毫微米元件使用平衡方程式方法的平行模擬
Parallel Simulation of Nanometer Devices Using Balance Equation Method

計畫編號：NSC89-2213-E009-051
執行期限：88/08/01～89/07/31
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一、 中文摘要(關鍵詞：毫微米元件、波茲曼傳輸方程式、平衡方程式、平行模擬、彈道二極體。)

本文從基本的波茲曼傳輸方程式推導出載子濃度、載子速度和載子能量的平衡方程式，用來模擬毫微米半導體元件的特性。利用牛頓反覆法來線性化這些耦合的平衡方程式和帕森方程式，且以左下右上三角矩陣(LU)分解法求解此線性系統。為了實現毫微米半導體元件的平行計算，亦可將 n, v_x, v_y, w_d, 和ϕ的五個方程式去耦合，並在平行虛擬機 PVM 的環境下同時求解。吾人係以毫微米彈道二極體為例，描述其在施予偏壓情況下的靜電位、電子濃度、速度和能量（溫度）的暫態分佈，並且觀察這些變量在不同偏壓下的穩態狀況。本數值模擬程式可以正確的預測出載子在毫微米元件中受熱而增加溫度和速度變化的情形，而速度的異常超射的情況並沒有在我們的模擬結果中出現。

英文摘要 (Keywords: nanometer devices, Boltzmann transport equation, balance equation method, Crank-Nicolson scheme, parallel simulation, ballistic diode.)

Numerical simulation for nanometer semiconductor devices based on the balance equation method has been developed in this work. The basic equations for electron concentration, electron velocity, and electron energy are derived from the Boltzmann transport equation. The time evolution is descritized according to the Crank-Nicolson scheme. The nonlinear equation system is linearized by Newton iteration and solved by LU decomposition method. This formulation is suitable to the implementation of parallel computation since each row or column of the grid points in a semiconductor device can be treated independently. A ballistic diode has been taken as an example. The transient behavior of the electrostatic potential, electron concentration, velocity, and energy under applied voltage are described. The distributions of all variables under steady state at various applied voltages are also shown. This model can accurately predict the carrier heating phenomena in nanometer device. However, the spurious velocity overshoot has not been observed in this work.

二、計劃緣由與目的

由於半導體元件的日益縮小，很多過去被忽略的物理現象，必須在新一代的元件分析中加以考慮。因為物理模式及元件結構日趨複雜，使得元件特性的模擬時間大幅地增加。因此很有必要採用平行計算，庶幾能在較少的時間內得到較準確的結果。

當元件尺寸的縮小時，半導體內部的電場以及載子的速度和能量隨之變大。傳統的漂移擴散模式僅計及載子的速度，而未曾涵蓋載子的能量。因此吾人需從基本的波茲曼傳輸方程式推導出含有載子能量平衡方程式的流體力學模式，較精確的模擬毫微米元件的特性。

三、研究方法

The classical carrier transport problem is based on the solution of Boltzmann transport equation for the distribution function $f(\bar{r},\bar{p},t)$ in the position $\bar{r}$ and momentum $\bar{p}$ spaces as a function of time t:

$$\frac{\partial f}{\partial t} = -\bar{v}\cdot\nabla f - e\nabla\phi\cdot\nabla_{\bar{p}} f + \left(\frac{\partial f}{\partial t}\right)_C \qquad (1)$$

where $\boldsymbol{v}$ is carrier velocity, $\boldsymbol{e}$ is the magnitude of electronic charge, and ϕ is the electrostatic potential arising from the space charges in semiconductor according to the Poisson equation.

$$\nabla^2\phi = -\frac{e}{\varepsilon_s}\left(N_D - n\right) \qquad (2)$$

where ε_s is the permittivity, N_D is the dopant

concentration, and n is the electron concentration.

