A Novel Approach to Carrier Temperature Calculation for Semiconductor Device Simulation using Monotone Iterative Method. Part I: Numerical Algorithm

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Abstract: - In this paper, we solve numerically a semiconductor device energy balance equation using monotone iterative method. With the proposed solution technique, we prove the solution of ¯nite volume discretized semiconductor device energy balance equation converges monotonically. The method presented here provides an e± cient approach for the numerical solution of energy balance equation in submicron semiconductor device simulation.

Key Words: - Energy Balance Equation, Semiconductor Device Simulation, Monotone Iterative Method

I. Introduction

For large scale or long channel semiconductor devices, the VLSI device design could be done with an empirical design rule or using a trial and error experimental approach, in past years. The device scale has been shrunk into deep submicron or nano meter region recently [1], and has become more di± cult to design or improve semiconductor device characteristics with such straightforwardly strategies. Consequently, the development of numerical device modeling and simulation provides an e± cient way not only for device optimal design but also insight into device physics [2, 3, 4, 5, 6, 7, 8, 9, 10, 11].

Semiconductor device simulation including energy balance equation has recently received great interests for modeling nonlocal and hot carrier e®ects in submicron semiconductor devices [2, 12, 13, 14, 15]. The energy balance equation is a nonlinear partial di®erential equation (PDE), so its numerical di± culties, such as convergence and stability have been discussed in semiconductor device simulation [2, 13, 14, 15]. For example, to solve the energy balance equation, the rapid variation of electron temperature between mesh points leads to a signi¯cant di± culty in semiconductor device simulation. Based on an assumption that the electron temperature T_n varies linearly between mesh points, a Scharfetter-Gummel liked discretization scheme for the energy balance equation, so-called Scharfetter-Gummel-Tang scheme was developed in semiconductor hydrodynamic device simulation. However, due to the electron temperature model problem is a singular nonlinear boundary value problem, the assumption of the Scharfetter-Gummel-Tang scheme holds only for ¯ne mesh arti¯cially. This leads to numerical stability and convergence problem when solving the system

of nonlinear algebraic equations arising from the discretization of energy balance equation.

In this paper, we propose a computational e±cient method for the numerical solution of semiconductor device energy balance equation using monotone iterative method [16, 17, 18]. This method for semiconductor device simulations with nonlinear Poisson equation, drift diffusion, and hydrodynamic models has been reported in our earlier work [4, 5, 6, 7, 8, 9, 10, 11]. First of all, applying a physical based new state variable ®, the energy balance equation can be transformed into a self-adjoint form and then discretized using ¯nite volume method [19, 20] with a very ¯ne nonuniform mesh. The discretized energy balance equation leads to a system of nonlinear algebraic equations with a diagonal dominate property [19]. We solve the nonlinear system by applying a monotone iterative method directly instead of Newton's iterative method. We prove the solution sequence constructed from the monotone iterative algorithm converges to the unique solution of the system of nonlinear algebraic equations monotonically. This solution method converges monotonically and is highly parallel.

We divide this study into two parts, Part I concerns theoretical work. Practical implementation algorithm and simulation results are described in Part II. This paper is organized as follows. Sec. 2 states semiconductor device energy balance equation. Sec. 3 shows the solution algorithm with monotone iterative method. We prove the solution sequence converges to the unique solution of the system of nonlinear algebraic equations monotonically. Sec. 4 draws the conclusions and suggests future works.

II. A Numerical Energy Balance Model

In steady state, we consider here a two-dimensional (2D) energy balance equation for electrons as follows [1, 2, 12, 13, 14, 15]

$$\begin{aligned} &\tau \cdot (v_d n \varepsilon + v_d n k_B T_n + Q_n) \\ &+ q n v_d \cdot E = (\tfrac{@W_n}{@t})_{coll:}; \end{aligned} \qquad (1)$$

where $\tau = (\frac{@}{@x}; \frac{@}{@y})$ is the spatial gradient vector, v_d is the electron drift velocity, ε is the average electron energy, q is the elementary charge, n is the electron concentration, and $E = ¡ \tau Á$ ($Á$ is the electrostatic potential) is the electric ¯eld. In addition, k_B is the Boltzmann's constant, and the electron temperature T_n is assumed to be a scalar quantity here , Q_n is the heat °ux, and $(\frac{@W_n}{@t})_{coll:}$ is the energy collision rate. For the hole, we have a similar energy balance equation.

