Computers and Mathematics with Applications 76 (2018) 451–470

Contents lists available at ScienceDirect

Computers and Mathematics with Applications

journal homepage: www.elsevier.com/locate/camwa

Numerical modeling and investigations of 3D devices with ferroelectric layer fully embedded in a paraelectric environment

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

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

ARTICLE INFO

Article history:
Received 3 October 2017
Received in revised form 19 March 2018
Accepted 20 April 2018
Available online 31 May 2018

MSC:
82D45
82D80
35Q56
47H10
65N30
49M15

Keywords:
Electroactive media
Ferroelectricity
Ginzburg–Landau systems
Finite elements
Inexact Newton methods
Numerical simulations

ABSTRACT

We investigate three-dimensional devices made up of a ferroelectric layer that is fully embedded in a paraelectric environment, by modeling based on the Ginzburg–Landau formalism as well as on the Electrostatics equations, and boundary conditions that are suitable for applications. From finite element approximations and inexact Newton techniques for solving numerically the resulting nonlinear system, we develop two numerical protocols. The first protocol concerns a determination of states related to the system and incorporates a process of heating as well as of cooling of devices, in terms of the temperature, whereas the second one is devoted to the existence study of hysteresis loops. The efficiency of these protocols is particularly emphasized from numerical simulations.

1. Introduction

In the frame of the development of new memory concepts, the main desired qualities are the non-volatility of the stored information, the low power consumption and the low writing/reading times. Among the emerging concepts, the ferroelectric memory (FeRAM) has a significant lead over its competitors (see, e.g., [1]). The FeRAM is based on ferroelectric devices which have a hysteretic behavior and thus allow to store bits. The miniaturization required for associated applications led to the discovery of new nanoscopic properties of devices, due to long-range Coulomb interactions which are no longer negligible (see, e.g., [2]). A notable property is that the ferroelectric body can be organized into a finite number of distinct regions, the *domains*, separated by *domain walls*, in which the electric polarization field is in opposite directions. A pertinent numerical investigation of such devices requires thus a description of the polarization texture as accurate as possible, in terms of the physical and geometrical parameters.

Usually, two numerical approaches are considered for studying such devices: the approach based on first-principles simulations (see, e.g., [3,4]), related to a good accuracy but having the particularity to be however subject to expensive

* Corresponding author.
E-mail addresses: pierre-william.martelli@univ-lorraine.fr (P.-W. Martelli), seraphin.mefire@univ-lorraine.fr (S.M. Mefire).

https://doi.org/10.1016/j.camwa.2018.04.027
0898-1221/

CPU costs, and the approach that consists of solving Partial Differential Equations, namely very suited to a description of the parameters dependence as regards the results.

Two phases are in association with a ferroelectric body. At high-temperature, we have the paraelectric phase, in which the polarization field depends linearly on the electric field. Below a certain temperature, called the Curie temperature (see, e.g., [2]), this dependence becomes nonlinear: it is the ferroelectric phase. In the 1940s, V.L. Ginzburg applied the Landau phase transition theory to ferroelectricity (see, e.g., [5]). E.V. Chenskii and V.V. Tarasenko [6] had the idea, in 1985, to complete the original model in order to take into account the long-range Coulomb interactions, in particular by making also use of the Electrostatics equations.

Recently, I.A. Luk'yanchuck et al. [7] have established the universal properties of ferroelectric domains from this model together with periodic conditions, for the context of 2D devices made up of a ferroelectric film partly embedded in a paraelectric environment. In this work, we are concerned with 3D devices made up of a ferroelectric layer that is fully embedded in a paraelectric environment, and where the geometrical configurations of nanofilms, nanorods or nanodots can be considered. We are namely interested in an extended frame of investigations in the sense that the considerations of the physical and geometrical parameters can be also the ones that are not systematically in correspondence with particular concrete situations, in contrast with [8] where the considerations of the parameters are essentially related to applications by involving furthermore the geometrical context of nanodots.

