A Monotone Iterative Method for Semiconductor Device Drift Diffusion Equations

YIMING LI
National Nano Device Laboratories, and
Microelectronics and Information Systems Research Center,
National Chiao Tung University,
1001 Ta-Hsueh Rd., Hsinchu city, Hsinchu 300,
TAIWAN

Abstract: - In this paper, we solve semiconductor device drift diffusion equations with the Gummel's decoupling and monotone iterative methods. With monotone iterative technique, we prove each Gummel's decoupled and finite volume discretized device equation converges monotonically. The proposed method here provides an alternative in the numerical solution of semiconductor device drift diffusion equations.

Key Words: - Drift Diffusion Model, Semiconductor Device, Monotone Iterative Method

1. Introduction

Numerical methods for the fundamental semiconductor device equations provide an alternative in the development of microelectronics [1, 2, 3, 4, 5, 6, 7, 8, 9]. The drift diffusion model consists of the Poisson, electron current continuity, and hole current continuity equations has been of great studied for semiconductor device simulation in the past years [10, 11, 12, 13, 14]. A widely approach to solve these equations efficiently is to decoupled them firstly with the Gummel's decoupling method [14, 13, 16]. Each decoupled equation is then discretized and solved with the Newton's iteration method subsequently. It is a traditional method for the solution of system of nonlinear algebraic equations and converges quadratically when the initial guess is in the neighborhood of the exact solution. However, to simulate the submicron and nano-scale semiconductor devices with an accurate initial guess is a difficult task and has involved many engineering works.

The monotone iterative method is not only a classical constructive technique for the solutions of PDEs but also useful for the numerical solutions of physical models [17, 18, 19]. In this work, we use this method to simulate device characteristics with exploiting the basic nonlinear property in drift diffusion model. By considering the quasi-Fermi levels in the approximation for carrier's density and electrostatic potential, the drift diffusion model in (ϕ, n, p) variables is transformed into a self-adjoint model with variables (ϕ, u, v) [11, 12, 13]. The transformed drift diffusion model is decoupled into three independent PDEs with the Gummel's decoupling scheme. The basic idea of this well-known Gummel's decoupled method is that the device equations are solved sequentially [14]. In the drift diffusion model, Poisson's equation is solved for $\phi^{(g+1)}$ given the previous states $u^{(g)}$ and $v^{(g)}$. The electron current continuity equation is solved for $u^{(g+1)}$ given $\phi^{(g)}$ and $v^{(g)}$. The hole current continuity equation is solved for $v^{(g+1)}$ given $\phi^{(g)}$ and $u^{(g)}$. Each decoupled PDE is discretized with finite volume method and then solved with the monotone iterative method. We prove this approach converges monotonically for all three decoupled equations. It means that we can solve the device equations with arbitrary initial guesses. Numerical results for various devices have been reported to demonstrate the robustness of the method in our earlier work [2, 3, 4, 5, 6, 7, 8, 9].

In Sec. 2 we state the drift diffusion model. Sec. 3 presents the monotone iterative methods for the Gummel's decoupled drift diffusion model. For each decoupled equation, we prove the convergence property for finite volume approximated equation by using monotone iterative method. Sec. 4 draws the conclusions and suggests future works.

2. Semiconductor Device Drift Diffusion Model

The steady state drift diffusion model of semiconductor devices is [10, 11, 12, 13, 14]

$$\begin{aligned} &\Delta\phi = \tfrac{q}{\varepsilon_s}(n-p+D),\\ &\tfrac{1}{q}\nabla\cdot J_n = R(\phi,n,p),\\ &\tfrac{-1}{q}\nabla\cdot J_p = R(\phi,n,p), \end{aligned}$$

where ϕ is the electrostatic potential, n and p are the electron and hole concentrations, q is the elementary charge, ε_s is the dielectric constant of semiconductor, D are ionized impurities, J_n and J_p are the electron and hole current densities, and $R(\phi,n,p)$ is the carrier recombination rate. The J_n, J_p, and Shockley-Read-Hall recombination rate $R(\phi,n,p)$ are as follows:

$$\begin{aligned} &J_n = -q\mu_n n\nabla\phi + qD_n\nabla n,\\ &J_p = -q\mu_p p\nabla\phi - qD_p\nabla p,\\ &R(\phi,n,p) = \tfrac{np-n_i^2}{\tau_n^0(p+p_T)+\tau_p^0(n+n_T)}, \end{aligned}$$

where n_i is the intrinsic carrier concentration, τ_n^0 and τ_p^0 are the electron and hole lifetimes, and p_T and n_T are the electron and hole densities associated with energy levels of the traps. The μ_n and μ_p are the doping- and field-dependent electron and hole mobilities [10, 11]. The diffusion coefficients of electrons and holes are expressed in the Einstein relations $D_n = V_T\mu_n$ and $D_p = V_T\mu_p$, where $V_T = \frac{kT}{q}$ is the thermal voltage, k is Boltzmann's constant, and T is temperature.

