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Electro-thermo-chemical computational models for 3D heterogeneous semiconductor device simulation

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ABSTRACT

In this article we propose and numerically implement a mathematical model for the simulation of three-dimensional semiconductor devices characterized by an heterogeneous material structure. The model consists of a system of nonlinearly coupled time-dependent diffusion–reaction partial differential equations with convection terms describing the principal electrical, thermal and chemical phenomena that determine the macroscopic electrical response of the device under the action of externally applied electrical and thermal forces. The system is supplied with suitable initial, boundary and interface conditions that account for the interaction occurring among the various regions of the device with the surrounding environment. Temporal semi-discretization of the problem is carried out with the Backward Euler Method while a fixed-point iteration of Gummel type is used for system decoupling. Numerical approximation of the linearized subproblems is carried out using an exponentially fitted stabilized Finite Element Method on unstructured tetrahedral grids. Several computational experiments are included to validate the physical accuracy of the proposed computational algorithm in the study of realistic device structures.

1. Introduction

The continuous scaling of semiconductor devices has pushed contemporary research and most prominent technologies towards the use of innovative materials where new physical phenomena occur. In this context, an important class of applications is represented by resistive memories. In the case of Phase Change Memories (PCM) the resistive state is determined by a controlled switch of a calchogenide between the crystalline and the amorphous phase [1]. Here recent studies have clearly demonstrated the onset of a significant mass transport among different components of the calchogenide alloys. In other devices, the Resistive Random Access Memories (ReRAM), the low and high resistance state [2] is realized by using and controlling non-equilibrium thermo-chemical reactions. Moreover, in most of these new applications, the active material of the device (where transport, diffusion and reaction processes occur) is no longer homogeneous but often displays a markedly heterogeneous structure, as in the case of advanced logic devices. Finally, during the specific device application, the main physical material properties are not constant but also evolve in time due to the extreme working conditions (i.e., high electric and/or thermal fields).

A multidisciplinary approach is clearly fundamental to describe the basic functionality of heterogeneous devices in the correct physical framework. As a matter of fact, even if the exploration of materials properties can be effectively understood

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and theoretically simulated with the help of "ab initio" calculations [3], the electrical response and the time scale of operation of such devices still need to be addressed with the advanced mathematical methods traditionally employed in electronic, mechanical and thermal simulation. The novel challenge introduced by the technological application considered in the present article is that theoretical elements of semiconductor device physics, chemical, thermal and mechanical properties, must be included within a unified model setting in order to allow self-consistent calculations that account for the mutual interplay among the various phenomena occurring in the same device. This strong requirement reflects into a similar constraint in the numerical treatment of the problem because standard simulation suites are no longer usable but they need to be integrated and in some cases completely developed from scratch.

For these reasons, in this article we have developed a general mathematical and numerical framework in which the different physical contributions to the simulation can be effectively incorporated and mutually coupled to reach the desired self-consistency and model accuracy.

The mathematical model consists of a system of nonlinearly coupled time-dependent diffusion–reaction partial differential equations (PDEs) with convection terms describing the principal electrical, thermal and chemical phenomena that determine the macroscopic electrical response of the device under the action of externally applied electrical and thermal forces (see [4–9]). The system is supplied with initial, boundary and interface conditions that account for the interaction occurring among the various regions of the device with the surrounding environment.

The numerical approximation of the problem is conducted in two distinct steps. In the first step, temporal semi-discretization is carried out with the Backward Euler Method using a non-uniform time stepping. In the second step, a fixed-point iteration of Gummel type is adopted for system decoupling [10]. This leads to solving a sequence of linearized advection–diffusion–reaction equations that are numerically treated using an exponentially fitted stabilized Finite Element Method (FEM) [11–13] on unstructured tetrahedral partition of the computational domain. The FEM is chosen in the present discrete formulation of our model because it can properly address the complexity of the three-dimensional geometry (3D), avoiding any requirement of symmetry often used as a simplification and offering at the same time the adequate flexibility to implement all the mathematical and physical models needed in these emerging applications.

An outline of the article is as follows. Section 2 illustrates the fundamental conservation laws that express mass and energy balance of a system of M charged species in a material medium under the combined effect of electrical, thermal and chemical forces. Section 3 is devoted to the description of the multi-domain geometrical structure of the 3D semiconductor device object of the present study while Section 4 describes how to adapt the general thermo-electrochemical theory of Section 2 to the mathematical modeling of the class of devices of Section 3. The resulting formulation deals with the case of a single negatively charged species (electrons, $M = 1$) and consists of a nonlinearly coupled system of advection–diffusion–reaction PDEs that have to be solved in a heterogeneous domain supplied by a set of initial and boundary conditions. Section 5 is, instead, devoted to illustrate the three main computational steps which allow to translate the differential problem of Section 4 into the successive solution of linear algebraic systems providing the approximate solution of the problem. Section 6 is devoted to the validation of the physical accuracy of the computational model through the simulation of 3D device structures under realistic working conditions. Section 7 draws the main conclusions reached in the present article and addresses possible future research developments. Appendix A contains a list of all the symbols introduced in the article, specifying for each symbol the associated physical meaning and units.

2. Modeling of thermo-electrochemical phenomena

In this section we introduce the fundamental conservation laws that express mass and energy balance of a charged multi-species system moving in a material medium under the combined effect of electrical, thermal and chemical forces. For a complete treatment of electrochemical phenomena and of the mathematical foundations of non-equilibrium thermodynamics, we refer to [4] and to, e.g., [5]. For the mathematical analysis of general reaction–diffusion thermo-chemically coupled systems, we refer, e.g., to [6–9] and to the bibliography cited therein.

Let $M \geqslant 1$ be the total number of chemicals flowing in the medium under the action of electrical, chemical and thermal forces. We denote by $N_i = N_i(\boldsymbol{x}, t),\ i = 1, \ldots, M$, the number density of the ith chemical at the spatial position $\boldsymbol{x}$ and time t, and by z_i its ionic valence (which is assumed to be non-zero throughout the article). We set $\mathbf{N} := [N_1, \ldots, N_M]^T$. We also introduce the dependent variables $T = T(\boldsymbol{x}, t)$ and $\boldsymbol{E} = \boldsymbol{E}(\boldsymbol{x}, t)$ representing the temperature of the medium and the electric field at the spatial position $\boldsymbol{x}$ and time t, respectively.

2.1. Conservation laws

The basic form of the mathematical model considered in this article is constituted by the following coupled system of PDEs in conservation form:

$$qz_i \frac{\partial N_i}{\partial t} + \operatorname{div} \boldsymbol{j}_i(N_i, T, \boldsymbol{E}) = qR_i(\mathbf{N}, T, \boldsymbol{E}) \quad i = 1, \ldots, M, \tag{1a}$$

$$\frac{\partial}{\partial t}(\rho c T) + \operatorname{div} \boldsymbol{j}_T(\mathbf{N}, T, \boldsymbol{E}) = \mathcal{Q}_T(\mathbf{N}, T, \boldsymbol{E}), \tag{1b}$$

$$\operatorname{div}(\varepsilon \boldsymbol{E}) = q\mathcal{D} + \sum_{i=1}^{M} q z_i N_i. \tag{1c}$$