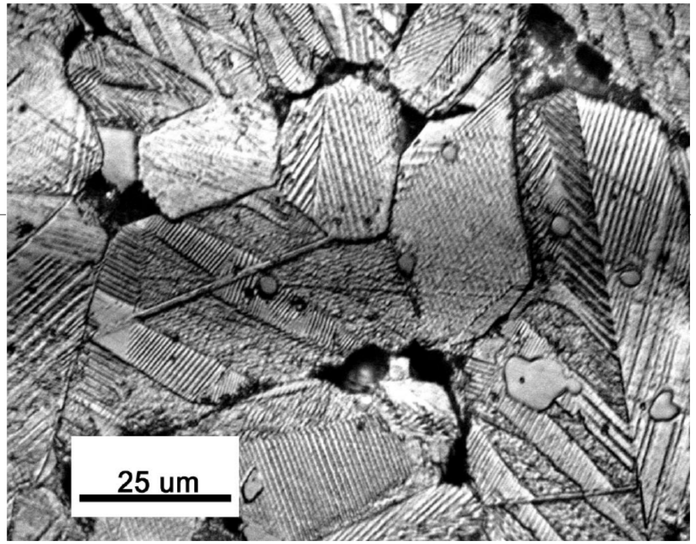
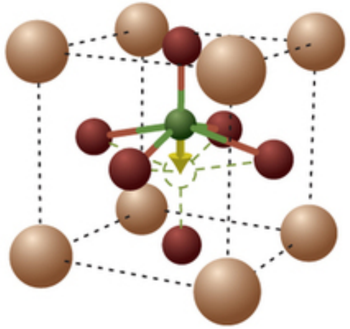


Figure: Domain structures in Barium Titanate[1].



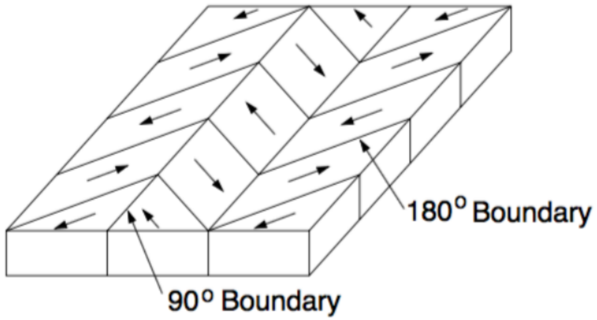


Figure: (Left) Unit cell width is approximately 4 angstroms.
http://www.nature.com/nmat/journal/v12/n7/fig_tab/nmat3669_F1.html
(Right) Polydomain structures - 180° and 90° domain wall boundaries.

1. Dong, Liang, Donald S. Stone, and Roderic S. Lakes. "Softening of bulk modulus and negative Poisson ratio in barium titanate ceramic near the Curie point." *Philosophical Magazine Letters* 90.1 (2010): 23-33.

Density Functional Theory (DFT)

- Lead Titanate
- Deform atomic positions – different polarization states
- Uncertainty:
  - Nuclei positions and electron density (5 atoms, each with 3 degrees of freedom)
  - Approximate as a polarization vector