This paper is subdivided in six sections. We start by describing a model based on the Ginzburg–Landau formalism and Electrostatics equations, together with boundary conditions that are suitable for applications, for studying such 3D devices. In Section 3, we associate a weak formulation with the nonlinear system that represents this model, and establish the existence of weak solutions. We are concerned, in Section 4, with a numerical approach using Finite Elements for the discretization of the formulation and inexact Newton techniques for solving the associated discrete nonlinear system. In Section 5, we develop two numerical protocols and present the obtained results. The first protocol is devoted to the determination of states, and incorporates also a process of heating as well as of cooling of devices, in terms of the temperature. The second one aims at investigating the existence of hysteresis loops. The performed numerical simulations deal with various considerations of geometrical and physical parameters. We report in Section 6 the concluding remarks.

2. The ferroelectric model

We are here interested in a model for the study of 3D devices made up of a ferroelectric layer that is fully embedded in a paraelectric environment. Let us represent geometrically such a device by an open bounded subset Ω of $\mathbf{R}^3$, and its fully embedded layer by an open subset Ω_f, $\overline{\Omega_f} \subset \Omega$, as well as its paraelectric environment by $\Omega_p = \Omega \setminus \overline{\Omega_f}$. Also, let us denote by S, $S = \partial\Omega$, the boundary of Ω, and by S_f, $S_f = \overline{\Omega_f} \cap \overline{\Omega_p}$, the interface between Ω_f and Ω_p. The region Ω is also such that two subparts of its boundary are included in two planes, $(z = -\gamma)$ and $(z = \gamma)$, so it is possible to affix there electrodes, in order to prescribe a voltage potential (see, e.g., Fig. 1). It is assumed that the ferroelectric body is *uniaxial*, namely that the dependence of the polarization field, $\mathbf{P}$, on the electric field is nonlinear through only one of its components (here, the third one). More precisely, if we represent by $\mathbf{E} = (E_x, E_y, E_z)^T$ the electric field, where E_x, E_y, E_z are of course scalar fields, and the superscript "T" denotes here as well as in the next sections the transpose, we then have (see, e.g., [2]) that:

$$\mathbf{P} = \frac{1}{4\pi}(\varepsilon\mathbf{E} - \mathbf{E}) + \begin{pmatrix} 0 \\ 0 \\ P \end{pmatrix} \quad \text{in } \Omega_f, \tag{1}$$

with P a scalar field, $P : \Omega_f \longrightarrow \mathbf{R}$, and ε the electric permittivity.

By making use of the general theory presented in [2] or of the same arguments as those described in [7], we have here that the generating functional energy, $\mathcal{E}$, is such that:

$$\mathcal{E}(\mathbf{P}, \mathbf{E}) = \int_\Omega \tilde{\mathcal{F}}(\mathbf{P}, \mathbf{E})\mathrm{dx}, \tag{2}$$

where $\tilde{\mathcal{F}}(\mathbf{P}, \mathbf{E})$ is expressed as follows,

$$\begin{cases} \tilde{\mathcal{F}}(\mathbf{P}, \mathbf{E}) &= \mathcal{F}(P, 0) - E_z P - \dfrac{\mathbf{E} \cdot (\varepsilon\mathbf{E})}{8\pi} & \text{in } \Omega_f, \\ \tilde{\mathcal{F}}(\mathbf{P}, \mathbf{E}) &= -\dfrac{\mathbf{E} \cdot (\varepsilon\mathbf{E})}{8\pi} & \text{in } \Omega_p, \end{cases}$$

with $\mathcal{F}(P, 0)$ the Ginzburg–Landau potential. The term "$-\int_{\Omega_f} E_z P\mathrm{dx}$" penalizes the energy if E_z and P are of opposed signs, and thus traduces the effect of depolarizing field. The energy "$-\frac{1}{8\pi}\int_\Omega \mathbf{E} \cdot (\varepsilon\mathbf{E})\mathrm{dx}$" represents the effect of the domain walls. Thanks to the Ginzburg–Landau theory of phase transitions (cf., e.g., [2,7]), the term $\mathcal{F}(P, 0)$ can be written with respect to powers of P,

$$\mathcal{F}(P, 0) = \frac{4\pi}{\varkappa_\parallel}\left(\frac{t}{2}P^2 + \frac{1}{4}\frac{1}{P_0^2}P^4 + \frac{1}{2}\nabla P \cdot (\xi\nabla P)\right),$$

with