次微米元件模擬程式的發展與平行計算

Development and Parallel Computation of Sub-Micron Device Simulator

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一、 中文摘要(關鍵詞：數值模擬、波茲曼傳輸方程式、平衡方程式、克藍-尼可森方案、交變方向隱含法、平行計算。)

本計畫發展出一套基於平衡方程式法的次微米半導體元件的數值模擬程式。載子濃度、載子速度、載子能量的基本方程式係導自波茲曼傳輸方程式。爲了簡化數學推導和數值計算，吾人將所有的物理量先對一些適當的因數化一，使所有的變數和參數成爲純數。載子行爲的時間演變是按照克藍-尼可森方案離散，非線性方程式系統是用牛頓反覆法線性化，而二維問題則以交變方向隱含法簡化成一維者。這種形成方法很容易以分行或分列的方式實現次微米金氧半場效體格點的平行計算。

點文摘要 (Keywords: numerical simulation, Boltzmann transport equation, balance equation method, Crank-Nicolson scheme, alternating-direction-implicit method, parallel computation.)

A numerical simulation program for submicron semiconductor devices has been developed based on the balance equation method. The basic equations for the carrier concentration, the carrier velocity, the carrier energy are derived from the Boltzmann transport equation. To simplify the mathematical derivation and numerical computation, it is convenient to normalize all physical quantities with respect to some proper factors so that we have equations of pure numbers. The transient behavior is descritized according to the Crank-Nicolson scheme. The nonlinear equation system is linearized by Newton iteration and the two dimensional problem is reduced to one dimension by an alternating-direction-implicit method. This formulation is very suitable to the implementation of parallel computation since each row or column of the grid points in a semiconductor device can be treated independently.

二、計劃緣由與目的

隨著半導體元件的持續往更微小的尺寸發展，很多過去被忽略的物理現象，必須在新一代的元件模擬軟體中加以考慮。由於物理模式及元件結構日趨複雜，使得模擬時間大幅地增加。因此很有必要利用平行處理技術發展一套新的元件模擬軟體，以便在較少的時間內得到較準確的結確。

爲了因應元件尺寸縮小所伴隨而來的複雜的二維、三維效應，運用單一處理器做純量模擬或是使用傳統數值方法求解線性化的方程式，往往需要耗費大量的計算時間，因此極需藉助具有平行處理能力的超級電腦並發展適於平行化的方程式解法。平行計算可說是未來電腦的發展趨未，因爲微處理器製程技術再怎麼進步，半導體元件總有量子力學上的極限，想要在現有的電腦技術架構上得到高效能的速度提昇，唯有藉助於多處理器及平行環境的使用。

三、研究方法

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

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

where v is carrier velocity, 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.

$$\nabla^2\varphi = -\frac{e}{\varepsilon_s}(N_D - n) \tag{2}$$

where ε, 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.

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

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

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

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 $\kappa \cong 5k_B^2 nT/2m^* \nu_p(w)$ 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

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

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

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

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

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

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

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:

$\nu_n = 0$

$\nu_p = \nu_{imp} + (\nu_{p3}w_d^3 + \nu_{p2}w_d^2 + \nu_{p1}w_d + \nu_{p0})(1 - ew_d)$

$\nu_w = (\nu_{w1}w_d + \nu_{w0})\cdot(1 - ew_d)$

where $\nu_{imp} = 5\times10^{13}(N_D/10^{25})^{0.4}$,

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

$\nu_{p0} = 6.782\times10^{12}$, $\nu_{p1} = 6.063\times10^{13}$,

$\nu_{p2} = 7.590\times10^{13}$, $\nu_{p3} = 1.174\times10^{13}$,

$\nu_{w0} = 2.500\times10^{12}$, $\nu_{w1} = 2.338\times10^{11}$,

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 $x_0 = \sqrt{\varepsilon_s k_B T/e^2 n_i}$, the time to $t_0 = x_0/v_0$. Therefore, (2), (3), (6), and (7) become

$$\nabla^2\varphi + (N_d - n) = 0 \tag{8}$$

$$\frac{\partial n}{\partial t} = -\nabla\cdot(\vec{v}_d n) - \nu_n(n - n_0) \tag{9}$$

$$\frac{\partial \vec{v}_d}{\partial t} = -\vec{v}_d \cdot \nabla \vec{v}_d - \frac{1}{3n}\nabla\left(nw_d - nv_d^2\right) + \frac{1}{2}\nabla\varphi - \nu_p \vec{v}_d \tag{10}$$

$$\frac{\partial w_d}{\partial t} = -\vec{v}_d \cdot \nabla w_d - \frac{2}{3n}\nabla\left[n\vec{v}_d\left(w_d - v_d^2\right)\right] + \frac{5}{6\nu_p}\nabla^2\left(w_d - v_d^2\right) + \nabla\varphi \cdot \vec{v}_d - \nu_w(w_d - w_0) \tag{11}$$

