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A Numerical Approximation Structured by Mixed Finite Element and Upwind Fractional Step Difference for Semiconductor Device with Heat Conduction and Its Numerical Analysis

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Abstract. A coupled mathematical system of four quasi-linear partial differential equations and the initial-boundary value conditions is presented to interpret transient behavior of three dimensional semiconductor device with heat conduction. The electric potential is defined by an elliptic equation, the electron and hole concentrations are determined by convection-dominated diffusion equations and the temperature is interpreted by a heat conduction equation. A mixed finite element approximation is used to get the electric field potential and one order of computational accuracy is improved. Two concentration equations and the heat conduction equation are solved by a fractional step scheme modified by a second-order upwind difference method, which can overcome numerical oscillation, dispersion and computational complexity. This changes the computation of a three dimensional problem into three successive computations of one-dimensional problem where the method of speedup is used and the computational work is greatly shortened. An optimal second-order error estimate in L^2 norm is derived by prior estimate theory and other special techniques of partial differential equations. This type of parallel method is important in numerical analysis and is most valuable in numerical application of semiconductor device and it can successfully solve this international famous problem.

AMS subject classifications: 65M015; 65M60; 65N30; 82D37
Key words: Three dimensional transient behavior of heat conduction problem, numerical simulation computation, mixed finite element, modified upwind fractional step difference, second-order error estimates in L^2 norm.

1. Introduction

Traditional numerical methods are generally invalid for modern simulation of semiconductor device, since semiconductor device develops greatly and its mathematical model, an

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initial-boundary value diffusion system of nonlinear partial differential equations is solved in consideration of multi-dimensional problem, complicated geometric domains and high order of accuracy. Therefore, modern numerical simulation techniques are introduced to find its discrete solutions [13, 18, 35, 36].

The mathematical model of transient behavior problem of three-dimensional semiconductor device of heat conduction is formulated by four nonlinear partial differential Eqs. [2, 8, 13, 14, 18, 29, 31, 35, 36]. The first equation is elliptic for describing the electric potential, the second and third equations are of convection-diffusion for finding the electron concentration and hole concentration and the fourth equation is of heat conduction for finding the temperature. The electric potential governs the concentrations and the temperature by its electric field intensity. Combined with corresponding boundary value conditions and initial value conditions, a whole system follows on a three-dimensional domain Ω [2, 8, 13, 14, 18, 29, 31, 35, 36].

$$-\Delta\psi = \nabla\cdot\underline{u} = \alpha(p-e+N(X)), \quad X=(x_1,x_2,x_3)^T\in\Omega,\ \ t\in J=(0,\hat{T}], \tag{1.1a}$$

$$\frac{\partial e}{\partial t} = \nabla\cdot\left[D_e(X)\nabla e+\mu_e(X)e\underline{u}\right]-R_e(e,p,T), \qquad (X,t)\in\Omega\times J, \tag{1.1b}$$

$$\frac{\partial p}{\partial t} = \nabla\cdot\left[D_p(X)\nabla p-\mu_p(X)p\underline{u}\right]-R_p(e,p,T), \qquad (X,t)\in\Omega\times J, \tag{1.1c}$$

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

In the above expressions, the electric potential ψ, the electron concentration e, the hole concentration p and the temperature T, the electric field intensity $\underline{u}=-\nabla\psi$ are unknown functions. The electric field potential is generated by the electric field intensity in the concentration equations and the heat conduction equation, and governs the above three equations. $\alpha=q/\varepsilon$ is defined by the quotient of two positive constants, the electronic load q and the dielectric coefficient ε. All coefficients in (1.1b)-(1.1d) have a positive upper bound and a positive lower bound. The diffusion coefficients $D_s(X)$, $s=e$ or p, are equal to $U_T\mu_s(X)$, a product of the mobility $\mu_s(X)$ and the heat U_T. A given function $N(X)$ is defined by $N_D(X)-N_A(X)$, the difference of impurity concentrations of the donor and the acceptor, whose values change rapidly as X approaches closely the semiconductor P-N junction. The symbols $R_e(e,p,T)$ and $R_p(e,p,T)$ denote generation-recombination rates of the electron, the hole and the temperature. The coefficient of heat conduction $\rho(X)$ is positive definite.

Initial value conditions are given by

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

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

Boundary value conditions of Dirichlet type are given by

$$\psi(X,t)\big|_{\partial\Omega}=0, \qquad\qquad e(X,t)|_{\partial\Omega}=\bar{e}(X,t), \tag{1.3a}$$

$$p(X,t)\big|_{\partial\Omega}=\bar{p}(X,t), \qquad\qquad T(X,t)|_{\partial\Omega}=\bar{T}(X,t),\ \ t\in J. \tag{1.3b}$$