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Numerical Study of Switching Behavior in Finite Media Subject to 3D Ferroelectric-Paraelectric Interactions and Inspection of Calibration Effects

P.-W. Martelli* and S.M. Mefire

Université de Lorraine, CNRS, IECL, F-54000 Nancy, France

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Abstract. We study numerically the switching behavior aspects and calibration effects relative to finite media embedding fully a three-dimensional ferroelectric layer in a paraelectric environment. Our approach makes use of the Ginzburg-Landau formalism in combination with the electrostatics equations. The associated discrete nonlinear system, which arises from finite element approximations, is solved by an inexact Newton method. The resulting numerical experiments highlight the effects of a balance between the physical and geometrical parameters. In particular, the same state switchings can be retrieved from different ferroelectric layer sizes by acting upon the physical characteristic of the paraelectric environment. Ferroelectric platelet samples are in parallelepipedic and cylindrical configurations involved in these experiments.

AMS subject classifications: 82D45, 82D80, 78A25, 35Q56, 47H10, 65N30, 49M15

Key words: Electroactive media, ferroelectricity, electrostatics, Ginzburg-Landau systems, finite elements, inexact Newton methods, numerical simulations.

1. Introduction

For performing a relevant numerical investigation of structures comprised of a ferroelectric layer embedded in a paraelectric environment, a method involving a description as accurate as possible of the interplay between the spontaneous polarization and the long-range depolarization electric field caused by the same polarization is particularly suitable. For a finite-size sample, the depolarization field is distributed in the inner space and in the surrounding environment at the cost of an additional electrostatic energy. A notable property is that, even in the absence of the application of an external field, this inner space can be organized into a finite number of distinct regions, called the *domains*, in which the electric polarization is arranged uniformly [18]. Namely, the

*Corresponding author. *Email address:* pierre-william.martelli@ac-nancy-metz.fr (P.-W. Martelli)

depolarization electric field splits the finite-size ferroelectric sample into polarization domains.

Of course, when an external field is applied, the polarization domain patterning is subject to a complex behavior; the system is then characterized by various ferroelectric states. Recently, a work has been developed [13] to explicit how the Landau-Kittel structure [7–9] of 180° polarization domains is formed in finite-scale nanodot samples. In particular, it is highlighted in [13] that field and temperature applications allow to realize a controllable multibit switching; an effect leading thus to the ability to increase the volume of the writable information per nanodot. The approach used in [13] was introduced by Chenskii and Tarasenko [3]. It consists of completing the model of Ginzburg [5] that was based on the theory of phase transitions developed by Landau [9], with the electrostatics equations, in order to take into account long-range Coulomb interactions. This method, particularly suited to an accurate description of the interplay aforementioned, has been used also in a two-dimensional context involving periodic boundary conditions [10]. Moreover, it has been applied in the frame of certain three-dimensional ferroelectric devices [12, 13].

We deal here with this approach, and to dissociate the depolarization effects from the lattice deformation impacts, we consider *uniaxial* ferroelectric materials for which the ferroelastic coupling is small. In particular, in presence of such a material, the dependence of the electric polarization field on the electric field is namely nonlinear through only one of its components. Unlike in [13], where the simulations were associated with a cylindrical configuration and without an investigation of the influence of geometrical parameters, we are concerned with numerical variations of geometrical and physical parameters, moreover with the parallelepipedic configuration context. In contrast with [12], where is also presented the model related to the mentioned approach, the interest is here devoted on the one hand to considerations that are above all concrete as regards temperature applications too and on the other hand to a study of calibration effects. This interest leads us to analyze here the influence of physical and geometrical parameters, then both under concrete considerations of voltage potential and temperature applications. The present work deals thus with extensive numerical investigations for which the associated findings would aim at impregnating physical experiments. In particular, reference is made here to physical experiments that could be carried out by selecting, for instance, Sodium Nitrite ($NaNO_2$) as the model material for the ferroelectric layer [17].

This paper is subdivided in five sections. We consider in Section 2 a weak formulation based on the Ginzburg-Landau formalism and electrostatics system, suitable for uniaxial ferroelectric materials. In Section 3, we present the main algorithm that is used for solving the discrete nonlinear system deriving from finite element discretizations of the weak formulation. This is an iterative algorithm that combines two inexact Newton techniques. The first technique is an approach globalized with a *linesearch method* [15], which slowly converges for a large choice of initializations, whereas the second, a more standard one, converges faster but for a restricted choice of initializations. In Section 4, we develop an extensive study of the switching behavior aspects