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

$$\frac{n_{i,j} - n_{i,j}^0}{\Delta t} = \frac{G_{n,i,j} + G_{n,i,j}^0}{2} \tag{12}$$

$$\frac{\vec{v}_{i,j} - \vec{v}_{i,j}^0}{\Delta t} = \frac{\vec{G}_{v,i,j} + \vec{G}_{v,i,j}^0}{2} \tag{13}$$

$$\frac{w_{i,j} - w_{i,j}^0}{\Delta t} = \frac{G_{w,i,j} + G_{w,i,j}^0}{2} \tag{14}$$

$$\frac{G_{\varphi,i,j} + G_{\varphi,i,j}^0}{2} = 0 \tag{15}$$

where

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

$$\vec{G}_v = -\vec{v}_d \cdot \nabla \vec{v}_d - \frac{2}{3n}\nabla\left(nw_d - nv_d^2\right) + \frac{1}{2}\nabla\varphi - \nu_p(w_d)\vec{v}_d$$

$$G_w = -\vec{v}_d \cdot \nabla w_d - \frac{2}{3n}\nabla\left[n\vec{v}_d\left(w_d - v_d^2\right)\right] + \frac{5}{6\nu_p}\nabla^2\left(w_d - v_d^2\right) + \nabla\varphi \cdot \vec{v}_d - \nu_w(w_d - w_0)$$

$$G_\varphi = \nabla^2\varphi + (N_d - n)$$

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 equation system can be written in the following forms:

$$\Phi_n\left(\eta_{i,j-1}, \eta_{i-1,j}, \eta_{i,j}, \eta_{i+1,j}, \eta_{i,j+1}\right) = \frac{2(n_{i,j} - n_{i,j}^0)}{\Delta t} - (G_{n,i,j} + G_{n,i,j}^0) = 0 \tag{16}$$

$$\Phi_{v_x}\left(\eta_{i,j-1}, \eta_{i-1,j}, \eta_{i,j}, \eta_{i+1,j}, \eta_{i,j+1}\right) = \frac{2(v_{x,i,j} - v_{x,i,j}^0)}{\Delta t} - (G_{vx,i,j} + G_{vx,i,j}^0) = 0 \tag{17}$$

$$\Phi_{v_y}\left(\eta_{i,j-1}, \eta_{i-1,j}, \eta_{i,j}, \eta_{i+1,j}, \eta_{i,j+1}\right) = \frac{2(v_{y,i,j} - v_{y,i,j}^0)}{\Delta t} - (G_{vy,i,j} + G_{vy,i,j}^0) = 0 \tag{18}$$

$$\Phi_w\left(\eta_{i,j-1}, \eta_{i-1,j}, \eta_{i,j}, \eta_{i+1,j}, \eta_{i,j+1}\right) = \frac{2(n_{i,j} - n_{i,j}^0)}{\Delta t} - (G_{w,i,j} + G_{w,i,j}^0) = 0 \tag{19}$$

$$\Phi_\varphi\left(\eta_{i,j-1}, \eta_{i-1,j}, \eta_{i,j}, \eta_{i+1,j}, \eta_{i,j+1}\right) = G_{\varphi,i,j} + G_{\varphi,i,j}^0 = 0 \tag{20}$$

where $\eta_{i,j}$ represents the unknown variables $n_{i,j}$, $v_{x,i,j}$, $v_{y,i,j}$, $w_{i,j}$ and $\varphi_{i,j}$ at the grid point (i,j).