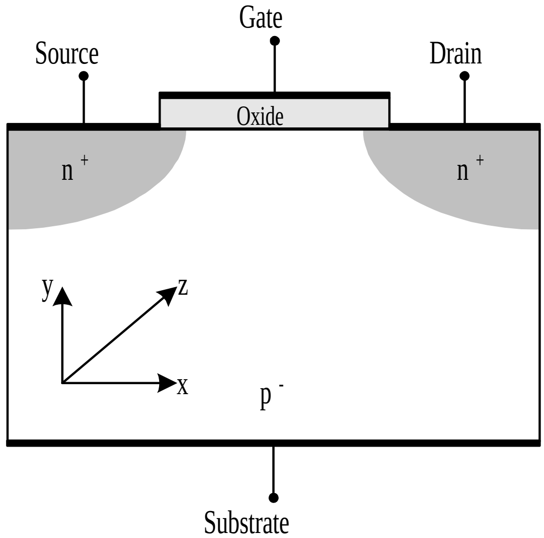

Fig. 1. A 2D domain for a submicron N-MOSFET device.

Using Boltzmann statistics, we write above equations as

$$\begin{aligned} &\Delta\phi = \tfrac{q(n_i(ue^{\frac{\phi}{V_T}} - ve^{\frac{-\phi}{V_T}})+D)}{\varepsilon_s},\\ &\nabla\cdot(D_n n_i e^{\frac{\phi}{V_T}}\nabla u) = R(\phi,u,v),\\ &\nabla\cdot(D_p n_i e^{\frac{-\phi}{V_T}}\nabla v) = R(\phi,u,v), \end{aligned} \qquad (1)$$

where $u = e^{\frac{-\varphi_n}{V_T}}$, and $v = e^{\frac{\varphi_p}{V_T}}$ are the exponential quasi-Fermi levels. The expressions for electrons and holes in terms of the quasi-Fermi potentials φ_n and φ_p are

$$\begin{aligned} &n = n_i e^{\frac{\phi-\varphi_n}{V_T}},\\ &p = n_i e^{\frac{\varphi_p-\phi}{V_T}}. \end{aligned}$$

The carrier recombination rate $R(\phi,n,p)$ becomes a nonlinear function in terms of ϕ, u, and v.

We have derived a self-adjoint semiconductor device drift diffusion model (1) with the state variables (ϕ, u, v) and it is favorable for the monotone iterative method. As shown in Fig. 1, [10] the model (1) is subject to boundary conditions on a rectangular domain - $\subset \mathbb{R}^2$. The domain is formed by the ohmic contact parts: source, gate, drain, and substrate and left and right boundaries. By the charge neutrality condition and the mass action law, the boundary conditions for three state variables are as follows [10].

The Dirichlet type boundary conditions are [11]

$$\begin{aligned} \phi &= V_O \\ &+ V_T \ln(\frac{\frac{N_A^- - N_D^+}{2} + (\frac{(N_A^- - N_D^+)^2}{4} + n_i^2)^{1/2}}{n_i}), \end{aligned}$$

$u = e^{\frac{-V_O}{V_T}}$, and $v = e^{\frac{V_O}{V_T}}$ on ∂- $_D$, where ∂- $_D$ consists of source, drain, and substrate contacts, $V_O = V_S$, V_D, or V_B, is the source, drain, or substrate applied voltage, respectively. On the left and right boundaries, we artificially assume that the normal components of the electric field $E = -\nabla\phi$ and current density are zero, and have the Neumann type boundary conditions $\frac{\partial \phi}{\partial \vec{\nu}} = 0$, $\frac{\partial u}{\partial \vec{\nu}} = 0$, and $\frac{\partial v}{\partial \vec{\nu}} = 0$ on ∂- $_N$, where ∂- $_N$ is the union of the left and right boundaries, $\vec{\nu}$ is the outward normal vector on ∂- $_N$. At the interface between semiconductor and oxide, we derive the Robin and Neumann types boundary conditions $\frac{t_{ox}\varepsilon_s}{\varepsilon_d}\frac{\partial \phi}{\partial \nu} + \phi = V_G$, $\frac{\partial u}{\partial \nu} = 0$, and $\frac{\partial v}{\partial \nu} = 0$ on ∂- $_R$, where ∂- $_R$ is the interface between semiconductor and oxide, V_G is the voltage applied on the gate, t_{ox} is the gate oxide thickness, and ε_d is the dielectric constant of the gate oxide.