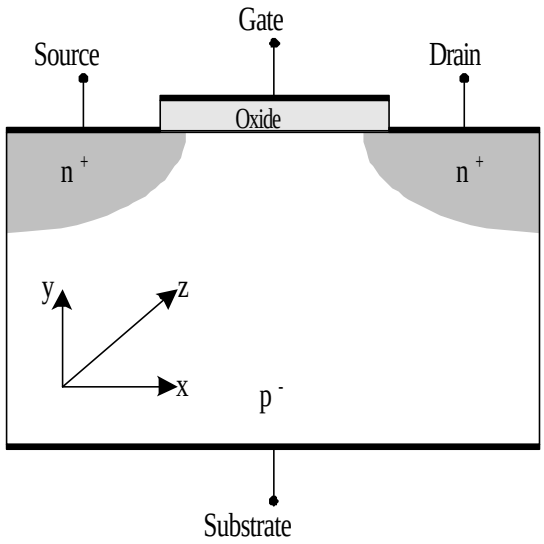

Fig. 1. A 2D domain for a submicron N-MOSFET device.

To proceed our derivation subsequently, we brie°y state the used physical models and assumptions [1, 2, 12, 13, 14, 15]: (a) the average electron energy ε is the sum of thermal energy $\frac{3}{2}k_B T_n$ and kinetic (drift) $\frac{1}{2}m_n^¤ jv_d j^2$ energy and $m_n^¤$ is the electron e®ective mass; (b) energy collision rate $(\frac{@W_n}{@t})_{coll:}$ can be represented as $¡ n(\varepsilon ¡ \varepsilon_0)=¿_\varepsilon(T_n)$ physically, average electron equilibrium thermal energy ε_0 is given by $\frac{3}{2}k_B T_L$, where T_L is the lattice temperature. An energy relaxation time model $¿_\varepsilon = \frac{3^1{}_{n0} k_B T_n T_L}{2q v^2_{sat:(Tn+T_L)}} + \frac{m_n^¤ {}^1{}_{n0} T_L}{2qT_n}$ is used in this work, where $v_{sat:}$ is the electron saturation velocity, $^1{}_{n0}$ is the electron mobility at low electric ¯eld, and the 2nd term on the right hand side of $¿_\varepsilon$ is so-called the momentum relaxation time; (c) consider here the

Weidmann-Franz physical model for semiconductor, we have heat °ow $Q_n = ¡ \cdot_c r T_n$, where $\cdot_c = 2T_n k_B^2 n^1{}_n/q$ is the thermal conductivity for electrons and $^1{}_n$ is the electron temperature dependent mobility model; (d) we further assume here the $T_n{}^1{}_n$ can be expressed a product of T_L and $^1{}_n^{E;D}$, where $^1{}_n^{E;D}$ is an electric ¯eld E and ionized carrier concentration D dependent mobility model; and (e) the electron current density can be written as $J_n = ¡ qnv_d$ directly.

With these physical models and assumptions (a)-(e) above, it is evident we can write Eq. (1) into this expression

$$r \cdot (\frac{5k_B T_n J_n}{2q} + \frac{m^¤_n |v_d|^2 J_n}{2q} + \frac{2T_L k_B^2 n^1{}_n^{E;D}}{q} r T_n) = f(T_n; T_L; n; Á; v_d; v_{sat:}; q; ^1{}_{n0}; k_B; m^¤_n) \quad (2)$$

where f can be directly calculated and it is a nonlinear function, and the unknown to be solved is T_n. Eq. (2) involves ¯rst order and second order derivate for T_n and the f is at least a nonlinear function in T_n, so it is a strongly nonlinear PDE. This leads to some di± culties in numerical solution, such as stability and convergence problems.

To apply monotone iterative method for the numerical solution of Eq. (2) e± ciently, we now assume Boltzmann statistics [1] holds for the approximation of electron concentration and electrostatic potential. With this physical observation, the Eq. (2) can be transformed into a self-adjoint form and hence has many advantanges in the numerical solution of energy balance equation. By considering the exponential quasi Fermi level approximation for electron concentration n and a similar approximation for electron temperature T_n [1, 15], we can further express Eq. (2)

$$r \cdot ((\frac{2n_i T_L^2 k_B^2 ^1{}_n^{E;D} e^{\frac{q(Á ¡ '_n)}{k_B T_L}}}{q}) e^{c'_n} r ®) = f(®; ©); \quad (3)$$

where f has new interpretation and it is a monotone function with respect to ®, n and T_n are implicitly de¯ned by

$$n = n_i u e^{\frac{q}{k_B T_L} Á}; \text{ and } T_n = T_L ® e^{c'_n}: \quad (4)$$

The u and ® in Eq. (4) can be uniquely de¯ned here, and the value c is also followed. Eq. (3) is an electron energy °ow continuity equation and the unknown to be solved is ®, where the u and other physical quanties can be solved from the solution of Poisson equation and electron-hole current continuity equations [4, 5, 6, 7, 8, 9, 10, 11].

