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

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Abstract: - In this paper, we apply our proposed computing algorithm for numerical solution of semiconductor device energy balance equation in carrier temperature simulation. This robust simulation based on finite volume discertization scheme and monotone iterative algorithm is successfully developed and implemented for intrinsic investigation of submicron MOSFET device. Simulation results demonstrate MOSFET electron temperature can be significantly controlled with lightly doped drain (LDD) structure. Global convergence behavior is also presented to show the robustness and efficiency of the method.

Key-Words: - Carrier Temperature Calculation, Monotone Iterative Algorithm, LDD, MOSFET

1. Introduction

Design and fabrication of deep submicron metal oxide semiconductor field effect transistor (MOSFET) have been of great interests in these decades [1]. The channel length scales in today's MOSFET devices are so small that high field, nonlocal, and hot carrier effects become important. Technology computer aided design (TCAD) (see [2] and references therein) provides an alternative tool to analyze the intrinsic and extrinsic electrical behavior of MOSFET structures at a very fundamental physical level. In recent years, ultra-small MOSFET device simulation has been become a very important tool in the development of new devices and fabrication technologies [3-9]. To study the effects mentioned above for ultra-short channel MOSFET devices, an energy balance equation should be solved numerically for carrier temperature distribution [10-13]. Computed intrinsic results can be used as a reference data for optimal design for ultra-small MOSFET device structures so that electrical characteristics of the device can be further improved.

To study the physical mechanism for carrier temperature distribution in MOSFET devices, the energy balance equation in device simulation should be included, and this model has been received many notices. Various simulation approaches have been proposed for the numerical solution of this equation efficiently [10-15]. In solving the energy balance equation, the rapid variation of electron temperature between mesh points leads to a significant difficulty in semiconductor device simulation. Based on an assumption that the electron temperature T_n varies linearly between mesh points, Scharfetter- Gummel-Tang discretization scheme was developed in semiconductor hydrodynamic device simulation [11]. 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 fine mesh artificially. 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 apply our proposed method for the numerical solution of semiconductor device energy balance equation using monotone iterative algorithm. First of all, we solve a set of drift diffusion (DD) equations with our developed device simulator earlier. The computed physical quantities, such as electron concentration, electrostatic potential, and electron current are used as the input data for carrier temperature simulation. At the beginning, the energy balance equation is transformed into a self-adjoint form equation and then discretized using finite

volume method [16, 17] with very fine nonuniform mesh. The discretized energy balance equation leads to a system of nonlinear algebraic equations with a diagonal dominate property. We solve the nonlinear system by applying a monotone iterative method directly. With the developed carrier temperature simulator, we study some basic physical mechanism for conventional as well as LDD submicron NMOSFET under high bias condition. Numerical results and convergence property of the algorithm is also reported in this work.

This paper is organized as follows. In Sec. 2, we briefly state drift diffusion model and energy balance equation associated physical models. In Sec. 3, we present the overall computational procedure and monotone iterative algorithm for the carrier temperature simulation. In Sec. 4, simulation results for submicron N-MOSFET devices are presented to demonstrate the robustness and efficiency of the method. Sec. 5 draws the conclusions.

2. Physical Computational Models

We first stat the drift diffusion model and then energy balance equation for a completeness. The DD model was derived from Maxwell's equation as well as charge conservation law. A set of the DD equations is as follows:

$$\Delta\phi = \frac{q}{\varepsilon_S}(n - p + D), \quad (1)$$

$$\frac{1}{q}\nabla\cdot\mathbf{J}_n = R(n,p), \quad (2)$$

$$\frac{1}{q}\nabla\cdot\mathbf{J}_p = -R(n,p), \quad (3)$$

$$\mathbf{J}_n = -q\mu_n n\nabla\phi + qD_n\nabla n, \quad (4)$$

$$\mathbf{J}_p = -q\mu_p p\nabla\phi - qD_p\nabla p. \quad (5)$$

Eq. (1) derived from Maxwell's equation is so-called the Poisson equation. The Eqs. (2) and (3) derived from the charge conservation law are the electron and hole continuity equations. The Eqs. (4) and (5) are electrons and holes current equations, respectively. The unknown ϕ = $\phi(x,y)$ to be solved is the electrostatic potential, n and p are electrons and holes concentrations. The function $D = -(N_D^+ - N_A^-)$, in Eq. (1), is the specified ionized net doping profile, and R = $R(n,p)$ is the recombination rate for electrons and holes [1]. The quantity $q = 1.60218\times10^{-19}\,C$ is the elementary charge, $\varepsilon_S = 11.9\varepsilon_0$ is silicon permittivity. The N_D^+, and N_A^- are ionized donor and acceptor impurities, and $\varepsilon_0 = 8.85418\times10^{-14}\,F/cm$ is the permittivity in vacuum. The D_n, D_p, μ_n, and μ_p are electron and hole diffusion coefficients and mobility functions, respectively [1, 10-15]. This model was solved numerically with our proposed method successfully in our earlier works [3-9]. To compute the carrier temperature for a submicron MOSFET device, we solve the following energy balance equations for electrons and holes:

$$\nabla\cdot\mathbf{S}_n = \mathbf{J}_n\cdot\mathbf{E} - \frac{n(\omega_n - \omega_0)}{\tau_{nw}(T_n)}, \quad (6)$$

$$\nabla\cdot\mathbf{S}_p = \mathbf{J}_p\cdot\mathbf{E} - \frac{p(\omega_p - \omega_0)}{\tau_{pw}(T_p)}. \quad (7)$$