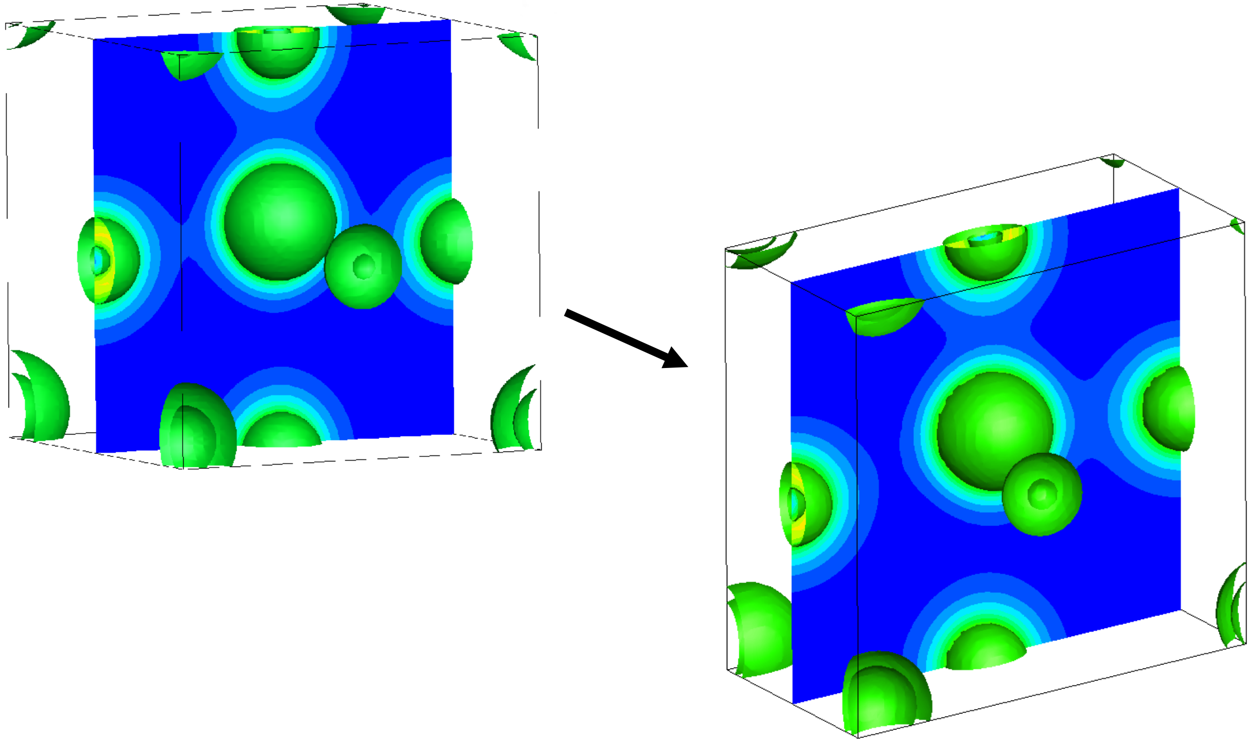


Figure: Example of the electron density solutions for (Left) the reference undeformed cubic structure and (Right) shear deformed state where the unit cell has been sheared such that the deformation gradient component F_{23} is non-zero.

DFT: Energy & Stress

- Shear:
  - Atoms moved based on estimates from shear deformation
  - Positive P_2 generated, P_3 reduced
- Calculate energy and stress at each polarization state
  - Energy: $u\left(P_i, P_{i,j}, \varepsilon_{ij}\right)$
  - Stress: $\sigma_{ij} = \dfrac{\partial u}{\partial \varepsilon_{ij}}$