As shown in Fig. 1, the boundary for electron temperature T_n is the Dirichlet type boundary conditions at ohmic contact parts: source, drain, and substrate. At $S_i ¡ S_iO_2$ interface, left and right hand sides, zero energy °ow is applied and it leads to a homogeneous Neumann type boundary condition for T_n. By the de¯nition of ® in Eq. (4) and boundary conditions for T_n, the boundary conditions for ® are followd.

To solve Eq. (3), we note the required physical quanties, such as Á; n; E; J_n; mobility, and recombination terms can be obtained from the numerical solution of Poisson equation and electron-hole current continuity equations.

Our monotone iterative method is applied to solve the nonlinear algebraic system resulting from the ¯nite volume discretization of Eq. (3). We prove the computed solution with monotone iterative method converges to the unique solution of the equation monotonically.

III. A Monotone Iterative Solution Technique

We state here a monotone iterative method for ¯nite volume discretized energy balance equation ¯rstly. The f(®; ©) is a monotone function in ®; and we have following result directly.

Theorem 1 The nonlinear term f(®; ©) in Eq. (3) is a monotone function in ®, i.e., there exists a positive constant c_0; such that $\frac{@f(®;©)}{@®} ¸ c_0$; for all ®:

Remark 1 We note the applied bias at device ohmic contact parts is ¯nite, so all of the physical quanties are bounded functions in the device simulation domain. Thus based on the physical de¯nition above, ® is bounded function.

Proof. With Remark 1 and calculation for the function, we have the results directly. ■

We discertized nonlinear Eq. (3) with ¯nite volume method and approximate the integrations with quadrature rule [19, 20]. The system of nonlinear algebraic equations for the equation is then solved by the monotone iterative method. The discretized system can be written as

$$\begin{aligned} &- \alpha_{i;j-1} z_{i;j-1} - \alpha_{i-1;j} z_{i-1;j} + \alpha_{i;j} z_{i;j} \\ &- \alpha_{i+1;j} z_{i+1;j} - \alpha_{i;j+1} z_{i;j+1} = - F(z_{i;j}); \end{aligned} \tag{5}$$

for all nodes $(x_i; y_j)$ in the device domain, where $z_{i;j} = z(x_i; y_j)$ represents the approximated value $\phi_{i;j}$ of the function ϕ at $(x_i; y_j)$ in Eqs. (3). The discretization coe± cients $\alpha_{i;j}$; $\alpha_{i+1;j}$; $\alpha_{i-1;j}$; $\alpha_{i;j-1}$; and $\alpha_{i;j+1}$ are associated with the operators as well as its boundary conditions. Similarly, F is associated with the nonlinear function f and boundary conditions. The coe± cients satisfy the conditions:

$$\begin{aligned} &\alpha_{i;j} \geq 0; \alpha_{i+1;j} \geq 0; \alpha_{i-1;j} \geq 0; \\ &\alpha_{i;j-1} \geq 0; \alpha_{i;j+1} \geq 0; \\ &\alpha_{i;j} \geq \alpha_{i+1;j} + \alpha_{i-1;j} + \alpha_{i;j-1} + \alpha_{i;j+1}; \end{aligned} \tag{6}$$

for all discretization index $(i; j)$ in the device domain. We write now Eq. (5) as a compact system of nonlinear algebraic equations,

$$AZ = -F(Z): \tag{7}$$

Theorem 2 The system of nonlinear algebraic equations (7) derived from energy balance equation (3) has at most a solution.

Remark 2 The matrix A in Eq. (7) is an M-matrix and since $\frac{\partial}{\partial z_{i;j}} f(z_{i;j}) > 0$, F is uniformly bounded and $\frac{\partial}{\partial z_{i;j}} F(z_{i;j}) \geq 0$.

