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NUMERICAL METHOD OF MIXED FINITE VOLUME-MODIFIED UPWIND FRACTIONAL STEP DIFFERENCE FOR THREE-DIMENSIONAL SEMICONDUCTOR DEVICE TRANSIENT BEHAVIOR PROBLEMS*

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Abstract Transient behavior of three-dimensional semiconductor device with heat conduction is described by a coupled mathematical system of four quasi-linear partial differential equations with initial-boundary value conditions. The electric potential is defined by an elliptic equation and it appears in the following three equations via the electric field intensity. The electron concentration and the hole concentration are determined by convection-dominated diffusion equations and the temperature is interpreted by a heat conduction equation. A mixed finite volume element approximation, keeping physical conservation law, is used to get numerical values of the electric potential and the accuracy is improved one order. Two concentrations and the heat conduction are computed by a fractional step method combined with second-order upwind differences. This method can overcome numerical oscillation, dispersion and decreases computational complexity. Then a three-dimensional problem is solved by computing three successive one-dimensional problems 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 using prior estimate theory and other special techniques of partial differential equations. This type of mass-conservative parallel method is important and is most valuable in numerical analysis and application of semiconductor device.

Key words three dimensional transient behavior of heat conduction problem; mixed finite volume element; modified upwind fractional step difference; second-order error

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estimate in L^2 norm; numerical computation

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1 Introduction

Since semiconductor device develops greatly, so it is necessary to consider the mathematical model on complicated regions and get numerical solutions more precisely. Therefore, traditional numerical methods are generally invalid for modern simulation of semiconductor device. The mathematical model is defined by an initial-boundary value diffusion system of nonlinear partial differential equations. Then some modern numerical simulation techniques were introduced in complicated simulation [1–4].

The mathematical model is formulated by four quasi-linear partial differential equations to describe transient behavior of three-dimensional semiconductor device with heat conduction [1–9]. The first equation of elliptic type describes electric potential. The next two equations of convection-diffusion determine electron concentration and hole concentration. The last one of heat conduction defines the temperature. Electric potential governs the concentrations and the temperature via its electric field intensity. Combined with corresponding boundary value conditions and initial value conditions, the details of the whole system were stated as follows on a three-dimensional domain Ω [1–9],

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

$$\frac{\partial e}{\partial t} = \nabla\cdot[D_e(X)\nabla e+\mu_e(X)e\underline{u}] - R_e(e,p,T), \quad (X,t)\in\Omega\times J, \tag{1.2}$$

$$\frac{\partial p}{\partial t} = \nabla\cdot[D_p(X)\nabla p-\mu_p(X)p\underline{u}] - R_p(e,p,T), \quad (X,t)\in\Omega\times J, \tag{1.3}$$

$$\rho\frac{\partial T}{\partial t} - \Delta T = \{(D_e(X)\nabla e+\mu_e(X)e\underline{u}) - (D_p(X)\nabla p-\mu_p(X)p\underline{u})\}\cdot\underline{u}, \ \ (X,t)\in\Omega\times J. \tag{1.4}$$

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 potential is generated by the electric field intensity in the concentration equations and the heat conduction equation, and governs the above three functions. $\alpha=q/\varepsilon$ is defined by the quotient of two positive constants, the electronic load q and the dielectric coefficient ε. All coefficients in (1.2)–(1.4) have a positive upper bound and a positive lower bound. The diffusion coefficients $D_e(X)$ and $D_p(X)$, are respectively equal to $U_T\mu_e(X)$ and $U_T\mu_p(X)$, where $\mu_e(X)$ and $\mu_p(X)$ mean the mobilities and U_T denotes the heat. 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 dependent on the electron, the hole and the temperature. The coefficient of heat conduction $\rho(X)$ is positive definite.

Initial value conditions are given by

$$e(X,0)=e_0(X), \ p(X,0)=p_0(X), \ T(X,0)=T_0(X), \quad X\in\Omega, \tag{1.5}$$

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