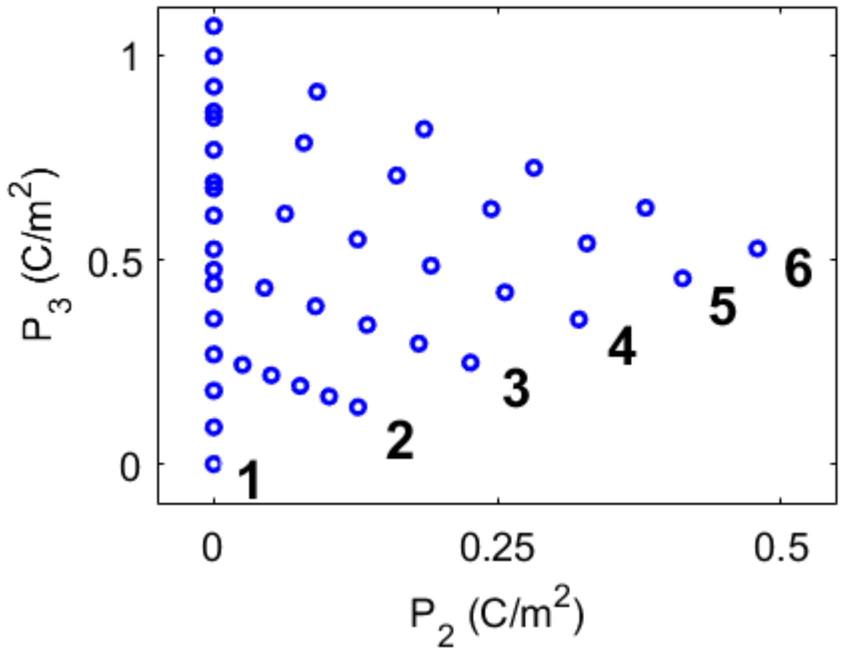


Figure: Polarization rotation – starting from five different locations of nonzero P_3 and $P_2 = 0$. Atoms moved along directions estimated from shear deformation states to generate positive P_2 values while reducing P_3. DFT computations performed by Justin Collins.

Theory

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

1. Cao, Wenwu, and L. E. Cross. "Theory of Tetragonal Twin Structures in Ferroelectric Perovskites with a First-Order Phase Transition." *Physical Review B* 44.1 (1991)

Monodomain Analysis

- Landau energy density

$$u_L(P_i) = \alpha_1(P_1^2 + P_2^2 + P_3^2) + \alpha_{11}(P_1^2 + P_2^2 + P_3^2)^2$$
$$+ \alpha_{12}(P_1^2 P_2^2 + P_2^2 P_3^2 + P_1^2 P_3^2) + \alpha_{111}(P_1^6 + P_2^6 + P_3^6)$$
$$+ \alpha_{112}[P_1^4(P_2^2 + P_3^2) + P_2^4(P_1^2 + P_3^2) + P_3^4(P_1^2 + P_2^2)]$$
$$+ \alpha_{123} P_1^2 P_2^2 P_3^2$$

- Unknown phenomenological parameters:

$\alpha_1, \alpha_{11}, \alpha_{12}, \alpha_{111}, \alpha_{112}, \alpha_{123}$

Uncertainty Quantification: Bayesian Statistics

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

$$\pi(\theta|M^{DFT}) = \frac{p(M|\theta)\pi_0(\theta)}{\int_{\mathbb{R}p} p(M|\theta)\,\pi_0(\theta)d\theta}$$

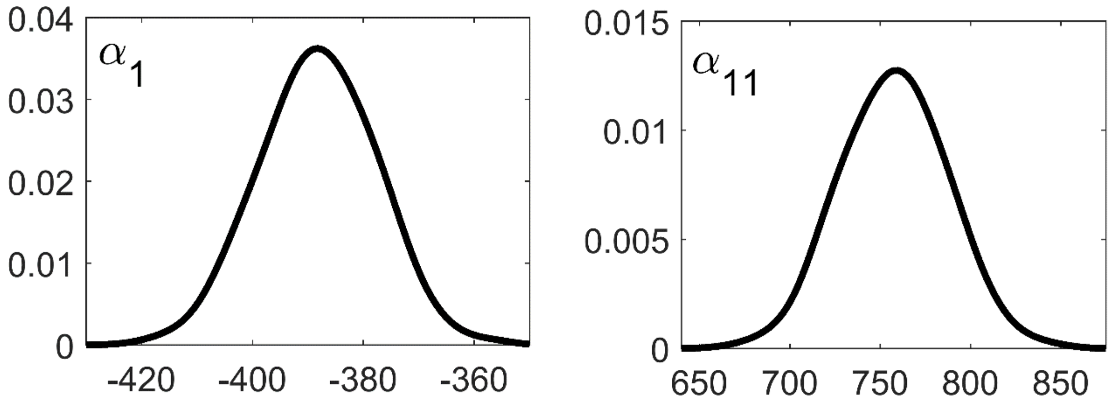
- Posterior density: $\pi(\theta|M^{DFT})$
- Prior density: $\pi_0(\theta)$
- Likelihood: $p(M|\theta) = \; e^{-\sum_{i=1}^{n}[M^{DFT}(i)-M(i;\theta)]^2/(2\sigma^2)}$
  - Assume observation errors are independent and identically distributed (iid) and $\varepsilon_i \sim N(0,\sigma^2)$.

