Modelling of Ferroelectric Vortex Lattice with COMSOL

Marvin Degen

COMSOL Nutzertreffen | June, 26th 2024

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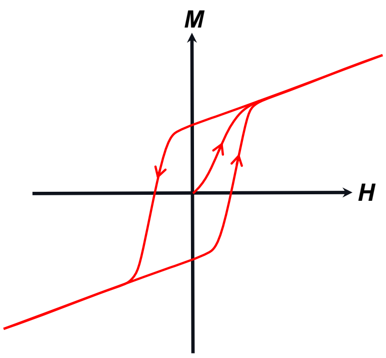
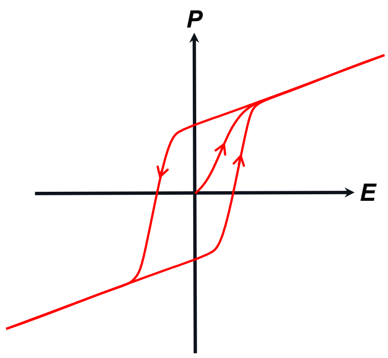
Introduction





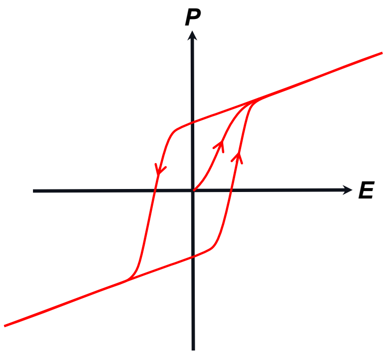
Introduction

Application

- Varactors (adjustable capacitor)
- Memory (RAM)
- Sensors (Piezeelectric properties)
- Integrated photonics
- …

Materials

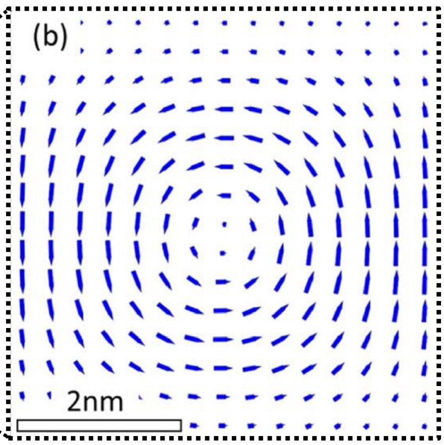
- $BaTiO_3$ (BTO)
- $SrTiO_3$ (STO)
- $PbTiO_3$ (PTO)
- $MgTiO_3$
- $CaTiO_3$
- …



Introduction

Strained multilayers

- New polarization topologies
  - Vortex-antivortex lattice
  - Skyrmions

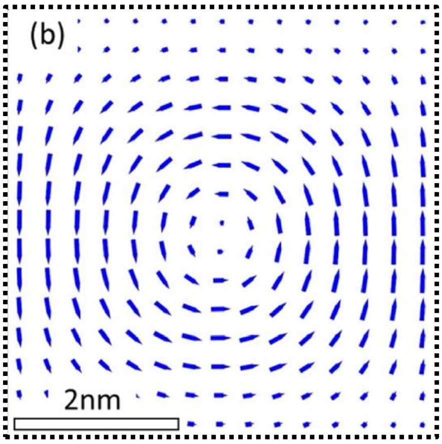


[1] Z. Hong et al., "Stability of Polar Vortex Lattice in Ferroelectric Superlattices," *Nano Letters*, vol. 17, no. 4, pp. 2246-2252, Apr. 2017.

Introduction

Strained multilayers

- New polarization topologies
  - Vortex-antivortex lattice
  - Skyrmions
- Interaction of EM-Waves with the Ferroelectric vortex lattice
  - → Anomalous scattering in the sub-THz band



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Numerical Modeling – Phase Field Model

Minimizing Free Energy

$$F = \int \left(\alpha_{ij} P_i P_j + \alpha_{ijk\ell} P_i P_j P_k P_\ell + \alpha_{ijklmn} P_i P_j P_k P_\ell P_m P_n + \frac{1}{2} g_{ijkl} \frac{\partial P_i}{\partial x_j} \frac{\partial P_k}{\partial x_\ell} + \frac{1}{2} c_{ijkl} \varepsilon_{ij} \varepsilon_{kl} - q_{ijkl} \varepsilon_{ij} P_k P_\ell - \frac{1}{2} \kappa_b E_i E_i - E_i P_i \right) \mathrm{d}V$$