The balance equations for the carrier density n, the momentum density $n\vec{p}_d$, and the energy density nw_d can be obtained by integrating both sides of the Boltzmann transport equation (1) for 1, $\vec{p}$ and w over the momentum space.

$$\frac{\partial n}{\partial t} = -\nabla \cdot (\vec{v}_d n) + \left(\frac{\partial n}{\partial t}\right)_C \quad (3)$$

$$\frac{\partial (n\vec{p}_d)}{\partial t} = -\nabla \cdot (n\vec{v}_d \vec{p}_d) + en\nabla Œ + \left(\frac{\partial (n\vec{p}_d)}{\partial t}\right)_C - \frac{2}{3}\nabla\left(nw_d - \frac{1}{2}m^* n v_d^2\right) \quad (4)$$

$$\frac{\partial (nw_d)}{\partial t} = -\nabla \cdot \left(n\vec{v}_d w_d\right) + en\nabla Œ \cdot \vec{v}_d + \left(\frac{\partial (nw_d)}{\partial t}\right)_C - \frac{2}{3}\nabla \cdot \left(n\vec{v}_d - \frac{/}{k_B}\nabla\right)\left(w_d - \frac{m^* v_d^2}{2}\right) \quad (5)$$

where $\vec{v}_d = \vec{p}_d / m^*$ is the average drift velocity, m^* is the effective mass, k_B is the Boltzmann constant, and $/ \cong 5k_B^2 nT / 2m^* €_p(w)$ is the thermal conductivity.

Since the quantities $n\vec{p}_d$ and nw_d on the left-hand-side of (4) and (5) are the products of two unknown quantities, these equations are slightly inconvenient. We must derive the equations in terms of the average carrier velocity $\vec{v}_d$ and average carrier energy w_d

$$\frac{\partial \vec{v}_d}{\partial t} = -\vec{v}_d \cdot \nabla \vec{v}_d + \frac{e}{m^*}\nabla Œ + \left(\frac{\partial v_d}{\partial t}\right)_c - \frac{2}{3nm^*}\nabla\left(nw_d - \frac{1}{2}m^* n v_d^2\right) \quad (6)$$

$$\frac{\partial w_d}{\partial t} = -\vec{v}_d \cdot \nabla w_d + e\nabla Œ \cdot \vec{v}_d + \left(\frac{\partial w_d}{\partial t}\right)_c - \frac{2}{3n}\nabla \cdot \left[\left(n\vec{v}_d - \frac{/}{k_B}\nabla\right)\left(w_d - \frac{m^* v_d^2}{2}\right)\right] \quad (7)$$

The collision terms in the balance equations can be represented by the ensemble relaxation rates.

$$(\partial n/\partial t)_C = -€_n(n - n_0),$$

$$(\partial \vec{v}_d / \partial t)_C = -€_p \vec{v}_d,$$

$$(\partial w_d / \partial t)_C = -€_w(w_d - w_0).$$

The Monte Carlo method is generally used to compute the ensemble relaxation rates as a function of energy. The results for silicon can be expressed as:

$$€_n = 0$$

$$€_p = €_{imp} + \left(€_{p3} w_d^3 + €_{p2} w_d^2 + €_{p1} w_d + €_{p0}\right)(1 - ew_d)$$

$$€_w = \left(€_{w1} w_d + €_{w0}\right) \cdot (1 - ew_d)$$

where $€_{imp} = 5 \times 10^{13}\left(N_D / 10^{25}\right)^{0.4}$,

$$ew = \min\left(\exp\left(\frac{-q(w - w_c)}{k_B T}\right), 1\right),$$

$€_{p0} = 6.782 \times 10^{12}$, $€_{p1} = 6.063 \times 10^{13}$,

$€_{p2} = 7.590 \times 10^{13}$, $€_{p3} = 1.174 \times 10^{13}$,

$€_{w0} = 2.500 \times 10^{12}$, $€_{w1} = 2.338 \times 10^{11}$,

and $w_c = 0.03$.

To simplify the mathematical derivation and numerical computation, it is convenient to normalize all physical quantities with respect to some factors so that we have equations of pure numbers. In general, the dopant and carrier concentrations are normalized to the intrinsic carrier concentration n_i, the potential to the thermal potential $V_{kT} = k_B T / e$, the energy to the thermal energy $w_0 = k_B T$, the velocity to $v_0 = \sqrt{2k_b T / m^*}$, the distance to the Debye length $x_0 = \sqrt{V_s k_B T / e^2 n_i}$, the time to $t_0 = x_0 / v_0$. Therefore, (2), (3), (6), and (7) become