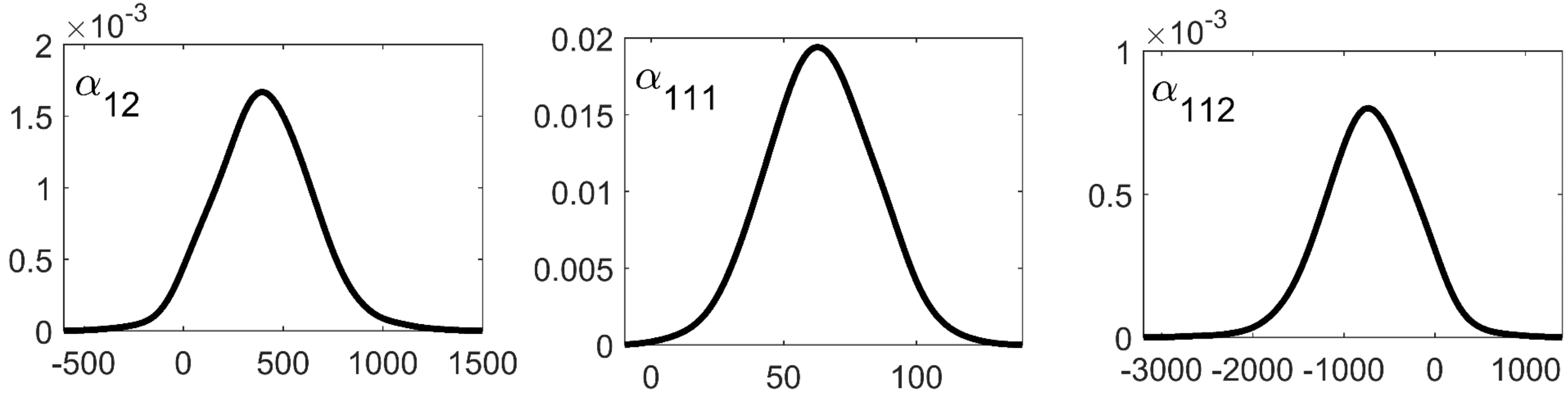
Monodomain Analysis: Uncertainty Quantification

- Posterior densities:

$$\pi(\theta|M^{DFT})$$

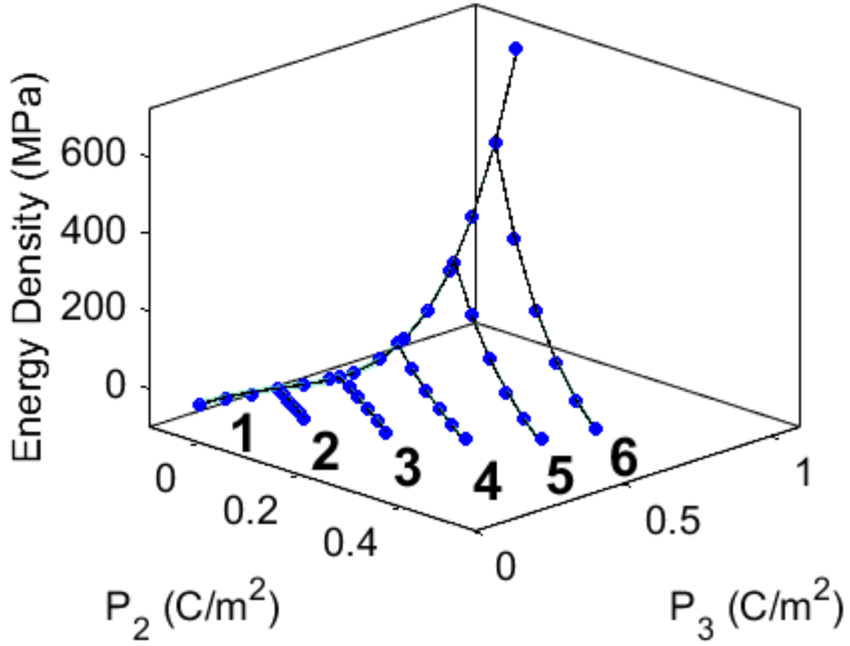
- Calibrated from DFT calculated energy





Monodomain Analysis: Uncertainty Propagation

$\theta = [\alpha_1, \alpha_{11}, \alpha_{12}, \alpha_{111}, \alpha_{112}, \alpha_{123}]$