- Dependant variables:
  - Polarization $\boldsymbol{P} = [P_x, P_y, P_z]^{\mathrm{T}}$
  - Mech. displacement $\boldsymbol{u} = [u_x, u_y, u_z]^{\mathrm{T}}$
  - El. potential φ

- Time-dependent Landau-Ginzburg-Devonshire equation: $\mu \ddot{P}_i + \gamma \dot{P} = -\frac{\delta F}{\delta P_i}$
- → Substrate effects and boundary conditions (including displacements) needs to be taken into account

$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial j} + \frac{\partial u_j}{\partial i}\right)$: total strain, α: Landau coefficients, g: gradient energy coefficients, c: Elastic stiffness, q: Electrostrictive coupling coefficients, κ_b: Background permittivity

Numerical Modeling – Simplyfied Model

Non-atomistic, steady state model

- Reducing complexity to a minimum:
  - All mechanical effects are considered in modified Landau coefficients a [1]
  - Considering only a single layer
  - Steady-State solution: $\frac{\mathrm{d}}{\mathrm{d}t} = 0$
  - Assuming 2D
- Free energy is expressed depending on $\boldsymbol{P} = \left[P_x, P_y\right]^{\mathrm{T}}$, $\boldsymbol{E} = \left[E_x, E_y\right]^{\mathrm{T}}$

$$2\, a_1 P_x + \mathrm{h.o.t.} - g_0 \left(\frac{\partial^2 P_x}{\partial x^2} + \frac{\partial^2 P_x}{\partial z^2}\right) = E_x \qquad (1.1)$$

$$2\, a_3 P_x + \mathrm{h.o.t.} - g_0 \left(\frac{\partial^2 P_z}{\partial x^2} + \frac{\partial^2 P_z}{\partial z^2}\right) = E_z \qquad (1.2)$$

$$\nabla \cdot \boldsymbol{D} = \boldsymbol{0} \quad \rightarrow \quad \frac{\partial D_x}{\partial x} + \frac{\partial D_z}{\partial z} = 0 \qquad (1.3)$$

$$\nabla \times \boldsymbol{E} = \boldsymbol{0} \quad \rightarrow \quad \frac{\partial E_x}{\partial z} = \frac{\partial E_z}{\partial x} \qquad (1.4)$$

$$F = \int \begin{pmatrix} a_1 P_x^2 + a_3 P_z^2 + a_{11} P_x^4 + a_{33} P_z^4 + a_{12} P_x^2 P_z^2 + a_{111}(P_x^6 + P_z^6) + a_{112}(P_x^4 P_z^2 + P_x^2 P_z^4) \\ + \frac{g_0}{2}\left[\left(\frac{\partial P_x}{\partial x}\right)^2 + \left(\frac{\partial P_x}{\partial z}\right)^2 + \left(\frac{\partial P_z}{\partial x}\right)^2 + \left(\frac{\partial P_z}{\partial z}\right)^2\right] - \frac{1}{2}\varepsilon_0 \varepsilon_{\mathrm{r},11} E_x^2 - \frac{1}{2}\varepsilon_0 \varepsilon_{\mathrm{r},33} E_z^2 - E_x P_x - E_z P_z \end{pmatrix} \mathrm{d}V$$

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Numerical Modeling – Simplyfied Model

Non-atomistic, steady state model

- Using $D_i = \varepsilon_0 \varepsilon_{\mathrm{r},jj}\, E_i + P_i$, (1.3) can be rewritten as
  $$\varepsilon_0 \varepsilon_{\mathrm{r},11} \frac{\partial E_x}{\partial x} + \varepsilon_0 \varepsilon_{\mathrm{r},33} \frac{\partial E_z}{\partial z} = -\frac{\partial P_x}{\partial x} - \frac{\partial P_z}{\partial z}$$
- (1.4) can be rewritten as
  $$\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} = 0$$

$$2\, a_1 P_x + \mathrm{h.o.t.} - g_0 \left(\frac{\partial^2 P_x}{\partial x^2} + \frac{\partial^2 P_x}{\partial z^2}\right) = E_x \qquad (1.1)$$

$$2\, a_3 P_x + \mathrm{h.o.t.} - g_0 \left(\frac{\partial^2 P_z}{\partial x^2} + \frac{\partial^2 P_z}{\partial z^2}\right) = E_z \qquad (1.2)$$

$$\frac{\partial D_x}{\partial x} + \frac{\partial D_z}{\partial z} = 0 \qquad (1.3)$$

$$\frac{\partial E_x}{\partial z} = \frac{\partial E_z}{\partial x} \qquad (1.4)$$