3. The Gummel's Decoupling and Monotone Iterative Methods

In this section, we briefly state the Gummel's decoupling method for the coupled drift diffusion equations. The monotone iterative method is then applied to compute the solution for each decoupled and finite volume discretized equation. In order to use the classical monotone iterative in the numerical solution for each decoupled and discretized equation directly, we state the Gummel's decoupling method firstly and the monotone iterative method for each equation will be addressed later on.

With a given initial guess $\left(\phi^{(0)}, u^{(0)}, v^{(0)}\right)$ and for each Gummel's iteration index g, $g = 0, 1, \ldots$, we first solve the nonlinear Poisson equation

$$\Delta \phi^{(g+1)} = \widehat{R^{\phi}}(\phi^{(g+1)}, ., .), \tag{2}$$

for $\phi^{(g+1)}$ where $\widehat{R^{\phi}}$ is the right hand side function of the Poisson equation in (1). We then solve the electron current continuity equation

$$\nabla \cdot (D_n n_i e^{\frac{\phi^{(g)}}{V_T}} \nabla u^{(g+1)}) = \widehat{R^{u}}(., u^{(g+1)}, .), \tag{3}$$

with the known functions $\phi^{(g)}$ and $v^{(g)}$ for $u^{(g+1)}$, and the $\widehat{R^{u}}$ is the right hand side function of the electron current continuity equation. Finally we solve the hole current continuity equation

$$\nabla \cdot (D_p n_i e^{\frac{-\phi^{(g)}}{V_T}} \nabla v^{(g+1)}) = \widehat{R^{v}}(., ., v^{(g+1)}), \tag{4}$$

with computed $\phi^{(g)}$ and $u^{(g)}$ for $v^{(g+1)}$. The $\widehat{R^{v}}$ is the right hand side function of the hole current continuity equation. The Gummel's iteration loops will be terminated when a pre-specified criterion for (ϕ, u, v) is satisfied. This method is widely used in semiconductor device simulation and some theoretical works for its convergence could be found in [12, 13, 15, 16]. Each decoupled equation in Gummel's algorithm leads to an independent nonlinear PDE to be solved. Conventionally, these decoupled and discretized equations (by using finite difference or finite volume methods) [20, 21] are solved with the Newton's iterative method. This method has quadratic convergence rate, however it encounters many initial guess problems in submicron and nano-scale semiconductor device simulation.

Our monotone iterative method is applied to solve the nonlinear algebraic system resulting from the discretization of each PDE. We prove for each decoupled PDE the computed solution with monotone iterative method converges to the unique solution of the equation monotonically.

Theorem 1 *For a fixed Gummel's index g, the nonlinear terms $\widehat{R}(z)$, $z = \phi^{(g+1)}$, $u^{(g+1)}$, and $v^{(g+1)}$, in the Poisson and electron-hole current continuity equations are monotone functions in z, that is $\exists c > 0, \rightarrow \frac{\partial \widehat{R}(z)}{\partial z} \geq c,\ \forall z$.*

Remark 1 *We note the applied voltage at device contacts is finite, so the electrostatic potential ϕ is bounded function in device domain. In addition, based on the physical definition, the exponential quasi-Fermi levels u and v are positive and bounded functions.*

Proof. With Remark 1 and direct calculation for these three functions, we have the results directly. ■

We discertized nonlinear PDEs (2)-(4) with finite volume method and approximate the integrations with quadrature rule. The system of nonlinear algebraic equations for each PDE is then solved by the monotone iterative method. We fix the Gummel's iteration index g for the following discussions. The three discretized systems can be written as

$$\begin{array}{l} -\xi_{i,j-1}z_{i,j-1} - \xi_{i-1,j}z_{i-1,j} + \xi_{i,j}z_{i,j} \\ -\xi_{i+1,j}z_{i+1,j} - \xi_{i,j+1}z_{i,j+1} = -F(z_{i,j}), \end{array} \tag{5}$$