$\theta = [q_{11}, q_{12}, q_{44}]$

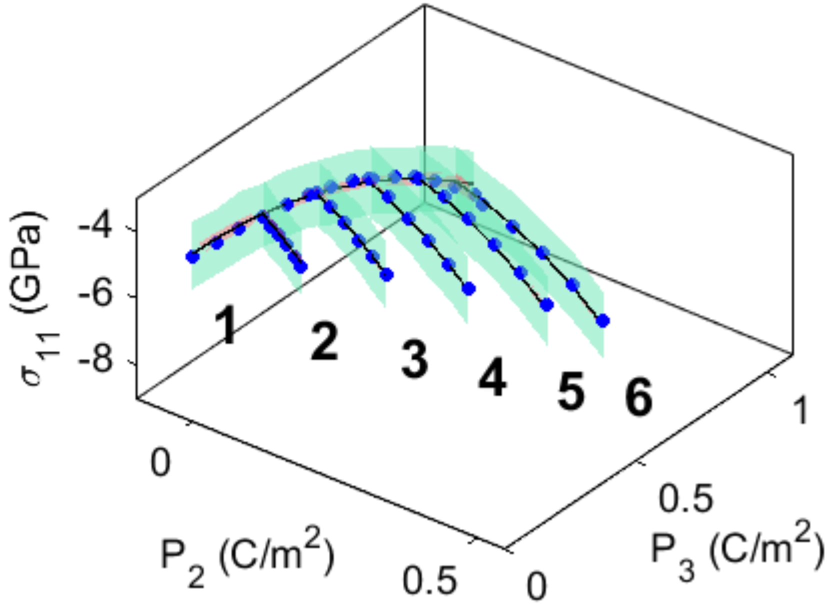


Figure: (Left) Uncertainty propagation through energy model. (Right) uncertainty in normal stress in the x_1 direction. Stress response not shown for σ_{22}, σ_{33}, and σ_{23}.

Polydomain Analysis: 180° Domain Walls

- Reported domain wall energy[3]

$$E_{180^\circ} = 132\frac{mJ}{m^2}$$

- Energy associated with domain wall

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

- Domain wall width
  - Same order as lattice constant
  - $L_{180^\circ} \sim a \approx 3.9$ Å

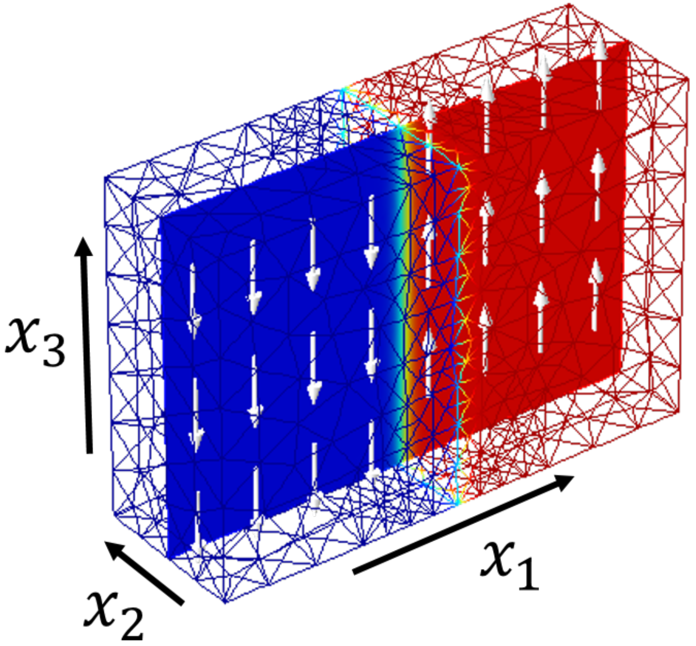


Figure: 180° domain wall – two distinct polarization regions. On the left (blue) we have polarization in the negative x_3 direction and on the right (red) the polarization is in the positive x_3 direction. The polarization switches by 180° as you pass through the domain wall.