$$\nabla^2 Œ + (N_d - n) = 0 \quad (8)$$

$$\frac{\partial n}{\partial t} = -\nabla \cdot (\vec{v}_d n) - €_n(n - n_0) \quad (9)$$

$$\frac{\partial \vec{v}_d}{\partial t} = -\vec{v}_d \cdot \nabla \vec{v}_d - \frac{1}{3n}\nabla\left(nw_d - nv_d^2\right) + \frac{1}{2}\nabla Œ - €_p \vec{v}_d \quad (10)$$

$$\frac{\partial w_d}{\partial t} = -\vec{v}_d \cdot \nabla w_d - \frac{2}{3n}\nabla\left[n\vec{v}_d\left(w_d - v_d^2\right)\right] + \frac{5}{6€_p}\nabla^2\left(w_d - v_d^2\right) + \nabla Œ \cdot \vec{v}_d - €_w(w_d - w_0) \quad (11)$$

The Crank-Nicolson method will be employed to solve the transient problem.

$$\frac{G_{Œ,i,j} + G^0_{Œ,i,j}}{2} = 0 \quad (12)$$

$$\frac{n_{i,j} - n^0_{i,j}}{\Delta t} = \frac{G_{n,i,j} + G^0_{n,i,j}}{2} \quad (13)$$

$$\frac{\vec{v}_{i,j}-\vec{v}^0_{i,j}}{\Delta t}=\frac{\vec{G}_{v,i,j}+\vec{G}^0_{v,i,j}}{2} \quad (14)$$

$$\frac{w_{i,j}-w^0_{i,j}}{\Delta t}=\frac{G_{w,i,j}+G^0_{w,i,j}}{2} \quad (15)$$

where

$$G_{\mathcal{E}}=\nabla^2\mathcal{E}+(N_d-n)$$

$$G_n=-\nabla\cdot(\vec{v}_d n)-\epsilon_n(n-n_0)$$

$$\vec{G}_v=-\vec{v}_d\cdot\nabla\vec{v}_d-\frac{2}{3n}\nabla\left(nw_d-nv_d^2\right)$$

$$+\frac{1}{2}\nabla\mathcal{E}-\epsilon_p(w_d)\vec{v}_d$$

$$G_w=-\vec{v}_d\cdot\nabla w_d-\frac{2}{3n}\nabla\left[n\vec{v}_d\left(w_d-v_d^2\right)\right]$$

$$+\frac{5}{6\epsilon_p}\nabla^2\left(w_d-v_d^2\right)+\nabla\mathcal{E}\cdot\vec{v}_d-\epsilon_w(w_d-w_0)$$

In the two dimensional problem, the velocity $\vec{v}_d$ should resolve along x and y directions as v_x and v_y, while the function $\vec{G}_v$ as G_{vx} and G_{vy}. The nonlinear equation system is solved by the Newton iteration method.

A simple alternating-direction-implicit (ADI) method is employed and the two dimensional problem can be reduced to one dimension under this condition. (a) Along y-direction (j inner loop, i outer loop)

$$\frac{\partial G_{i,j}}{\partial y_{i,j-1}}uy_{i,j-1}+\left(\frac{\partial G_{i,j}}{\partial y_{i,j}}-\frac{2}{\Delta t}\right)uy_{i,j}+\frac{\partial G_{i,j}}{\partial y_{i,j+1}}uy_{i,j+1}$$

$$=\frac{2(y_{i,j}-y^0_{i,j})}{\Delta t}-\left[G_{i,j}+G^0_{i,j}\right]$$

$$-\frac{\partial G_{i,j}}{\partial y_{i-1,j}}uy^0_{i-1,j}-\frac{\partial G_{i,j}}{\partial y_{i+1,j}}uy^0_{\mathrm{i+1,j}} \quad (16)$$

(b) Along x-direction (i inner loop, j outer loop)

$$\frac{\partial G_{i,j}}{\partial y_{i-1,j}}uy_{i-1,j}+\left(\frac{\partial G_{i,j}}{\partial y_{i,j}}-\frac{2}{\Delta t}\right)uy_{i,j}+\frac{\partial G_{i,j}}{\partial y_{i+1,j}}uy_{i+1,j}$$

$$=\frac{2(y_{i,j}-y^0_{i,j})}{\Delta t}-\left[G_{i,j}+G^0_{i,j}\right]$$

$$-\frac{\partial G_{i,j}}{\partial y_{i,j-1}}uy^0_{i,j-1}-\frac{\partial G_{i,j}}{\partial y_{i,j+1}}uy^0_{\mathrm{i,j+1}} \quad (17)$$

This formulation is suitable to the implementation of parallel computation since each row or column of the grid points in a semiconductor device can be treated independently.