Proof. It is a direct result with the monotone property of $F(Z)$. For a given vector $\vec{\zeta} = (\zeta_1; \ldots; \zeta_M)^T$, the diagonal matrix $D(\vec{\zeta})$ is de-¯ned by

$$D(\vec{\zeta}) = \begin{pmatrix} \frac{\partial F_1}{\partial z}(\zeta_1) & & 0 \\ & \ddots & \\ 0 & & \frac{\partial F_M}{\partial z}(\zeta_M) \end{pmatrix}:$$

Let Z^1 and Z^2 be two solutions of the system (7) and set $Z = Z^1 - Z^2$. Then $[A + D(\vec{\zeta})] Z = 0$, for some vector $\vec{\zeta}$. Since A is an M-matrix and diagonal matrix $D(\vec{\zeta})$ is nonnegative, $A + D(\vec{\zeta})$ is an M-matrix [19]. Thus $A + D(\vec{\zeta})$ is invertible and $Z = Z^1 - Z^2 = 0$, i.e, $Z^1 = Z^2$ ■

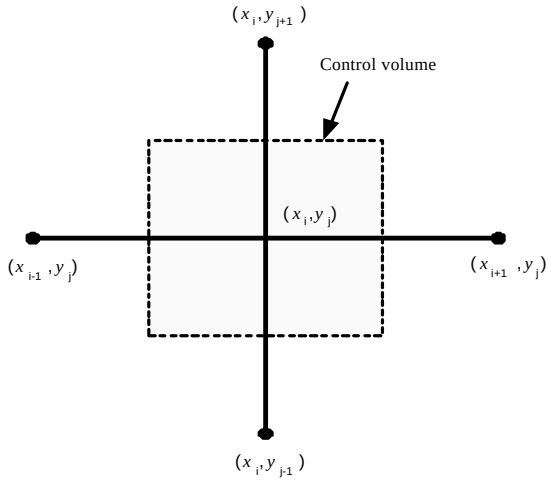

Fig. 2. An illustration of mesh points in $x - y$ plane for ¯nite volume discretization.

The proposed monotone iterative scheme for the nonlinear system are now written explicitly in terms of nodal points $(x_i; y_j)$ in the device domain and the monotone iteration index m, $m = 0; 1; \ldots$. The abstract iterative scheme is

$$\begin{aligned} \phi_{i;j}^{(m+1)} &= \frac{LU(\phi_{i;j}^{(m)}) - f(\phi_{i;j}^{(m)}) + \rho_{i;j}^{(m)} \phi_{i;j}^{(m)}}{\alpha_{i;j} + \rho_{i;j}^{(m)}}; \\ \rho_{i;j}^{(m)} &= \frac{\partial}{\partial \phi_{i;j}^{(m)}} f(\phi_{i;j}^{(m)}; \zeta); \end{aligned} \tag{8}$$

for all nodes $(x_i; y_j)$ in the device domain, where $A = D - L - U$, D constructed from the $\rho_{i;j}^{(m)}$ and inentidy matrix is the diagonal matrix of A, L and U are lower and upper matrices of A. The value $\phi_{i;j}^{(m+1)}$ is an approximation of the potential function ϕ at the node $(x_i; y_j)$ and $LU(\phi_{i;j}^{(m)})$ is the sum of the corresponding coe± cients (see Fig. 2) at m iteration. We further express above Eq. as the following computational algorithm

$$z_{i;j}^{(m+1)} = \frac{1}{\rho_{i;j}^{(m)} + \alpha_{i;j}} \{\alpha_{i+1;j} z_{i+1;j}^{(m)} + \alpha_{i-1;j} z_{i-1;j}^{(m)}$$

$$+ \quad \gg_{i;j\,i\,1} z^{(m)}_{i;j\,i\,1} + \gg_{i;j+1} z^{(m)}_{i;j+1} \;i\; f(z^{(m)}_{i;j})$$
$$+ \quad ,^{(m)}_{i;j} z^{(m)}_{i;j}\}; \qquad (9)$$

for all nodes $(x_i; y_j)$ in the device domain and for all m.

Theorem 3 Let $z^{(0)}_{i;j}$ be an arbitrary solution sequence and $z^{\alpha}_{i;j}$ be the solution of Eq. (5). Let $\{z^{(m)}_{i;j}\}_{m=1}^{1}$ be a solution sequence of Eq. (9). Then $z^{(m)}_{i;j} \,i\,! \, z^{\alpha}_{i;j}$ as $m \,i\,! \, 1$, for all $(x_i; y_j)$ in the device domain.

