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An Approximation of Three-Dimensional Semiconductor Devices by Mixed Finite Element Method and Characteristics-Mixed Finite Element Method

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Abstract. The mathematical model for semiconductor devices in three space dimensions are numerically discretized. The system consists of three quasi-linear partial differential equations about three physical variables: the electrostatic potential, the electron concentration and the hole concentration. We use standard mixed finite element method to approximate the elliptic electrostatic potential equation. For the two convection-dominated concentration equations, a characteristics-mixed finite element method is presented. The scheme is locally conservative. The optimal L^2-norm error estimates are derived by the aid of a post-processing step. Finally, numerical experiments are presented to validate the theoretical analysis.

AMS subject classifications: 65M15; 65M60

Key words: Three-dimensional semiconductor devices, characteristics-mixed finite element method, mixed finite element method, post-processing step, error bound.

1. Introduction

The numerical simulation of the transient behavior of semiconductor devices is of great value both in theory and in practice (cf. [6, 17]). The production of actual semiconductor devices is mainly based on a planar technology. However, the down-scaling of the devices brings some severe problems such as increase of power densities and noise effects. The use of multi-gate field-effect transistors is a possible solution to reduce the noise. In such devices, the gate contact encloses the channel region from different sides to lead to smaller no-signal currents. But such devices require to be modeled and numerically simulated in three space dimensions. In this paper, we will consider the drift-diffusion model of three-dimensional semiconductor devices. The

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mathematical model is a coupled system of three quasi-linear partial differential equations with initial and boundary conditions (cf. [2, 4, 12, 18, 19]). The equation for the electrostatic potential is a Poisson equation. The continuity equations for the electrons and holes are of convection-dominated diffusion type. The model is described by the following system

$$-\Delta\psi = \nabla \cdot u = \alpha(p - e + F(x)), \qquad (x,t) \in \Omega \times [0,T], \tag{1.1a}$$

$$\frac{\partial e}{\partial t} = \nabla \cdot [D_e(x)\nabla e + \mu_e(x)eu] - R(e,p), \qquad (x,t) \in \Omega \times J, \tag{1.1b}$$

$$\frac{\partial p}{\partial t} = \nabla \cdot [D_p(x)\nabla p - \mu_p(x)pu] - R(e,p), \qquad (x,t) \in \Omega \times J, \tag{1.1c}$$

where $J = (0,T]$, and Ω is a bounded domain in $\mathcal{R}^3$. Here ψ, e and p are the electrostatic potential, the electron and hole concentrations, respectively. $u = -\nabla\psi$ is the electric field. $\alpha = q/\vartheta$, where $q > 0$ is the electronic charge and $\vartheta > 0$ is the dielectric permittivity. $D_s(x)(s = e, p)$ are the diffusion coefficients which are related to the carrier mobilities $\mu_s(x)(s = e, p)$ through the Einstein relation $D_s(x) = U_T\mu_s(x)$, with U_T being the thermal voltage. $R(e,p)$ is the net recombination rate. $F(x) = N_D(x) - N_A(x)$ is the doping profile in the device, where $N_D(x)$ and $N_A(x)$ are the donor and acceptor impurity concentrations, respectively.

We consider the following boundary and initial conditions

$$-\left.\frac{\partial\psi}{\partial\nu}\right|_{\partial\Omega} = u \cdot \nu = 0, \qquad \left.\frac{\partial e}{\partial\nu}\right|_{\partial\Omega} = 0, \qquad \left.\frac{\partial p}{\partial\nu}\right|_{\partial\Omega} = 0, \quad t \in J, \tag{1.1d}$$

$$e(x,0) = e_0(x),\ p(x,0) = p_0(x), \quad x \in \Omega, \tag{1.1e}$$

where ν is the unit outward normal vector on boundary $\partial\Omega$.

The following compatibility condition (cf. [17])

$$\int_\Omega (p_0 - e_0 + F)dx = 0 \tag{1.1f}$$

must be imposed on the data in order that a solution is possible. In addition, we apply the conditions

$$\int_\Omega \psi dx = 0,\ 0 \le t \le T \tag{1.1g}$$

to determine a unique ψ for each t.

In reality (1.1b) and (1.1c) might be strongly convection-dominated when $D_s(s = e, p)$ are quite small. In such circumstance, the standard Galerkin or difference scheme does not work well any more. In order to obtain better approximations, a variety of numerical techniques, such as characteristic finite element method (cf. [18]), characteristic finite difference method (cf. [4, 19]), upwind finite volume method (cf. [14–16]), etc., have been used for (1.1) in two or three space dimensions.

Although the modified method of characteristic finite element method (MMOC-Galerkin) (cf. [5, 9]) has advantages of avoidance of numerical diffusion and nonphysical oscillations and smaller time-truncation, it fails to preserve local mass balance. Preserving mass locally is of great importance in practice. In [1], Arbogast and Wheeler