Phase-field simulation and design of a ferroelectric nano-generator

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1. Introduction

We study the behavior of ferroelectric material (BaTiO₃) for the design of a nano-generator to convert mechanical into electrical energy. We simulate structured ultrathin layers of ferroelectric material epitaxially sputtered onto a substrate. Thin films adopt to the lattice parameters of the substrate which cause interfacial strains in case of lattice misfit. Our investigations consider a standard finite element method with electro-mechanical phase-field theory having the electric polarization as state variable.

2. Foundation of the model

To determine domain evolution mechanisms phase-field modeling is an appropriate method since all necessary electrical and mechanical boundary conditions can be incorporated. Polarization is accompanied with lattice distortion resulting in spontaneous strain ε_s. Within the ferroelectric body B the electrostatic field equations for the electrical field E and the electric displacement D are fulfilled via

\[ E := \text{Grad}[φ]\text{, } \text{Div}[D] = q \text{ in } B \]

where \( φ \) is the electric potential and \( q \) is the volume charge density. The standard balance equations appear as

\[ \text{Div}[σ] + b = 0 \text{ , } σ = σ^T \text{ in } B \]

with the Cauchy stress tensor \( σ \) and the body forces per unit volume \( b \). The boundary conditions on the surface are

\[ φ = \tilde{ψ} \text{ , } D \cdot n = \tilde{ω} \text{ , } u = \tilde{u} \text{ , } ε \cdot n = \tilde{t} \text{ on } ∂B . \]

The unit vector \( n \) is normal to the surface, \( ω \) is the surface charge density, \( u \) is the displacement vector, and \( t \) are the surface tractions. Following the Landau-Devonshire theory we consider the Helmholtz free energy density:

\[ \psi = \frac{1}{2} \left[ \frac{1}{2} (L_{ij} P P^{T}) + \frac{1}{2} (L_{ij} P P^{T}) + \frac{1}{2} (L_{ij} P P^{T}) \right] + \frac{1}{2} \left( \frac{1}{2} L_{ij} P P^{T} + \frac{1}{2} L_{ij} P P^{T} + \frac{1}{2} L_{ij} P P^{T} \right) \]

Herein, terms \( (a,b) \) denote scalar products of the arguments \( a \) and \( b \) being vectorial or tensorial quantities \( P \) is the material polarization and \( ε_0 = 8.854 \times 10^{-12} \text{ C/Vm} \) is the permittivity of the free space. The tensors \( a_{ijkl}, b_{ijkl}, c_{ijkl}, d_{ijkl} \) represent the continuum material parameters of BaTiO₃.

3. Nano-generator simulation

We consider a thin film of 10 nm thickness deposited on an electrically conductive substrate and structured to the dimensions in Fig. 1. The biaxial epitaxial strain \( ε_b = 0.5, 0 = 0.41\% \) at the interface is provoked by differing lattice parameters.

Figure 1: Design and dimensions of the nano-generator. The lithographically patterned partial top electrode covers 75% of the top surface.

A partial top electrode covers 75% of the surface. The finite element mesh for the simulation uses 16 elements in lateral direction, 96 elements in longitudinal direction and 16 elements in thickness direction.

The mechanical straining process deforms the conductive substrate uniaxial and homogeneous, e.g. via bending. Two hysteresis loops \( ε_b / ε_0 ∈ [0,0.5] \) and \( ε_b / ε_0 ∈ [0.5, −0.3] \) are simulated, both starting with the intrinsic strain of \( ε_b / ε_0 = 0.5 \). Compressing the substrate periodically to \( ε_b = 0 \) leads to a fully reversible domain shifting process, shown in Fig. 2 a) - c).

In the second hysteresis loop the nano-generator acquires an interfacial strain up to \( ε_b / ε_0 = −0.3 \). A realignment of domains can be observed, depicted in Fig. 2 a) - h). This leads to a polarity reversal within the ferroelectric. The normalized hysteresis loop for the averaged polarization \( P_{av} \) in thickness direction as a function of the interfacial strain \( ε_b \) is shown in Fig. 3.

Figure 3: Normalized hysteresis loop caused by mechanical deformation as function of the interfacial strain \( ε_b \). Red loop is in case of a strain interval \( ε_b / ε_0 ∈ [0,0.5] \), blue loop from \( ε_b / ε_0 ∈ [0.5, −0.3] \). Prominent points a) - h) accord to the states in Fig. 2.