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Numerical Modeling – Simplyfied Model

Non-atomistic, steady state model

$$\boxed{\nabla\cdot\Gamma = f}$$

$$\nabla\cdot\overbrace{\begin{bmatrix} -g_0\dfrac{\partial P_{x(y)}}{\partial x}\\ -g_0\dfrac{\partial P_{x(y)}}{\partial z}\end{bmatrix}}^{\Gamma} = \overbrace{E_{x(y)} - 2\,a_{1(3)}P_{x(y)} - \mathrm{h.o.t.}}^{f}$$

$$\nabla\cdot\begin{bmatrix}\varepsilon_0\varepsilon_{\mathrm{r},11}\,E_x\\ \varepsilon_0\varepsilon_{\mathrm{r},33}\,E_z\end{bmatrix} = -\frac{\partial P_x}{\partial x} - \frac{\partial P_z}{\partial z}$$

$$\nabla\cdot\begin{bmatrix}-E_z\\ E_x\end{bmatrix} = 0$$

$$2\,a_1P_x + \mathrm{h.o.t.} - g_0\left(\frac{\partial^2P_x}{\partial x^2}+\frac{\partial^2P_x}{\partial z^2}\right) = E_x \quad (1.1)$$

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$$\varepsilon_0\varepsilon_{\mathrm{r},11}\frac{\partial E_x}{\partial x} + \varepsilon_0\varepsilon_{\mathrm{r},33}\frac{\partial E_z}{\partial z} = -\frac{\partial P_x}{\partial x} - \frac{\partial P_z}{\partial z} \quad (1.3)$$

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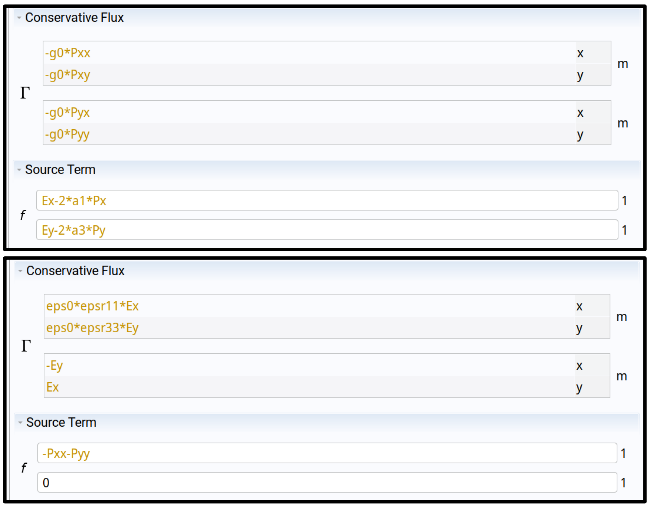
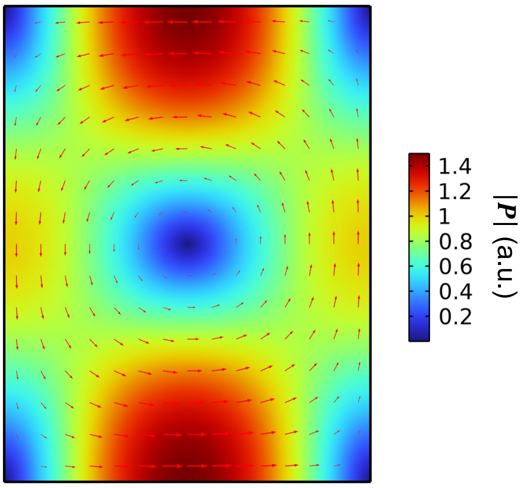


Numerical Modeling – Simplyfied Model

Non-atomistic, steady state model

- Dirichlet boundary condition for E_x and E_y at all boundaries
- Zero flux boundary condition for P_x and P_y
- Anti-periodic boundary condition P_x and P_y at left & right boundary