四、結果與討論

In this report, a n^+nn^+ Si ballistic diode will be taken as an example. In the following numerical experiments we apply 0.7V to the ballistic diode with a time step $\Delta t = 0.5$fs. The time evolution of the internal distributions of electrostatic potential, electric field, electron velocity and electron temperature are shown in Figs. 1 ~ 4. The system reaches steady state in approximately 3ps.

As shown in Fig. 1, the potentials in n^+ regions are maintained at constant values and the applied voltage is dropped across the n region. Correspondingly, as shown in Fig. 2, the electric fields approximate to zero in n^+ regions. The positive and negative peaks of electric field in n^+n and nn^+ junctions are due to the formulation of space charge regions. The velocity distribution given in Fig. 3 also shows two peaks at the beginning. The spurious velocity overshoot predict by some hydrodynamic models is not observed in our numerical calculation. Fig. 4 shows that the electron temperature in the n region is higher than the lattice temperature and this is related to the velocity distribution given in Fig. 3.

Fig. 5 shows the distribution of electron concentration under steady state for various biases. The injection of excess electrons from the left junction creates a potential barrier shown in Fig. 1. The transient behavior of current density under various biases is shown in Fig.6. The current density oscillates terribly initially and converges to a constant value gradually

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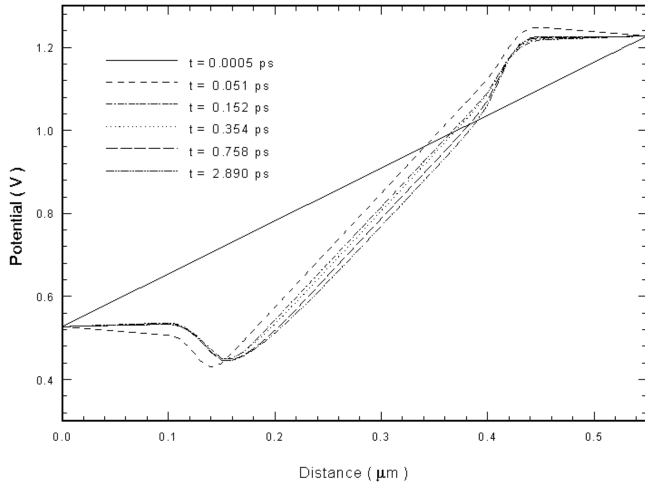
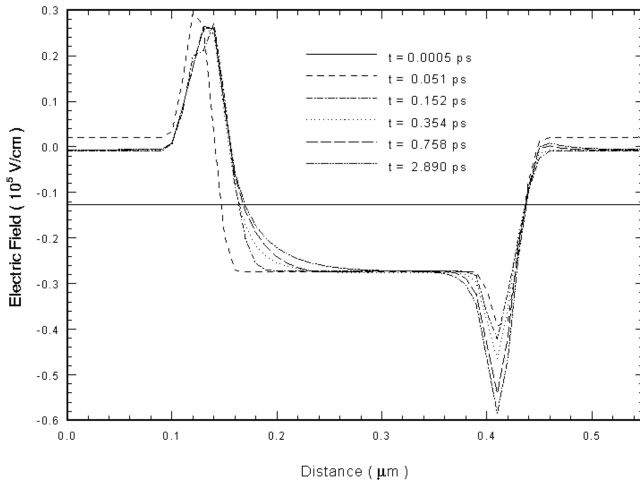
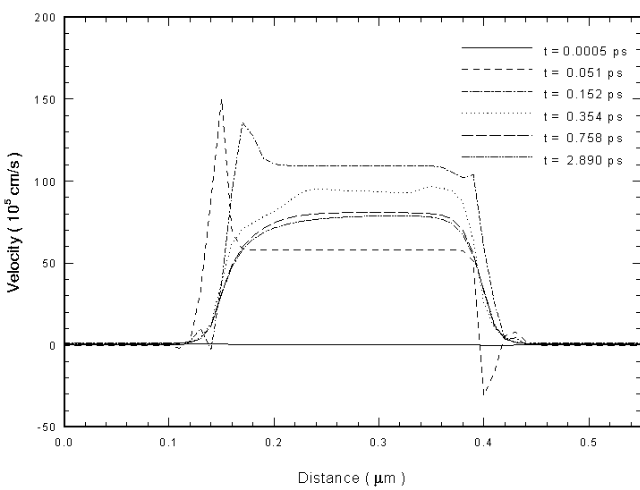


