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An Upwind-Block-Centered Multistep Difference Method for a Semiconductor Device and Numerical Analysis

Yirang Yuan[1,*], Changfeng Li[1,2] and Huailing Song[3]

[1] *Institute of Mathematics, Shandong University, Jinan, Shandong 250100, China*
[2] *School of Economics, Shandong University, Jinan, Shandong 250100, China*
[3] *College of Mathematics and Econometrics, Hunan University, Changsha, Hunan 410082, China*

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Abstract. Numerical simulation of a three-dimensional semiconductor device is a fundamental problem in information science. The mathematical model is defined by a nonlinear system of initial-boundary problem including four partial differential equations: an elliptic equation for electrostatic potential, two convection-diffusion equations for electron concentration and hole concentration, a heat conduction equation for temperature. The electrostatic potential appears within the concentration equations and heat conduction equation, and the electric field strength controls the concentrations and the temperature. The electric field potential is solved by the conservative block-centered method, and the order of the accuracy is improved by the electric potential. The concentrations and temperature are computed by the upwind block-centered multistep method, where three different numerical methods are involved. The multistep method is adopted to approximate the time derivative. The block-centered method is used to discretize the diffusion. The upwind scheme is applied to approximate the convection to avoid numerical dispersion and nonphysical oscillation. The block-centered difference simulates diffusion, concentrations, temperature, and the adjoint vector functions simultaneously. It has the local conservation of mass, which is an important nature in numerical simulation of a semiconductor device. By using the variation, energy estimates, induction hypothesis, embedding theorem and the technique of a priori estimates of differential equations, convergence of the optimal order is obtained. Numerical examples are provided to show the effectiveness and viability. This method provides a powerful tool for solving the challenging benchmark problem.

AMS subject classifications: 65M06, 65N06, 65N30, 82D37

Key words: Three-dimensional semiconductor device, upwind block-centered multistep difference, local conservation of mass, convergence analysis, numerical computation.

*Corresponding author.
Emails: yryuan@sdu.edu.cn (Y. Yuan), cfli@sdu.edu.cn (C. Li)

1 Introduction

Numerical simulation of a three-dimensional semiconductor device of heat conduction is a fundamental problem in information science. The mathematical model is defined by four nonlinear partial differential equations with initial-boundary conditions: 1) an elliptic equation for electric potential, 2) two convection-diffusion equations for electron concentration and hole concentration, 3) a heat equation for temperature. The electric potential appears within the concentration equations and heat equation, and the electric field strength controls the concentrations and the temperature. The mathematical model is formulated by a nonlinear partial differential system with initial-boundary conditions on a three-dimensional domain Ω [1–4],

$$-\Delta\psi=\alpha(p-e+N(X)), \qquad X=(x,y,z)^T\in\Omega, \quad t\in J=(0,\bar{T}], \tag{1.1a}$$

$$\frac{\partial e}{\partial t}=\nabla\cdot[D_e(X)\nabla e-\mu_e(X)e\nabla\psi]-R_1(e,p,T), \qquad (X,t)\in\Omega\times J, \tag{1.1b}$$

$$\frac{\partial p}{\partial t}=\nabla\cdot\left[D_p(X)\nabla p+\mu_p(X)p\nabla\psi\right]-R_2(e,p,T), \quad (X,t)\in\Omega\times J, \tag{1.1c}$$

$$\rho\frac{\partial T}{\partial t}-\Delta T=\Big\{(D_p(X)\nabla p+\mu_p(X)p\nabla\psi) -(D_e(X)\nabla e-\mu_e(X)e\nabla\psi)\Big\}\cdot\nabla\psi, \quad (X,t)\in\Omega\times J. \tag{1.1d}$$

The electric potential, electron concentration, hole concentration and temperature are the objective functions, denoted by ψ, e, p and T, respectively. All the coefficients of (1.1a)-(1.1d) are bounded by two positive constants. $\alpha=q/\varepsilon$, where q and ε are positive constants and they denote the electronic load and the permittivity, respectively. U_T is the thermal voltage. The diffusion $D_s(X)$ is related to the mobility $\mu_s(X)$, i.e., $D_s(X)=U_T\mu_s(X)$, ($s=e$ for the electron and $s=p$ for the hole). $N_D(X)$ and $N_A(X)$ are the donor impurity concentration and acceptor impurity concentration, respectively. $N(X)$, defined by $N(X)=N_D(X)-N_A(X)$, changes rapidly as X approaches nearby the P-N junction. $R_1(e,p,T)$ and $R_2(e,p,T)$ are the recombination rates of the electron, hole and temperature. $\rho(X)$ is the heat transfer coefficient. It is important to consider a nonuniform partition in numerical simulation [5,6].

Initial conditions:

$$e(X,0)=e_0(X), \quad p(X,0)=p_0(X), \quad T(X,0)=T_0(X), \quad X\in\Omega, \tag{1.2}$$

where $e_0(X)$, $p_0(X)$ and $T_0(X)$ are given positive functions.

In this paper, we concentrate on the Neumann boundary conditions:

$$\frac{\partial\psi}{\partial\gamma}\Big|_{\partial\Omega}=\frac{\partial e}{\partial\gamma}\Big|_{\partial\Omega}=\frac{\partial p}{\partial\gamma}\Big|_{\partial\Omega}=\frac{\partial T}{\partial\gamma}\Big|_{\partial\Omega}=0, \quad t\in J, \tag{1.3}$$

where $\partial\Omega$ is the boundary of Ω, and γ is the unit outer normal vector of $\partial\Omega$.