3. Meyer, B. and Vanderbilt, D., “First-principles investigation of ferroelectricity in perovskite compounds,” *Physical Review B* **49**(9), 5828 (1994)

Polydomain Analysis: Theory

- Recall: $u\left(P_i, P_{i,j}, \varepsilon_{ij}\right) = u_M\left(\varepsilon_{ij}\right) + u_L(P_i) + \ u_C\left(P_i, \varepsilon_{ij}\right) + u_G\left(P_{i,j}\right)$
- Gradient energy

$$u_G = \frac{g_{11}}{2}\left(P_{1,1}^2 + P_{2,2}^2 + P_{3,3}^2\right) + g_{12}\left(P_{1,1}P_{2,2} + P_{1,1}P_{3,3} + P_{2,2}P_{3,3}\right)$$

$$+ \frac{g_{44}}{2}\left[\left(P_{1,2} + P_{2,1}\right)^2 + \left(P_{1,3} + P_{3,1}\right)^2 + \left(P_{2,3} + P_{3,2}\right)^2\right]$$

- Governing equation

$$\left(\frac{\partial u}{\partial P_{3,1}}\right)_{,1} - \frac{\partial u}{\partial P_3} = 0 \longrightarrow$$

$$2(\alpha_1 - q_{11}\varepsilon_{33} - q_{12}(\varepsilon_{11} + \varepsilon_{22}))\, P_3 + 4\alpha_{11}P_3^3 + 6\alpha_{111}P_3^5 = g_{44}P_{3,11}$$

Polydomain Analysis: Theory

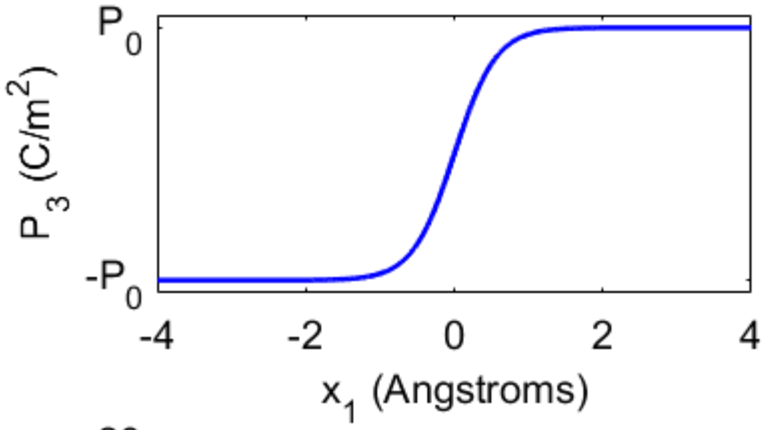
- Solution

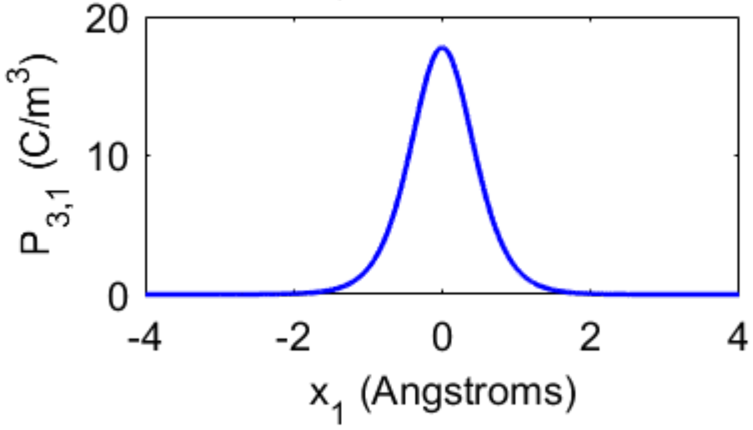
$$P_3(x_1) = \frac{P_0 \sinh\left(\frac{x_1}{\xi_{180}}\right)}{\left[A + \sinh^2\left(\frac{x_1}{\xi_{180}}\right)\right]^{1/2}}$$