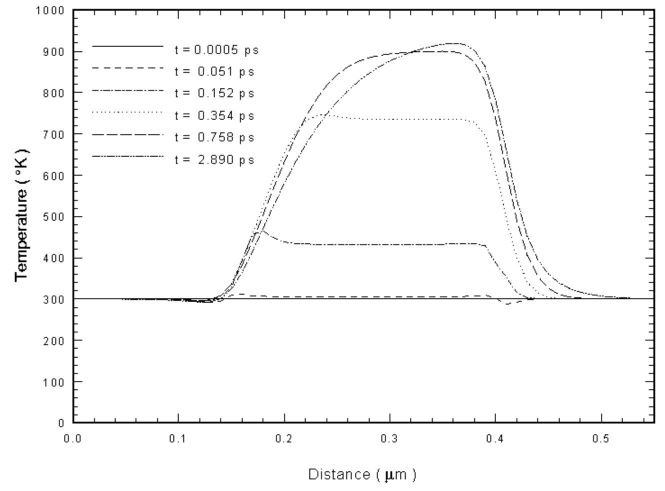
圖一 電位分佈之時間演變



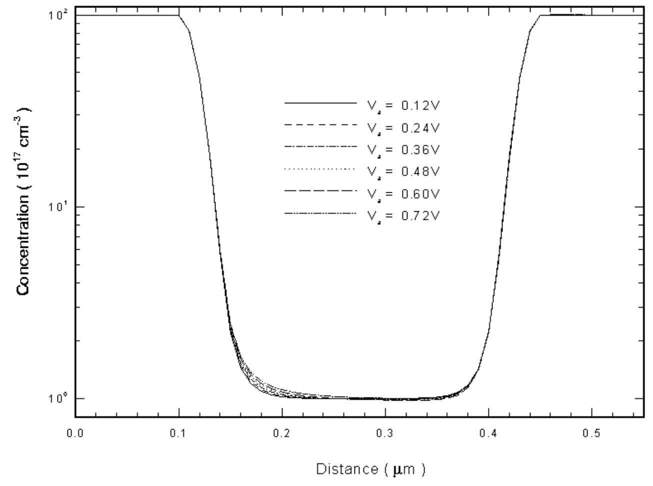
圖二 電場分佈之時間演變



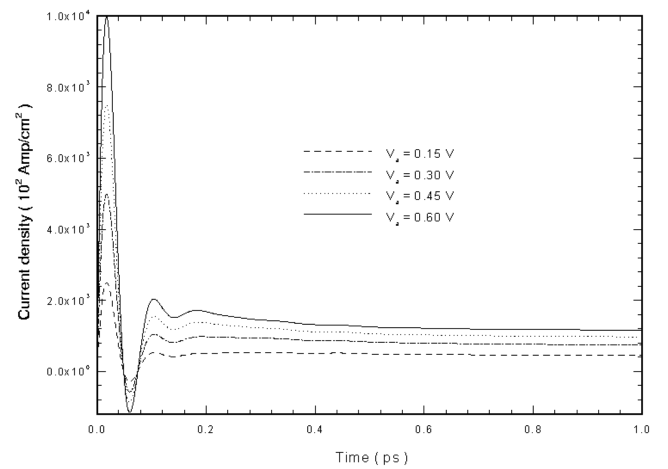
圖三 電子速度之時間演變



圖四 電子溫度之時間演變



圖五 電子濃度在不同電壓下的分佈



圖六 電流在不同電壓下的時間演變