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Phase-field simulation of Piezoresponse Force Microscopy

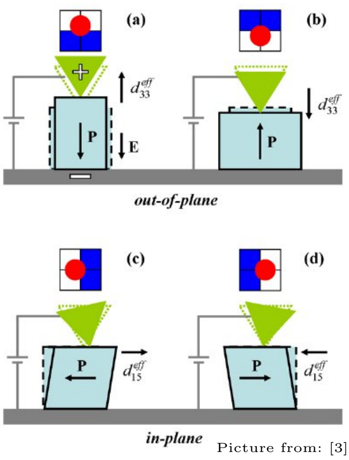
ITN NANOMOTION (project 1D: Finite-element modeling of electromechanically coupled materials)

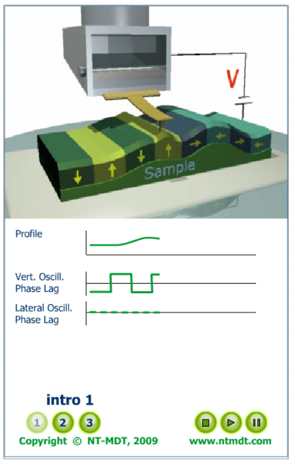
The overall goal of the Initial Training Network (ITN) NANOMOTION is to investigate the properties of multi-functional materials (as e.g. piezoelectrics, ferroelectrics, multiferroics) by using nano-electro-mechanical techniques. New nano-electro-mechanical tools like Piezoresponse Force Microscopy (PFM), Electrochemical Strain Microscopy (ESM), and their combination with traditional Scanning Probe Microscopies (SPM) can be used to study these materials in detail. The present project focuses on the modeling of non-linear electro-mechanical effects that occur during PFM measurements based on the phase-field method.

`http://www.itn-nanomotion.eu`

Piezoresponse Force Microscopy

The Piezoresponse Force Microscopy (PFM) can be used for the investigation of domain structures of ferroelectric materials. Its functionality is based on the electro-mechanical coupling of the ferroelectric material itself: by applying an electric bias through a tiny tip mounted at the end of a cantilever a deformation of the ferroelectric material is induced. The deformation is dependent on the orientation of the spontaneous polarization below the tip. By measuring the tip displacement detailed information can be derived about the domain configuration of the material [1].





Picture from: [3]

Thermodynamical framework: phase-field model

For the description of the ferroelectric material we use a phase-field formulation. The underlying potential is given as (c.f. [2])

$$H := H^{bulk}(\boldsymbol{\varepsilon}, \boldsymbol{E}, \boldsymbol{P}^r) + H^{int}(\nabla \boldsymbol{P}^r) + H^{sep}(\boldsymbol{P}^r)$$

where H^{bulk} is the bulk material electric enthalpy, H^{int} is the interface energy, and H^{sep} is the phase-separation energy. The idea of phase-field modeling is to choose an order parameter for the description of the phases of the material (here given by the remanent polarization $\boldsymbol{P}^r$) and to use the time-dependent Ginzburg-Landau equation for the evolution of the order parameter.

The evolution equation for the remanent polarization arises as

$$\dot{\boldsymbol{P}}^r = -\alpha \frac{\delta H}{\delta \boldsymbol{P}^r} = -\alpha \left(\frac{\partial H}{\partial \boldsymbol{P}^r} - \operatorname{div} \frac{\partial H}{\partial \nabla \boldsymbol{P}^r} \right) \quad \text{with} \quad \alpha > 0.$$

The kinematical quantities and balance equations are given by

$$\boldsymbol{\varepsilon} = \nabla^s \boldsymbol{u} \qquad \mathbf{E} = -\nabla \phi$$
$$\nabla \cdot \boldsymbol{\sigma} + \boldsymbol{f} = \mathbf{0} \qquad \nabla \cdot \mathbf{D} = q$$

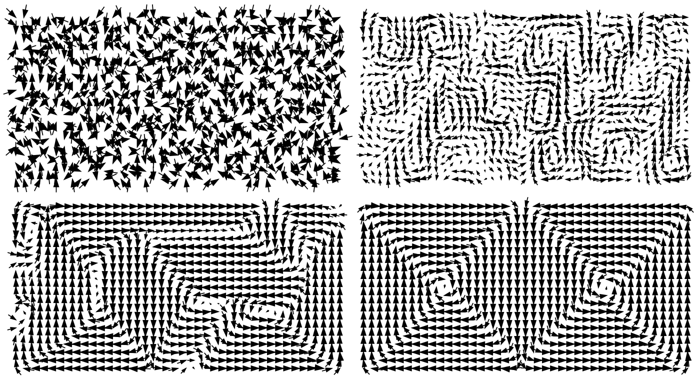
The model is implemented into the Finite-Element Method. For the time discretization we use the implicit Euler scheme

$$\dot{\boldsymbol{P}}^r \approx \frac{\boldsymbol{P}^r - \boldsymbol{P}^r_n}{\Delta t}$$

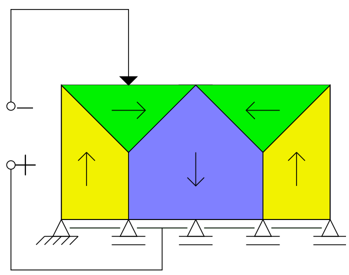
where $\boldsymbol{P}^r_n$ at time t_n is known and $\boldsymbol{P}^r$ is the unknown.

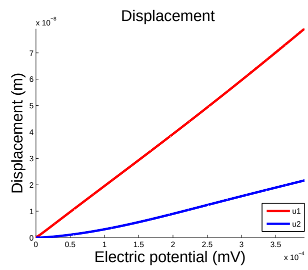
Numerical examples

As a first example we simulate the domain evolution of a rectangular body under charge-free boundary conditions. The initial configuration is given by randomized remanent polarizations.



In a second example, we analyze the deformation of a ferroelectric microstructure under electric bias applied by a PFM tip.





As expected, the surface displacement is proportional to the electric bias. Future developments will aim at simulating PFM by using a fully resolved tip geometry in contact with the sample.

References

[1] A. L. Kholkin, S. V. Kalinin, A. Roelofs, and A. Gruverman, in: *Scanning Probe Microscopy* pp.173–214, 2006.

[2] D. Schrade, R. Müller , B.-X. Xu and D. Gross, *Comput. Mech. in App. Mech. Eng.* 196:4365–4374, 2007.

[3] http://www.azonano.com: Piezoresponse Force Microscopy (PFM) - Introduction, Principles and Instrumental Aspects of Piezoresponse Force Microscopy by NT-MDT

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