The nonlinear equation system is solved by the Newton iteration method.

$$\frac{\partial G_{i,j}}{\partial \eta_{i,j-1}}\delta\eta_{i,j-1} + \frac{\partial G_{i,j}}{\partial \eta_{i-1,j}}\delta\eta_{i-1,j} + \left(\frac{\partial G_{i,j}}{\partial \eta_{i,j}} - \frac{2}{\Delta t}\right)\delta\eta_{i,j} + \frac{\partial G_{i,j}}{\partial \eta_{i+1,j}}\delta\eta_{i+1,j} + \frac{\partial G_{i,j}}{\partial \eta_{i,j+1}}\delta\eta_{i,j+1} = \frac{2(\eta_{i,j} - \eta_{i,j}^0)}{\Delta t} - \left[G_{i,j} + G_{i,j}^0\right] \tag{21}$$

where

$$\frac{\partial G_{i,j}}{\partial \eta_{k,l}} \equiv \begin{bmatrix} \frac{\partial G_{n,i,j}}{\partial n_{k,l}} & \frac{\partial G_{n,i,j}}{\partial vx_{k,l}} & \frac{\partial G_{n,i,j}}{\partial vy_{k,l}} & \frac{\partial G_{n,i,j}}{\partial w_{k,l}} & \frac{\partial G_{n,i,j}}{\partial \varphi_{k,l}} \\ \frac{\partial G_{vx,i,j}}{\partial n_{k,l}} & \frac{\partial G_{vx,i,j}}{\partial vx_{k,l}} & \frac{\partial G_{vx,i,j}}{\partial vy_{k,l}} & \frac{\partial G_{vx,i,j}}{\partial w_{k,l}} & \frac{\partial G_{vx,i,j}}{\partial \varphi_{k,l}} \\ \frac{\partial G_{vy,i,j}}{\partial n_{k,l}} & \frac{\partial G_{vy,i,j}}{\partial vx_{k,l}} & \frac{\partial G_{vy,i,j}}{\partial vy_{k,l}} & \frac{\partial G_{vy,i,j}}{\partial w_{k,l}} & \frac{\partial G_{vy,i,j}}{\partial \varphi_{k,l}} \\ \frac{\partial G_{w,i,j}}{\partial n_{k,l}} & \frac{\partial G_{w,i,j}}{\partial vx_{k,l}} & \frac{\partial G_{w,i,j}}{\partial vy_{k,l}} & \frac{\partial G_{w,i,j}}{\partial w_{i,j}} & \frac{\partial G_{w,i,j}}{\partial \varphi_{k,l}} \\ \frac{\partial G_{\varphi,i,j}}{\partial n_{k,l}} & \frac{\partial G_{\varphi,i,j}}{\partial vx_{k,l}} & \frac{\partial G_{\varphi,i,j}}{\partial vy_{k,l}} & \frac{\partial G_{\varphi,i,j}}{\partial w_{k,l}} & \frac{\partial G_{\varphi,i,j}}{\partial \varphi_{k,l}} \end{bmatrix}$$

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)

$$\frac{\partial G_{i,j}}{\partial \eta_{i,j-1}}\delta\eta_{i,j-1}+\left(\frac{\partial G_{i,j}}{\partial \eta_{i,j}}-\frac{2}{\Delta t}\right)\delta\eta_{i,j}+\frac{\partial G_{i,j}}{\partial \eta_{i,j+1}}\delta\eta_{i,j+1}$$
$$=\frac{2(\eta_{i,j}-\eta^0_{i,j})}{\Delta t}-\left[G_{i,j}+G^0_{i,j}\right]$$
$$-\frac{\partial G_{i,j}}{\partial \eta_{i-1,j}}\delta\eta^0_{i-1,j}-\frac{\partial G_{i,j}}{\partial \eta_{i+1,j}}\delta\eta^0_{\mathrm{i+1,j}} \qquad (22)$$

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

$$\frac{\partial G_{i,j}}{\partial \eta_{i-1,j}}\delta\eta_{i-1,j}+\left(\frac{\partial G_{i,j}}{\partial \eta_{i,j}}-\frac{2}{\Delta t}\right)\delta\eta_{i,j}+\frac{\partial G_{i,j}}{\partial \eta_{i+1,j}}\delta\eta_{i+1,j}$$
$$=\frac{2(\eta_{i,j}-\eta^0_{i,j})}{\Delta t}-\left[G_{i,j}+G^0_{i,j}\right]$$
$$-\frac{\partial G_{i,j}}{\partial \eta_{i,j-1}}\delta\eta^0_{i,j-1}-\frac{\partial G_{i,j}}{\partial \eta_{i,j+1}}\delta\eta^0_{\mathrm{i,j+1}} \qquad (23)$$

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

本計畫原來打算在現有的包含帕松方程式及電子-電洞連續性方程式的半導體元件模擬程式中加入能量平衡力程式，使之可以用來計算出次微米元件的特性。經過多方探討發現，此一構想未能適用於豪微米元件，因改採較爲基本的平衡方程式法而進度雖略有延誤，但已有初步的結結。