for all nodes (x_i, y_j) in the device domain, where $z_{i,j} = z(x_i, y_j)$ represents the approximated value $\phi_{i,j}$, $u_{i,j}$, and $v_{i,j}$ of the function ϕ, u, and v at (x_i, y_j) in Eqs. (2), (3), and (4), respectively. The discretization coefficients $\xi_{i,j}$, $\xi_{i+1,j}$, $\xi_{i-1,j}$, $\xi_{i,j-1}$, and $\xi_{i,j+1}$ are associated with the operators as well as their boundary conditions. Similarly, the nonlinear function F is associated with each nonlinear function $\widehat{R}$ and boundary conditions. It can be verified that the coefficients satisfy the conditions:

$$\begin{array}{l} \xi_{i,j} \geq 0, \xi_{i+1,j} \geq 0, \xi_{i-1,j} \geq 0, \\ \xi_{i,j-1} \geq 0, \xi_{i,j+1} \geq 0, \\ \xi_{i,j} \geq \xi_{i+1,j} + \xi_{i-1,j} + \xi_{i,j-1} + \xi_{i,j+1}, \end{array} \tag{6}$$

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

$$\mathcal{A}Z = -F(Z). \tag{7}$$

Theorem 2 *The system of nonlinear algebraic equations (7) has at most a solution.*

Remark 2 *The matrix $\mathcal{A}$ in Eq. (7) is an M-matrix [20] and since $\frac{\partial}{\partial z_{i,j}}\widehat{R}(z_{i,j}) > 0$, the function 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 $F(Z)$. ■

The iterative scheme for each 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 first iterative scheme is

$$\begin{array}{l} \phi_{i,j}^{(m+1)} = \frac{\mathcal{LU}(\phi_{i,j}^{(m)}) - \widehat{R}(\phi_{i,j}^{(m)}) + \lambda_{i,j}^{\phi-(m)}\phi_{i,j}^{(m)}}{\xi_{i,j} + \lambda_{i,j}^{\phi-(m)}}, \\ \widehat{R^{\phi}}(\phi_{i,j}^{(m)}) = \widehat{R^{\phi}}(\phi_{i,j}^{(m)}, ., .), \\ \lambda_{i,j}^{\phi-(m)} = \frac{\partial}{\partial \phi_{i,j}^{(m)}}\widehat{R^{\phi}}(\phi_{i,j}^{(m)}), \end{array} \tag{8}$$

for all nodes (x_i, y_j) in the device domain where $\phi_{i,j}^{(m+1)}$ is an approximation of the potential function ϕ at the node (x_i, y_j) and $\mathcal{LU}(\phi_{i,j}^{(m)})$ is the sum of the corresponding coefficients at m iteration. Similarly, for all nodes (x_i, y_j) we can write the iterative schemes

$$\begin{array}{l} u_{i,j}^{(m+1)} = \frac{\mathcal{LU}(u_{i,j}^{(m)}) - \widehat{R}(u_{i,j}^{(m)}) + \lambda_{i,j}^{u-(m)}u_{i,j}^{(m)}}{\xi_{i,j} + \lambda_{i,j}^{u-(m)}}, \\ \widehat{R^{u}}(u_{i,j}^{(m)}) = \widehat{R^{u}}(., u_{i,j}^{(m)}, .), \\ \lambda_{i,j}^{u-(m)} = \frac{\partial}{\partial u_{i,j}^{(m)}}\widehat{R^{u}}(u_{i,j}^{(m)}), \end{array} \tag{9}$$

and

$$\begin{array}{l} v_{i,j}^{(m+1)} = \frac{\mathcal{LU}(v_{i,j}^{(m)}) - \widehat{R}(v_{i,j}^{(m)}) + \lambda_{i,j}^{v-(m)}v_{i,j}^{(m)}}{\xi_{i,j} + \lambda_{i,j}^{v-(m)}}, \\ \widehat{R^{v}}(v_{i,j}^{(m)}) = \widehat{R^{v}}(., ., v_{i,j}^{(m)}), \\ \lambda_{i,j}^{v-(m)} = \frac{\partial}{\partial v_{i,j}^{(m)}}\widehat{R^{v}}(v_{i,j}^{(m)}), \end{array} \tag{10}$$

for electron and hole current continuity equations. We express above Eqs. as

$$\begin{aligned} z_{i,j}^{(m+1)} &= \frac{1}{\lambda_{i,j}^{(m)} + \xi_{i,j}}\{\xi_{i+1,j}z_{i+1,j}^{(m)} + \xi_{i-1,j}z_{i-1,j}^{(m)} \\ &+ \xi_{i,j-1}z_{i,j-1}^{(m)} + \xi_{i,j+1}z_{i,j+1}^{(m)} - \widehat{R}(z_{i,j}^{(m)}) \\ &+ \lambda_{i,j}^{(m)}z_{i,j}^{(m)}\}, \end{aligned} \tag{11}$$

