Adaptive Time Discretization for a Transient Quantum Drift-Diffusion Model

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Abstract

This paper describes a numerical method for a time-dependent quantum drift-diffusion model with emphasis on adaptive time discretization. The adaptive time step algorithm is proposed by introducing the derivative of the free energy of the system. The algorithm is evaluated for carrier transport simulations in n^+-n-n^+ structures. The new algorithm significantly reduces the total number of time step required to reach the stationary state.

1 Introduction

For the modeling of the semiconductor transport, the quantum drift-diffusion (QDD) model has been introduced as a generalization of the classical drift-diffusion model [1]. This model is suited to incorporate quantum confinement and tunneling effects in scaled semiconductor devices. An iterative method and numerical schemes of the stationary QDD model have been developed to realize the accurate prediction of such physical phenomena [2]-[4]. In this work, we propose a numerical method for the transient QDD model with emphasis on adaptive time discretization. The adaptive time step algorithm is designed by calculating the free energy of the system.

2 A Transient Quantum Drift-Diffusion Model

Considering only electrons, the QDD model is described as

$$\varepsilon \Delta \varphi = q(n - C) \tag{1}$$

$$\frac{\partial n}{\partial t} + \mathrm{div}(\mu_n n \nabla \varphi_n) = -R \tag{2}$$

$$\varphi_n = \varphi + \gamma_n - \frac{kT}{q} \log \frac{n}{n_i}, \quad \gamma_n = 2b_n \frac{\nabla^2 \sqrt{n}}{\sqrt{n}} \tag{3}$$

where φ is the electrostatic potential, n the electron density, and φ_n the generalized quasi-Fermi level. R is the recombination rate, ε the dielectric permittivity, q the electronic charge, k the Boltzmann constant, T the temperature, C the ionized impurity density. μ_n is an electron mobility, $b_n = \hbar^2/(12qm_n^*)$, $\hbar$ the Planck constant, m_n^* the effective mass for the electrons, and n_i is the intrinsic carrier density.
The free energy form of the system is important to determine the asymptotic behavior of the solutions of the time dependent problem. In order to understand the asymptotic

behavior of the solutions to the stationary state, we can define the derivative of the relative free energy W as follows:

$$H(t) = \frac{dW}{dt} = \int_\Omega J_n \cdot \nabla(\varphi_n - \varphi_n^*) dx \tag{4}$$

where φ_n^* is a stationary solution and J_n denotes the current density. An important property satisfied by the QDD model is the entropy dissipation and hence the adaptive time step algorithm for time discretization can be designed by calculating the free energy of the system.

3 Discretization

For time discretization, we apply a backward Euler scheme. By employing an exponential transformation of variables $S = \sqrt{n} = \sqrt{n_i}\exp(\frac{qu}{kT})$ in (3), space discretization is performed in terms of the variables (φ, u, n) [3]. Then we obtain high-order conservative schemes to the QDD equation:

$$\begin{aligned}\frac{1}{\tau_k}(n^k - n^{k-1}) =& \frac{\mu_{n_{i+1/2}}}{h_{i+1}}(B(\Phi_{i+1}^k - \Phi_i^k)n_{i+1}^k - B(\Phi_i^k - \Phi_{i+1}^k)n_i^k) \\ &- \frac{\mu_{n_{i-1/2}}}{h_i}(B(\Phi_i^k - \Phi_{i-1}^k)n_i^k - B(\Phi_{i-1}^k - \Phi_i^k)n_{i-1}^k)) \end{aligned} \tag{5}$$

$$\begin{aligned}\sqrt{n_i} b_n \frac{h_i + h_{i+1}}{2}\Big(&\frac{1}{h_{i+1}} e^{u_{i+1}} B(u_{i+1} - u_i)(u_{i+1} - u_i) \\ &- \frac{1}{h_i} e^{u_i} B(u_i - u_{i-1})(u_i - u_{i-1})\Big) - \Lambda_i u_i = -\frac{\varphi_i - \varphi_{ni}}{2}\Lambda_i \end{aligned} \tag{6}$$

where $\Phi = \varphi + \gamma_n$ and $\Lambda_i = \int_{x_{i-1/2}}^{x_{i+1/2}} S dx$. $\tau_k = t_k - t_{k-1} > 0$ is the time step. All of potentials are scaled by the Boltzmann voltage.

4 Adaptive Time Step Control

An effective way for the time step control is to look at the ratio of consecutive gradients of the free energy as follows:

$$\theta = \frac{W_{k+1} - W_k}{W_k - W_{k-1}} = \frac{\int_{t_k}^{t_{k+1}} H(t) dt}{\int_{t_{k-1}}^{t_k} H(t) dt}. \tag{7}$$

If θ is near 1 then the system approaches the stationary state and hence the time step size can be increased. If θ is far from 1 then the system is dynamically changed and hence the step size is kept to be constant. An adaptive time step algorithm is constructed as

$$\tau_{k+1} = \alpha(\theta)\tau_k \tag{8}$$

$$\alpha(\theta) = \begin{cases} 1 & \theta \le 1 - \varepsilon \\ 1.2 & -\varepsilon \le |\theta - 1| \le \varepsilon \\ 1 & \theta \ge 1 + \varepsilon \end{cases}. \tag{9}$$

In (7) $H(t)$ is approximated by the Lagrange interpolating polynomial $P(t)$. As $\tau_{k+1} = \tau_k$, θ at $t = t_{k+1}$ is predicted by using $P(t)$ in (7). Then, $\alpha(\theta)$ is estimated in (9). Using (8), the next time step τ_{k+1} is corrected. The initial time step is set to the minimum step size due to the large variation of W at the initial stage. The simulation is performed for different n^+-n-n^+ structures. The n^+ and n doping concentration is 5×10^{17} cm^{-3} and 2×10^{15} cm^{-3}, respectively. Fig. 1 and 2 show the evolution of adaptive time step. The results indicate the nonuniform step sizes and different evolutions of time step between short and long channel devices.

