Seminar

17. Februar 2010 15:30h HS 44-465

TECHNISCHE UNIVERSITÄT KAISERSLAUTERN

zu folgendem Vortrag wird herzlich eingeladen:

Evolution of ferroelectric domain structures on the nanoscale

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With the use of a phase field model we investigate tetragonal ferroelectric single crystals on the nanoscale. Such crystals have six crystal variants, each with its own particular polar direction and strain state. The geometric arrangement of the domains is a crucial factor that determines the behaviour of a nanostructure. Depending on the size and the boundary conditions of the single crystal the domain structure adopts a low-energy, compatible configuration. On the nanoscale, only small numbers of domains are expected. Therefore, commonly occurring arrangements of domains with particular properties evolve.

Our simulations focus on the evolution of domain structures in cuboidal regions of single crystal material of length l and height h, with electrically insulated and traction-free surfaces. We limit consideration to problems with no internal charges or body forces. Depending on the aspect ratio h/l we demonstrate the existence of transitions in the equilibrium domain topology. A rotationally symmetric hexadomain vortex structure is identified as an equilibrium state of the cube (aspect ratio = 1), see Münch & Huber [1]. However, relatively small changes in aspect ratio result in a transition to a well-known four domain plane vortex structure. Then, the evolution of these structures under mechanical and electrical loads is studied.

In previous work, the existence of known domain topologies has been used to analyze ferroelectric microstructure and its evolution under electrical and mechanical loads, see e.g. Huber & Cocks [2], Rödel [3], Weng & Wong [4]. Two dimensional plane strain models of domain evolution are widespread and are able to characterize a great spectrum of ferroelectric single crystal behaviour. However the real crystals have three dimensional nature and produce microstructure domain topologies that cannot be found in two dimensions. This motivates the present, three dimensional study.

In this work, a 3D phase field model is used which has its origins in the work of Fried & Gurtin [5, 6], Gurtin [7], Su & Landis [8, 9]. The model uses electrical polarization $\mathbf{P}$ as the order parameter. For isothermal processes below the Curie temperature this model yields the commonly accepted Ginzburg-Landau equation for the evolution of the polarization. From a physical point of view, this describes the rearrangement of atoms within unit cells when phase interfaces move through the material. Mechanically, the model assumes a Boltzmann continuum with small deformations and rotations. This gives a symmetric Cauchy stress $\boldsymbol{\sigma}$ and motivates the symmetric strain measure $\boldsymbol{\varepsilon} := \mathrm{sym}[\mathrm{Grad}[\mathbf{u}]]$, where $\mathbf{u}$ is the displacement field. The standard balance of momentum as well as the Cauchy theorem are also incorporated. Electrically, the model assumes the Maxwell-Faraday equations for quasi-static electromagnetic fields. Analogous to the mechanical displacement is an electric potential φ from which the curl free, quasi-static electric field $\mathbf{E} := -\mathrm{Grad}[\varphi]$ is derived.

We follow the work of Landis [8, 9] who postulated a form of free energy which matches the elastic, piezoelectric, and dielectric properties of the tetragonal ferroelectric barium titanate. A three field (polarization, displacement and electric potential) variational statement enforces the weak form of the Ginzburg-Landau equation as well as the mechanical and electrical equilibrium laws described above. This is the basis of a standard finite element formulation that allows equilibrium states to be found. Since the initial conditions in the model are often far from equilibrium, a backward Euler scheme is used for time integration, with a mobility associated with the polarization. The resulting polarization rates follow the Ginzburg-Landau equation and satisfy the second law of thermodynamics. The mobility thus provides a physically consistent way of approaching equilibrium solutions while maintaining computational stability.

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