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Phase Field Simulations of Ferroelectric Materials Using Open Source Software

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Summary

Ferroelectric materials are currently a topic of great interest in electronics. They are the electric equivalent of ferromagnetic materials, where the material polarization can be switched between stable states by the application of an electric field. The effect is nonlinear, and can be modeled with phase field simulations using the polarization as a variable of state. In this presentation, I demonstrate how the phase field simulations can be set up using the open source finite elements software package FEniCSx.

1 Introduction

The ferroelectric effect occurs in materials where several stable states of spontaneous polarization exist, with both pyroelectric and piezoelectric effects [1–3]. A classical phenomenological model is the Landau-Khalatnikov equation to be solved together with Gauss' law [4]

$$\frac{\partial P}{\partial t} = \nabla \cdot (g \nabla P) - \alpha P - \beta P^3 - \gamma P^5 - \sigma \frac{\partial V}{\partial z} \tag{1}$$

$$0 = \nabla \cdot [\varepsilon(-\nabla V) + P\hat{z}] \tag{2}$$

This can be considered as a nonlinear reaction-diffusion equation, often seen in chemical engineering. A typical length scale at steady state and zero potential emerges as $\sqrt{g/|\alpha|}$, which is the approximate domain wall thickness, which may be as thin as only a few lattice constants.

2 Finite element implementation

The system of equations is put in weak form by multiplying with test functions Q and ϕ, and integrating over the domain of interest Ω (enforcing Dirichlet conditions on electrode boundaries by embedding them into the function space, and assuming Neumann boundary conditions on remaining boundaries):

$$\int_\Omega Q \frac{\partial P}{\partial t}\,\mathrm{d}x = -\int_\Omega \nabla Q \cdot g \nabla P\,\mathrm{d}x - \int_\Omega Q(\alpha P + \beta P^3 + \gamma P^5)\,\mathrm{d}x - \int_\Omega Q\sigma \frac{\partial V}{\partial z}\,\mathrm{d}x - \int_\Omega \nabla\phi \cdot \nabla V\,\mathrm{d}x + \int_\Omega \nabla\phi \cdot P\hat{z}\,\mathrm{d}x \tag{3}$$

This equation can be implemented almost verbatim using the Unified Form Language (UFL) in the open source finite element software FEniCSx, `https://fenicsproject.org/`. The time derivative can be discretized, and the resulting system stepped in time using a Newton solver.

3 Results

As an example, a structure consisting of a slab of ferroelectric material in combination with a dielectric and a sinusoidal voltage source as depicted in Figure 1 has been implemented. The switching dynamics as the voltage changes sign is depicted using the traditional hysteresis diagram in the right part of Figure 1, as well as the time evolution of the polarization for different amplitudes of the voltage. It is seen that low voltages are not able to switch the ferroelectric, whereas high voltages significantly distort the sinusoidal waveform. The spatial distribution of the initial stages of the switching is depicted in Figure 2, starting from a random state.

4 Conclusions

We have demonstrated how ferroelectric materials can be simulated using phase field models in open source software. This enables a flexible and transparent simulation platform at low cost. Further examples will be elaborated upon in the presentation.

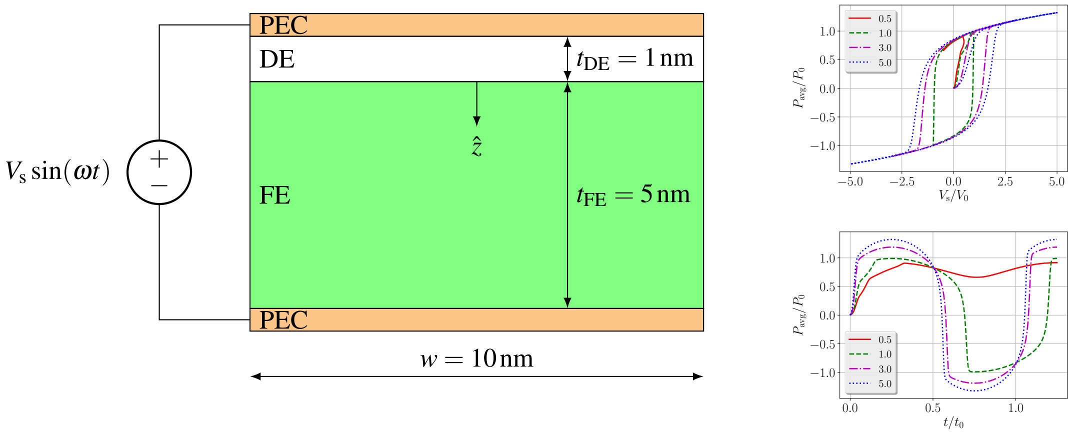

Figure 1. Geometry of the simulation, a ferroelectric slab (FE) interacting with a dielectric (DE) and clamped between two perfect electric conductors (PEC) with a time varying voltage $V_{\mathrm{s}}\sin(\omega t)$. The graphs on the right show the hysteresis and time evolution of the polarization for different amplitudes V_{s}.

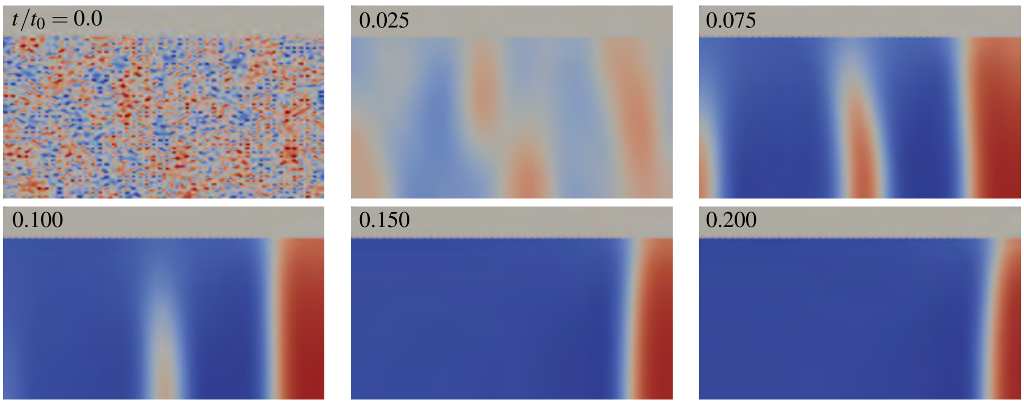

Figure 2. Switching dynamics of the setup in Figure 1. The graphs depict the distribution between positive polarization (blue) and negative polarization (red) at different times.

References

[1] K. M. Rabe, M. Dawber, C. Lichtensteiger, C. H. Ahn, and J.-M. Triscone, "Modern physics of ferroelectrics: Essential background," *Physics of Ferroelectrics*, pp. 1–30, 2007.

[2] V. Fridkin and S. Ducharme, *Ferroelectricity at the Nanoscale*, ser. NanoScience and Technology,. Berlin, Heidelberg :: Springer Berlin Heidelberg, 2014. [Online]. Available: http://dx.doi.org/10.1007/978-3-642-41007-9

[3] A. K. Saha and S. K. Gupta, "Negative capacitance effects in ferroelectric heterostructures: A theoretical perspective," *Journal of Applied Physics*, vol. 129, no. 8, p. 080901, 2021.

[4] A. Maslovskaya, L. Moroz, A. Y. Chebotarev, and A. E. Kovtanyuk, "Theoretical and numerical analysis of the Landau–Khalatnikov model of ferroelectric hysteresis," *Communications in Nonlinear Science and Numerical Simulation*, vol. 93, p. 105524, 2021.