Proof. The nodal values ¯xed on boundary part are uniquely determined by their associated values. We prove now the result for all interior nodes of the device domain. De¯ne

$$'^{(m)}_{i;j} = z^{(m)}_{i;j} \,i\, z^{\alpha}_{i;j}$$

for all $(x_i; y_j)$ in the device domain. Since $z^{\alpha}_{i;j}$ is the solution of Eq. (5), we have

$$z^{\alpha}_{i;j} = \frac{1}{\gg_{i;j}}\{\gg_{i+1;j} z^{\alpha}_{i+1;j} + \gg_{i\,i\,1;j} z^{\alpha}_{i\,i\,1;j}$$
$$+ \quad \gg_{i;j\,i\,1} z^{\alpha}_{i;j\,i\,1} + \gg_{i;j+1} z^{\alpha}_{i;j+1}$$
$$i \quad f(z^{\alpha}_{i;j})\}. \qquad (10)$$

From Eqs. (9) and (10) we derive

$$'^{(m+1)}_{i;j} = \frac{1}{,^{(m)}_{i;j} + \gg_{i;j}}\{\gg_{i+1;j} '^{(m)}_{i+1;j} + \gg_{i\,i\,1;j} '^{(m)}_{i\,i\,1;j}$$
$$+ \quad \gg_{i;j\,i\,1} '^{(m)}_{i;j\,i\,1} + \gg_{i;j+1} '^{(m)}_{i;j+1} \;i\; (z^{(m)}_{i;j})$$
$$+ \quad f(z^{\alpha}_{i;j}) + ,^{(m)}_{i;j} '^{(m)}_{i;j}\}$$
$$= \frac{1}{,^{(m)}_{i;j} + \gg_{i;j}}\{\gg_{i+1;j} '^{(m)}_{i+1;j} + \gg_{i\,i\,1;j} '^{(m)}_{i\,i\,1;j}$$
$$+ \quad \gg_{i;j\,i\,1} '^{(m)}_{i;j\,i\,1} + \gg_{i;j+1} '^{(m)}_{i;j+1} + (,^{(m)}_{i;j}$$
$$i \quad \frac{f(z^{(m)}_{i;j}) \,i\, f(z^{\alpha}_{i;j})}{'^{(m)}_{i;j}})'^{(m)}_{i;j}\}. \qquad (11)$$

Since f is increasing function, there exists a positive constant c_0 such that

$$\frac{f(z^{(m)}_{i;j}) \,i\, f(z^{\alpha}_{i;j})}{'^{(m)}_{i;j}} \;, \; c_0 > 0;$$

where the constant c_0 can be calculated in Theorem 1. We calculate the estimation from Eq. (11) and note the Eq. (6), the following expression can be derived directly

$$\|'^{(m+1)}_{i;j}\|_1 \;.\; \circ\|'^{(m)}_{i;j}\|_1;$$

where the positive parameter ° is given by

$$\circ = \max_{i;j}\left(\frac{,^{(m)}_{i;j} + \gg_{i;j} \,i\, c_0}{,^{(m)}_{i;j} + \gg_{i;j}}\right) < 1;$$

for all nodes $(x_i; y_j)$ in the device domain. Therefore,

$$\|'^{(m+1)}_{i;j}\|_1 \;.\; \circ\|'^{(m)}_{i;j}\|_1$$
$$\;.\; \circ 2\|'^{(m\,i\,1)}_{i;j}\|_1$$
$$\;.\; ¢¢¢$$
$$\;.\; \circ m+1\|'^{(0)}_{i;j}\|_1$$

for all $z^{(0)}_{i;j}$ and nodes $(x_i; y_j)$ in the whole device domain, and the result follows. ■

IV. Conclusions

Based on monotone iterative technique, we have presented a novel numerical solution method for semiconductor device energy balance equation. We further proved the solution sequences converge to the solution of the nonlinear system monotonically. This approach provided an alternative in the numerical solution of electrons and holes energy balance equations. Practical implementation algorithm for the carrier temperature calculation and simulation results are given in Part II. This method is inherently parallel and can be systematically extended to simulate, such as advanced semiconductor hydrodynamic model and spherical harmonic expanded Boltzmann transport equation.

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