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THE CHARACTERISTIC FINITE ELEMENT ALTERNATING-DIRECTION METHOD WITH MOVING MESHES FOR THE TRANSIENT BEHAVIOR OF A SEMICONDUCTOR DEVICE

YIRANG YUAN

Abstract. For the transient behavior of a semiconductor device, the modified method of characteristics finite element alternating-direction procedures with moving meshes are put forward. Some techniques, such as calculus of variations, operator-splitting, characteristic method, generalized L^2 projection, energy method, negative norm estimate and prior estimates and techniques are employed. Optimal order estimates in L^2 norm are derived for the error in the approximation solution. Thus the well-known theoretical problem has been thoroughly and completely solved.

Key Words. semiconductor device, alternating-direction, moving meshes, characteristic finite element, L^2 error estimate

1. Introduction

With the rapid development of semiconductor devices, the traditional approximate method is no longer applicable. We must study the initial boundary value problems of quasilinear partial differential equations, namely, the so-called diffusion model. For high-dimensional problems, new numerical simulation techniques[1−3] are needed to obtain the solutions for semiconductor devices in complicated geometric shapes.

The mathematical model of the two-dimensional semiconductor device of heat conduction is described with the initial boundary value problem made up of four quasilinear partial differential equations[1−4]: one equation of the elliptic type for the electric potential, two of the convection-dominated diffusion type for the conservation of electron and hole concentrations, and the last one for heat conduction. The four equations, relevant initial condition and boundary condition make up a closed system. For two-dimensional problems, there are

$$-\Delta\psi = \alpha(p - e + N(X)), \quad X = (x_1, x_2)^T \in \Omega, \ \ t \in J = (0, \bar{T}], \tag{1}$$

$$\frac{\partial e}{\partial t} = \nabla \cdot \{D_e(X)\nabla e - \mu_e(X)e\nabla\psi\} - R_1(e, p, T), \quad (X, t) \in \Omega \times J, \tag{2}$$

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$$\frac{\partial p}{\partial t} = \nabla \cdot \{D_p(X)\nabla p + \mu_p(X)p\nabla\psi\} - R_2(e,p,T), \quad (X,t) \in \Omega \times J, \tag{3}$$

$$\rho(X)\frac{\partial T}{\partial t} - \Delta T = \{(D_p(X)\nabla p + \mu_p p\nabla\psi) - (D_e(X)\nabla e - \mu_e(X)e\nabla\psi)\} \cdot\nabla\psi, \quad (X,t) \in \Omega \times J. \tag{4}$$

The unknown functions are electrostatic potential ψ and electron and hole concentrations e, p and temperature T. All coefficients appearing in (1) $\sim$ (4) are positive. $\alpha = \frac{q}{\varepsilon}$, q and ε are constants (q is the electron charge, ε is the dielectric permittivity). The diffusion coefficients $D_s(X)$ $(s = e, p)$ are related to the mobilities $\mu_s(X)$ by the relation $D_s(X) = U_T\mu_s(X)$, where U_{T} is the thermal voltage. $N(X) = N_D(X) - N_A(X)$ is a given function, $N_D(X)$ and $N_A(X)$ being the donor and acceptor impurity concentrations. $R_i(e,p,T)(i = 1,2)$ is the recombination term. $\nabla = (\frac{\partial}{\partial X_1}, \frac{\partial}{\partial X_2})^T$ and $\Delta = \frac{\partial^2}{\partial X_1^2} + \frac{\partial^2}{\partial X_2^2}$.

The initial conditions is

$$e(X,0) = e_0(X),\ p(X,0) = p_0(X),\ T(X,0) = T_0(X), \quad X \in \Omega. \tag{5}$$

Boundary condition:

$$\psi|_{\partial\Omega} = 0, \ \left.\frac{\partial e}{\partial\gamma}\right|_{\partial\Omega} = \left.\frac{\partial p}{\partial\gamma}\right|_{\partial\Omega} = \left.\frac{\partial T}{\partial\gamma}\right|_{\partial\Omega} = 0, \quad (X,t) \in \partial\Omega \times J, \tag{6}$$

where γ is the outer normal vector of Ω.

In 1964 Gummel first proposed sequence iterative computation methods to treat this kind of problem[5], thus opening up a new field. Douglas et al. put forward the finite difference method for one-dimensional and two-dimensional simple models (without considering the temperature's effect or constant coefficients). They solved some practical problems and first obtained the theoretical analysis result[6,7]. However, optimal order error estimates in l^2 norm were not obtained yet. Based on what has been achieved, the author considers the finite difference method for a semiconductor device of heat conduction, and optimal order estimates in l^2 norm are obtained [8]. And the author first considers characteristic finite element method and theoretical analysis for numerical simulation of a semiconductor device [9,10]. In this paper, for modern numerical simulation the problems met are often large-scale and large-scope, and the mode number is as large as tens of thousands or even hundreds of millions. Thus we need the operator-splitting method to solve the problem. We shall apply the finite element method with moving meshes to concentration equations and heat-conduction equation. Moreover, in the process of solution, the electron, hole concentrations and heat conduction distribution front will push forward with increasing time, so the finite element mesh near the front will be locally densified. In such a way, we can ensure the accuracy of the numerical results without increasing the computation time as a whole. The densified meshes must move forward as time goes on, to keep themselves always near the concentration and temperature distribution front. At this point we need the new technique of alternating-direction and moving meshes mutual association scheme to solve the problem [11−15].

This thesis puts forward a kind of modified method of characteristics finite element alternating-direction procedures with moving meshes. Some techniques, such as calculus of variations, operator-splitting, characteristic methods, generalized L^2 projection, energy method, negative norm estimate and prior estimates are employed. Optimal order estimates in L^2 norm are derived for the error in approximate solution. The research is important both theoretically and practically for the model