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

Theorem 3 *Let $z_{i,j}^{(0)}$ be an arbitrary solution sequence and $z_{i,j}^*$ be the solution of Eq. (5). Let $\left\{z_{i,j}^{(m)}\right\}_{m=1}^{\infty}$ be a solution sequence of Eq. (11). Then $z_{i,j}^{(m)} \longrightarrow z_{i,j}^*$ as $m \longrightarrow \infty$, for all (x_i, y_j) in the device domain.*

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

$$\omega_{i,j}^{(m)} = z_{i,j}^{(m)} - z_{i,j}^*$$

for all (x_i, y_j) in the device domain. Since $z_{i,j}^*$ is the solution of Eq. (5), we have

$$\begin{aligned} z_{i,j}^* &= \frac{1}{\xi_{i,j}}\{\xi_{i+1,j} z_{i+1,j}^* + \xi_{i-1,j} z_{i-1,j}^* \\ &+ \xi_{i,j-1} z_{i,j-1}^* + \xi_{i,j+1} z_{i,j+1}^* \\ &- \widehat{R}(z_{i,j}^*)\}. \end{aligned} \quad (12)$$

From Eqs. (10) and (11) we derive

$$\begin{aligned} \omega_{i,j}^{(m+1)} &= \frac{1}{\lambda_{i,j}^{(m)} + \xi_{i,j}}\{\xi_{i+1,j}\omega_{i+1,j}^{(m)} + \xi_{i-1,j}\omega_{i-1,j}^{(m)} \\ &+ \xi_{i,j-1}\omega_{i,j-1}^{(m)} + \xi_{i,j+1}\omega_{i,j+1}^{(m)} - (z_{i,j}^{(m)}) \\ &+ \widehat{R}(z_{i,j}^*) + \lambda_{i,j}^{(m)}\omega_{i,j}^{(m)}\} \\ &= \frac{1}{\lambda_{i,j}^{(m)} + \xi_{i,j}}\{\xi_{i+1,j}\omega_{i+1,j}^{(m)} + \xi_{i-1,j}\omega_{i-1,j}^{(m)} \\ &+ \xi_{i,j-1}\omega_{i,j-1}^{(m)} + \xi_{i,j+1}\omega_{i,j+1}^{(m)} + (\lambda_{i,j}^{(m)} \\ &- \frac{\widehat{R}(z_{i,j}^{(m)}) - \widehat{R}(z_{i,j}^*)}{\omega_{i,j}^{(m)}})\omega_{i,j}^{(m)}\}. \end{aligned} \quad (13)$$

Since $\widehat{R}$ is increasing function, there exists a positive constant c such that

$$\frac{\widehat{R}(z_{i,j}^{(m)}) - \widehat{R}(z_{i,j}^*)}{\omega_{i,j}^{(m)}} \geq c > 0,$$

where the constant c can be calculated in Theorem 1. We calculate the estimation from Eq. (13) and note the Eq. (6), the following expression can be derived directly

$$\left\|\omega_{i,j}^{(m+1)}\right\|_\infty \leq \gamma \left\|\omega_{i,j}^{(m)}\right\|_\infty,$$

where the positive parameter γ is given by

$$\gamma = \max_{i,j}\left(\frac{\lambda_{i,j}^{(m)} + \xi_{i,j} - c}{\lambda_{i,j}^{(m)} + \xi_{i,j}}\right) < 1,$$

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

$$\begin{aligned} \left\|\omega_{i,j}^{(m+1)}\right\|_\infty &\leq \gamma \left\|\omega_{i,j}^{(m)}\right\|_\infty \\ &\leq \gamma^2 \left\|\omega_{i,j}^{(m-1)}\right\|_\infty \\ &\leq \cdots \\ &\leq \gamma^{m+1} \left\|\omega_{i,j}^{(0)}\right\|_\infty \end{aligned}$$

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

4. Conclusions

Based on the Gummel's decoupling and monotone iterative methods, we have presented a numerical solution method for semiconductor device drift diffusion equations. With monotone iterative technique, we have proved each Gummel's decoupled and finite volume discretized device equation converges monotonically. The proposed method here provided an alternative in the numerical solution of semiconductor device equations. Computational results for PN diode, MOSFET, DTMOS devices have been reported in our earlier work [2, 3, 4, 5, 6, 7, 8, 9] to demonstrate the robustness of the method. This method is inherently parallel and can be systematically extended to simulate not only VLSI circuit but also biological transportation.

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