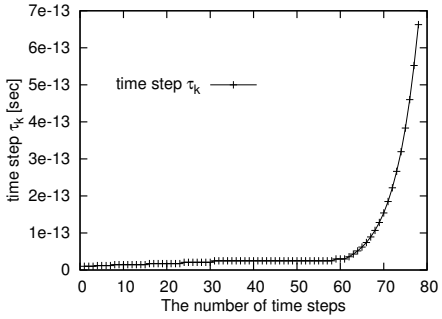

Figure 1: Evolution of adaptive time step for the n^+-n-n^+ device with $l = 0.1$ μm.

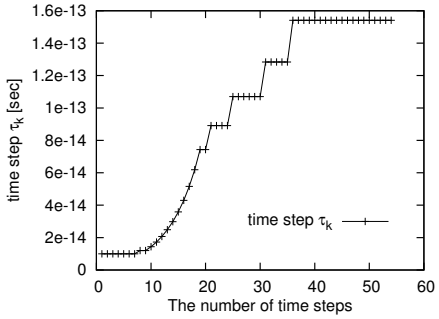

Figure 2: Evolution of adaptive time step for the n^+-n-n^+ device with $l = 0.3$ μm.

5 Numerical Results

The resulting algorithm was validated in n^+-n-n^+ structures. Fig. 3 shows electron density distributions for the n^+-n-n^+ device with the channel length of 0.1μm, calculated by different time step algorithms. Fig. 4 shows the derivative of the free energy of the system. In both cases, our proposed algorithm represents the exact solutions calculated using the fine time step of 0.01 psec. As shown in Fig. 5 and 6, the adaptive time discretization exhibits the exact results at different drain voltages and at short and long channel devices. The number of time steps required to reach the stationary state at different devices are summarized in Table 1. It is found that the adaptive time step algorithm significantly reduces the total number of time steps required to reach the stationary state.

6 Conclusion

The adaptive time step algorithm for the transient QDD model has been newly developed by introducing the derivative of the free energy of the system. The new algorithm significantly reduces the total number of time step required to reach the stationary state.

References

[1] M.G. Ancona and G.J. Iafrate, "Quantum correction to the equation of state of an electron gas in a semiconductor," Phys. Rev. B, vol.39, pp.9536-9540, 1989.

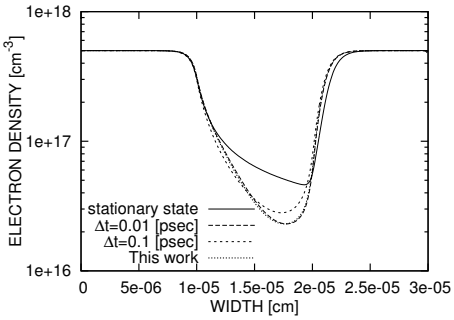

Figure 3: Electron density distributions calcalculated by different time step algorithms.

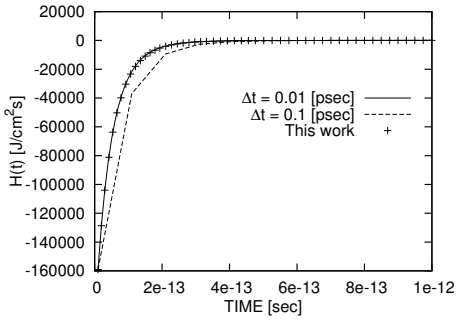

Figure 4: The derivative of free energy calculated by different time step algorithms.

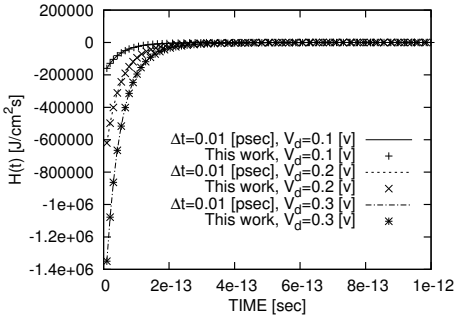

Figure 5: The derivative of free energy at different drain voltages.

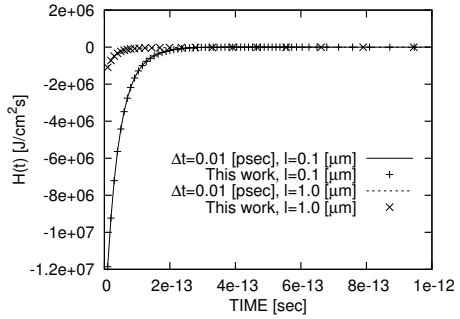

Figure 6: The derivative of free energy at short and long channel devices.

	$l = 0.1$ [μm]		$l = 0.2$ [μm]		$l = 0.3$ [μm]	
	time [p sec]	The number of time step	time [p sec]	The number of time step	time [p sec]	The number of time step
$\Delta t = 0.01$	0.89	89	2.5	250	4.85	485
$\Delta t = 0.1$	0.61	7	1.31	14	2.41	25
This work	0.924	48	2.62	52	5.13	54

Table 1: The number of time steps required to reach the stationary state. l is the channel length of the n^+-n-n^+ device. The drain voltage is 0.1 V.

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