Where

$$\xi_{180} = \frac{\sqrt{g_{44}}}{P_0\left(6\alpha_{111}P_0^2 + 2\alpha_{11}\right)^{\frac{1}{2}}}$$

$$A = \frac{\left(3\alpha_{111}P_0^2 + \alpha_{11}\right)}{2\alpha_{111}P_0^2 + \alpha_{11}}$$





Polydomain Analysis: Uncertainty Quantification

- Exchange parameter uncertainty is small
  - Deviation $\sim \mathcal{O}(10^{-7})$
  - Calibrating scalar energy

- How does uncertainty from monodomain affect the energy?

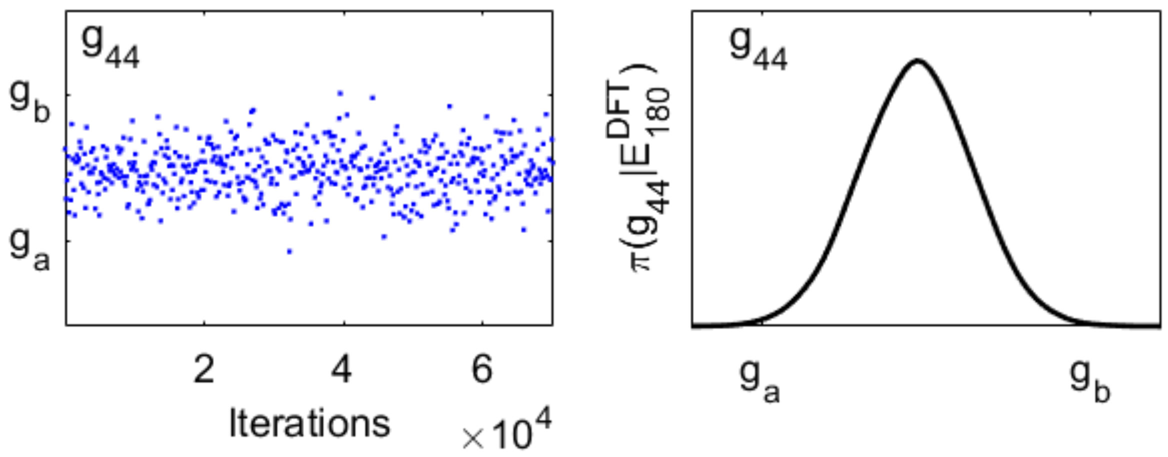


Figure: (a) Marginal posterior density for g_{44}. (b) Sample chain from MCMC simulation of parameter g_{44}. The axes labels are: $[g_a, g_b] = [5.587741948\times10^{-6}, 5.587741962\times 10^{-6}]$.