Polarization



Numerical Modeling – Simplyfied Model

Non-atomistic, steady state model

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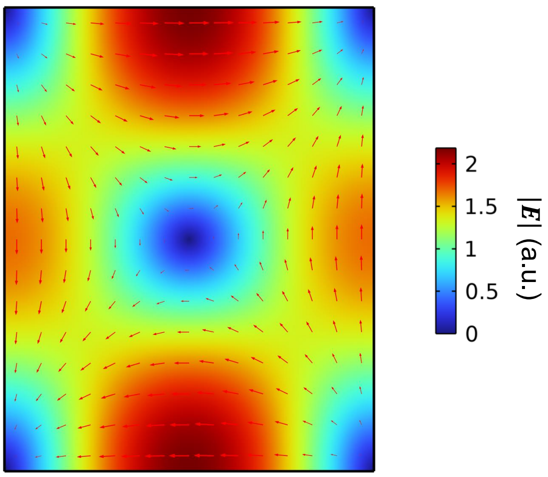
Electric Field



Outlook

Electrodynamic Model

- Modelling the evolution of polar vortices by solving the time-dependent Landau-Ginzburg-Devonshire equation:
  $\mu \ddot{P}_i + \gamma\, \dot{P} = -\frac{\delta F}{\delta P_i}$
- Modelling the interaction with an external Electromagnetic wave
- Electrodynamic model:
  - $\nabla \times \boldsymbol{E} = -\mu_0 \frac{\partial \boldsymbol{H}}{\partial t} \leftrightarrow \frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} = -\mu_0 \frac{\partial H_z}{\partial t}$
  - $\nabla \times \boldsymbol{H} = \frac{\partial \boldsymbol{D}}{\partial t} \leftrightarrow \frac{\partial H_z}{\partial y} = \frac{\partial D_x}{\partial t} = \varepsilon_0 \varepsilon_{\mathrm{r},11} \frac{\partial E_y}{\partial t} + \frac{\partial P_y}{\partial t}$
- Dependent variables: P_x, P_y, E_x, E_y, H_z

Governing Equations

$$-L\left(2a_1 P_x + \mathrm{h.o.t.} - g_0 \left[\frac{\partial^2 P_x}{\partial y^2} + \frac{\partial^2 P_x}{\partial x^2}\right] - E_x\right) = \frac{\partial P_x}{\partial t}$$

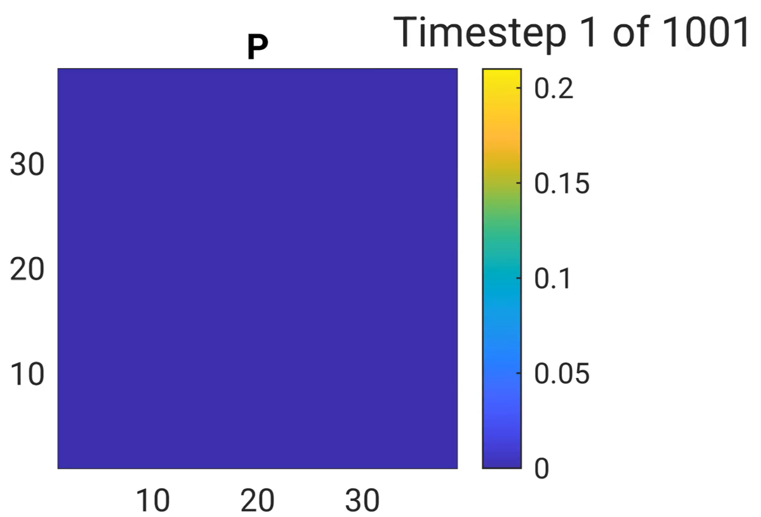
$$-L\left(2a_3 P_y + \mathrm{h.o.t.} - g_0 \left[\frac{\partial^2 P_y}{\partial y^2} + \frac{\partial^2 P_y}{\partial x^2}\right] - E_y\right) = \frac{\partial P_y}{\partial t}$$

$$\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} = -\mu_0 \frac{\partial H_z}{\partial t}$$

$$\varepsilon_0 \varepsilon_{11} \frac{\partial E_x}{\partial t} + \frac{\partial P_x}{\partial t} = \frac{\partial H_z}{\partial y}$$

$$\varepsilon_0 \varepsilon_{33} \frac{\partial E_y}{\partial t} + \frac{\partial P_y}{\partial t} = -\frac{\partial H_z}{\partial x}$$

Outlook



Thank you for your attention!

Marvin Degen
University of Duisburg-Essen, Faculty of Engineering
General and Theoretical Electrical Engineering (ATE)
marvin.degen@uni-due.de

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