爲了測試所編寫的平衡方程式法數值模擬程式，吾人紀錄n^+nn^+結構的若干模擬過程及結結。圖一和圖二分別顯示電子濃度和電子速度在施加0.5v電壓下的分佈及時間演變，而圖三則顯示在施加0.3v電壓下的電流分佈及時間演變。圖四顯示電流在四同電壓下由暫態演變至定態。

五、參考文獻

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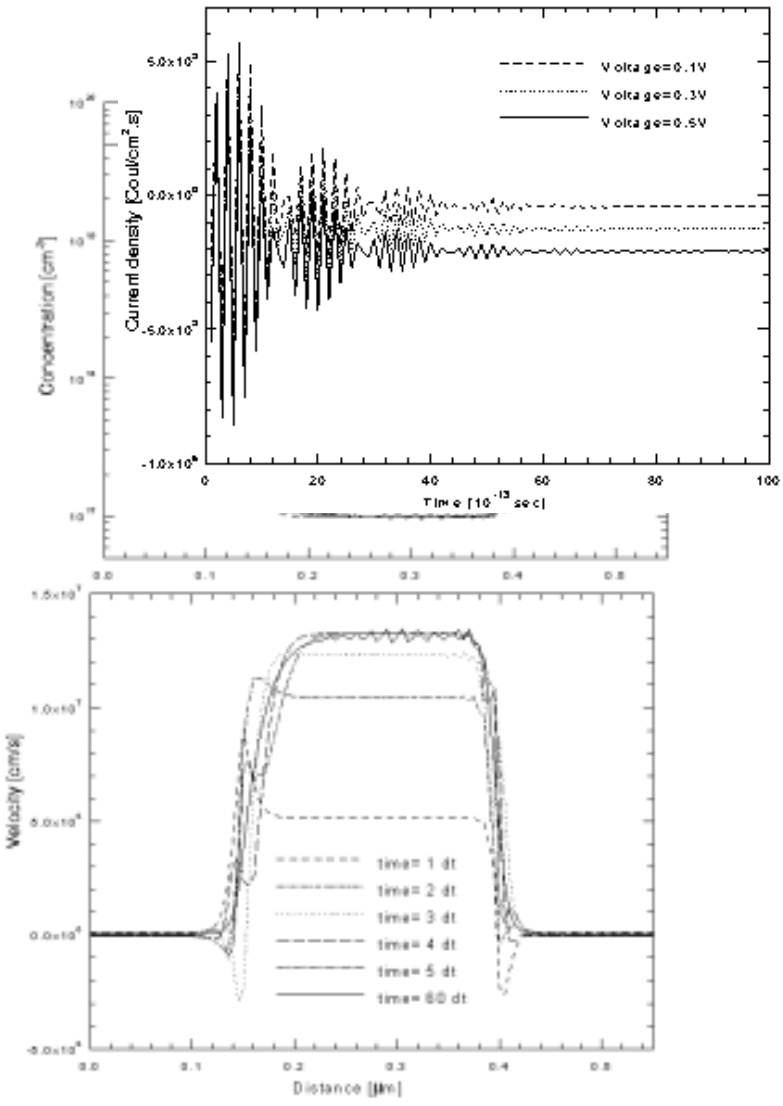
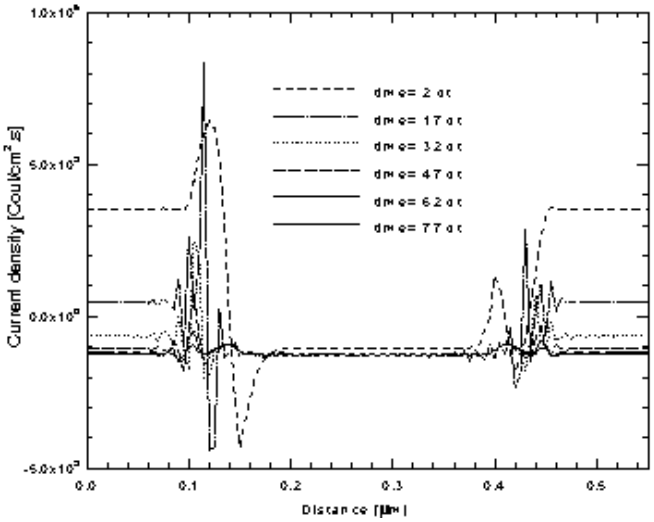


圖一 電子濃度分佈及時間演變

圖二 電子速度分佈及時間演變



圖三 電流分佈及時間演變

圖四 電流在四同電壓下的時間演變