NUMERICAL MATHEMATICS
A Journal of Chinese Universities (English Series)

Vol. **15** No. 3, pp. 278-288
August 2006

A Finite Difference Scheme for a Semiconductor Device Problem on Grids with Local Refinement in Time and Space[†]

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Received June 1, 2005; Accepted (in revised version) March 23, 2006

Abstract. The momentary state of a semiconductor device is described by a system of three nonlinear partial differential equations. A finite difference scheme for simulating transient behaviors of a semiconductor device on grids with local refinement in time and space is constructed and studied. Error analysis is presented and is illustrated by numerical examples.

Key words: Semiconductor device; local refinement; finite difference scheme; error estimate.

AMS subject classifications: 65M06, 65M12, 65M50

1 Introduction

We shall consider a system of three nonlinear partial differential equations in a bounded domain Ω, which forms a basic model of one-dimensional transient behavior of a semiconductor device [1-3]:

$$\begin{aligned}
&(a)\ -\frac{\partial^2\psi}{\partial x^2} = \alpha(p-e+N(x)), \quad x\in\Omega, t\in J=(0,T],\\
&(b)\ \frac{\partial e}{\partial t} = \frac{\partial}{\partial x}\left\{D_e(x)\frac{\partial e}{\partial x} - \mu_e(x)e\frac{\partial\psi}{\partial x}\right\} - R(e,p), \quad (x,t)\in\Omega\times J,\\
&(c)\ \frac{\partial p}{\partial t} = \frac{\partial}{\partial x}\left\{D_p(x)\frac{\partial p}{\partial x} + \mu_p(x)p\frac{\partial\psi}{\partial x}\right\} - R(e,p), \quad (x,t)\in\Omega\times J.
\end{aligned} \tag{1}$$

The electrostatic potential equation is elliptic. The electron and the hole density equations are parabolic equations. The unknowns are the electrostatic potential ψ and the electron and the hole densities e and p. All coefficients appearing in (1) are supposed to be suitably smooth functions

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[†]Supported by the Major State Basic Research of China (Grant No. G1999032803), the National Natural Science Foundation of China (Grant No. 10372052,10271066) and the Doctorate Foundation of the Ministry of Education of China (Grant No. 20030422047).

and have positive lower and upper bounds. $\alpha = q/\varepsilon$, where q and ε are positive constants(q is the electron charge, ε is the permittivity). $D_s(x)$ and $\mu_s(x)(s = e, p)$ are the diffusion coefficient and the transient respectively. $N(x)$ is a given function and changes rapidly near the p-n node of a semiconductor device. $R(e, p)$ is the recombination rate.

In addition, we have initial and boundary conditions:

$$e(x,0) = e_0(x), \quad p(x,0) = p_0(x), \quad x \in \Omega, \tag{2}$$

$$\psi|_{\partial\Omega} = \bar{\psi}(x,t), e|_{\partial\Omega} = \bar{e}(x,t), \quad p|_{\partial\Omega} = \bar{p}(x,t), \quad (x,t) \in \partial\Omega \times J. \tag{3}$$

Douglas and Yuan put forward practical finite difference methods for one and two dimensional semiconductor models and provide some theoretical analyses [2,3]. According to practical numerical simulations of semiconductor devices, grids near the p-n node need to be refined locally. In this way, we can improve computational precision greatly with a little increase of computational cost [4]. Ewing and Lazarov proposed some finite difference approximations of the ellipse equation on grids with local refinement in space [5]. Cai and Mccormick analyze stationary local grid refinement for the diffusion equation [6]. Ewing, Lazarov and Vassilevski derive implicit schemes on the basis of a finite volume approach [7]. Ewing and Lazarov construct and study finite difference schemes for transient convection-diffusion problems on grids with local refinement in time and space [8].

In this paper, we study a finite difference scheme on grids with local refinement in time and space for one-dimensional transient behavior of a semiconductor device. The electrostatic potential equation is approximated by a central difference scheme. The electron and the hole density equations are discretized by modified upwind schemes. Linear interpolation is utilized at the slave nodes. We derive the error estimate in the maximum norm for the electron and the hole density equations. Finally, numerical examples illustrating the theory are given. It is of great importance for the research on theory and application of numerical simulations of semiconductor devices.

The paper is organized as follows. In Sections 2-4 we consider the finite difference scheme with local refinement in time. In Section 2 we introduce the necessary notations. In Section 3 the finite difference scheme is constructed. The error analysis is addressed in Section 4. In Section 5 we consider schemes on grids with local refinement in time and space, and again discuss their approximation properties. Finally in Section 6 we present some numerical experiments.

2 Notations

First, $\Omega = [0, 1]$ is discretized using a regular grid with a parameter h. The spatial nodes of the grid on Ω are then defined by $x = nh$, where $n = 0, 1, \cdots, N$, $h = 1/N$. Next, we introduce closed intervals $\{\Omega_k\}_{k=1}^{M}$, which are subsets of Ω with boundaries aligned with the spatial discretizaton already defined. Further, it is required that $\bigcup_{k=1}^{M} \Omega_k \subset \Omega$, and we set $\Omega_0 = \Omega \setminus \bigcup_{k=1}^{M} \Omega_k$. In order to avoid unnecessary complications, we assume that $dist(\Omega_i, \Omega_j) \geq lh \ for \ i, j > 0$, where $l > 1$ is an integer.

With each subdomain Ω_i, we associate corresponding sets of nodal points: ω_i is defined to be the set of all nodes of the discretizaton of Ω that are in Ω_i. We require $\omega_i \bigcap \omega_j = \emptyset, \ for \ i \neq j, \ i, j = 0, \cdots, M$. And assume that there is no spatial refinement. In each $\omega_i, i = 0, \cdots, M$, we define a subset of boundary nodes γ_i as the nodes which have at least one neighbor not in ω_i, γ_i contains only nodes which do not reside on the boundary of Ω in case $\partial\Omega_i \cap \partial\Omega \neq \emptyset$. Then set $\omega = \bigcup_{i=0}^{M} \omega_i$.