Polydomain Analysis: Uncertainty Propagation

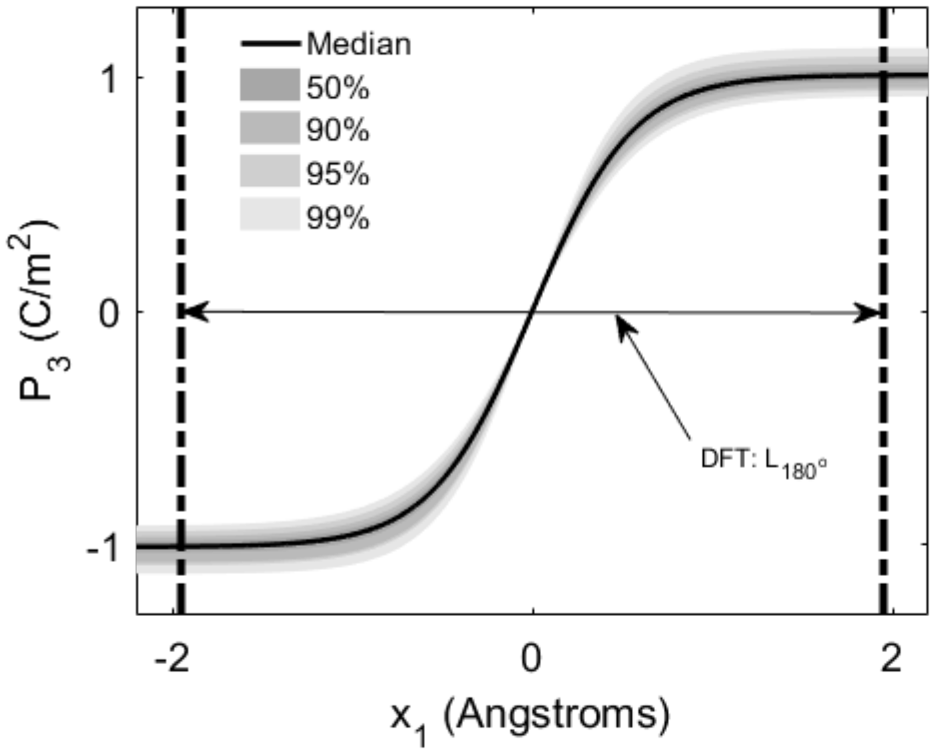


Figure: Polarization in 180° domain wall.

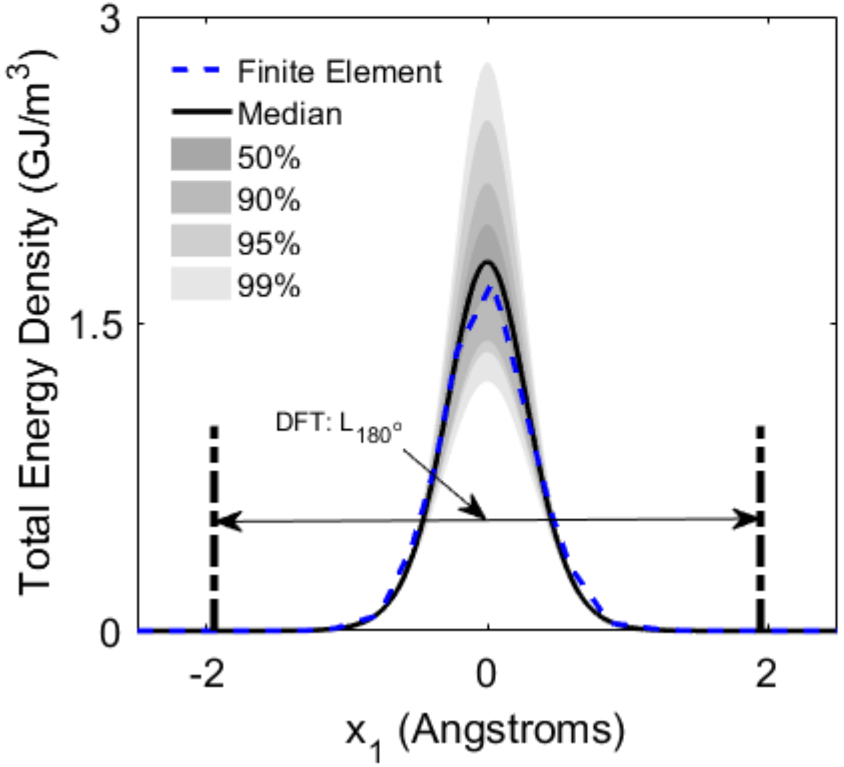


Figure: 180° domain wall – excess energy along x_1 axis as you go through the domain wall.

Conclusions & Future Work:

- Conclusions:
  - Quantified uncertainty in phase field model parameters.
  - Propagated uncertainty to assess model limitations.
  - Compared theoretical solution of $180°$ domain wall with finite element model.
- Future Work:
  - Uncertainty analysis of $90°$ domain wall?
  - Parameter correlation: monodomain & polydomain structures?
  - Global sensitivity[4]?

4. Collaborative effort with Dr. Ralph Smith and Lider Leon at North Carolina State University.

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