The energy flow equations are

$$\mathbf{S}_n = \frac{\mathbf{J}_n}{-q}\omega_n + \frac{\mathbf{J}_n}{-q}k_B T_n + \mathbf{Q}_n, \quad (8)$$

$$\mathbf{S}_p = \frac{\mathbf{J}_p}{-q}\omega_p + \frac{\mathbf{J}_n}{+q}k_B T_p + \mathbf{Q}_p, \quad (9)$$

where the notations and physical models follow the discussions in Part. I. We solve the above carrier balance equations with computed physical quantities from DD equations to obtain carrier temperature distribution over the device structure.

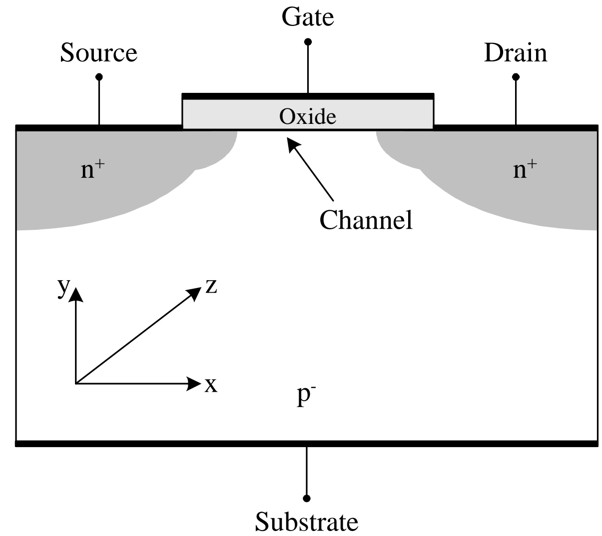

Fig. 1. A two-dimensional domain of a submicron LDD N-MOSFET device.

As shown in Fig. 1, the DD equations (1)-(5) and energy balance equations (6)-(9) are subject to mixed

type boundary conditions in a two-dimensional simulation domain. On the left and right sides, the homogeneous Neumann type boundary condition is considered. On the Source, Gate, Drain and Substrate contacts, the Dirichlet type boundary condition is applied [1, 10-15]. The solution procedure for the numerical solution of these equations is discussed in Sec. 3.

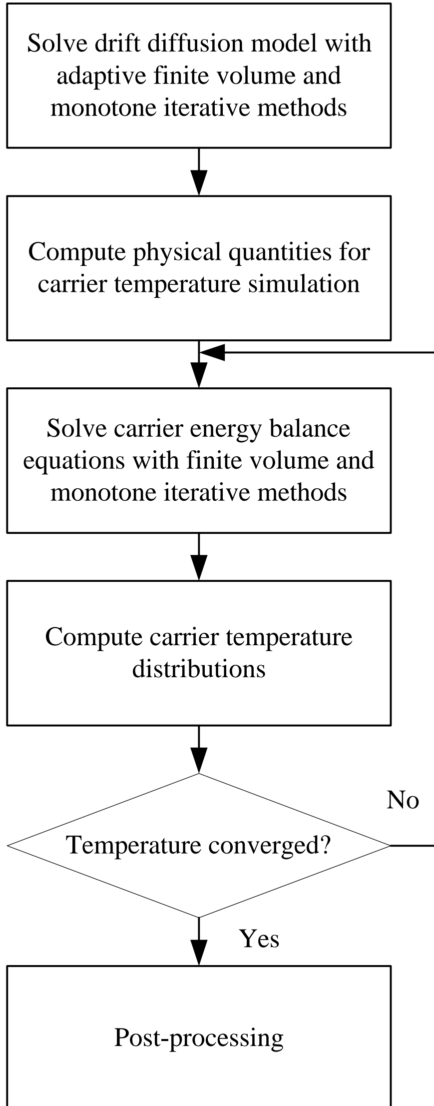

Fig. 2. An overall simulation procedure for carrier temperature calculation.

3. Simulation Techniques

As shown in Fig. 2, with the computed results from DD model, we solve energy balance equations, subsequently. To calculated electrostatic potential, electric field, carrier concentrations, and current flows, Eqs. (1)-(5), the drift diffusion equations are solved with Gummel's decoupled algorithm [18, 19] and monotone iterative method [3-9]. Here we briefly state the flowchart and numerical methods for the solutions of drift diffusion model can be found in our earlier works [3-9]. The well-known Gummel's decoupled method is that the device equations are solved sequentially (see Fig. 3).

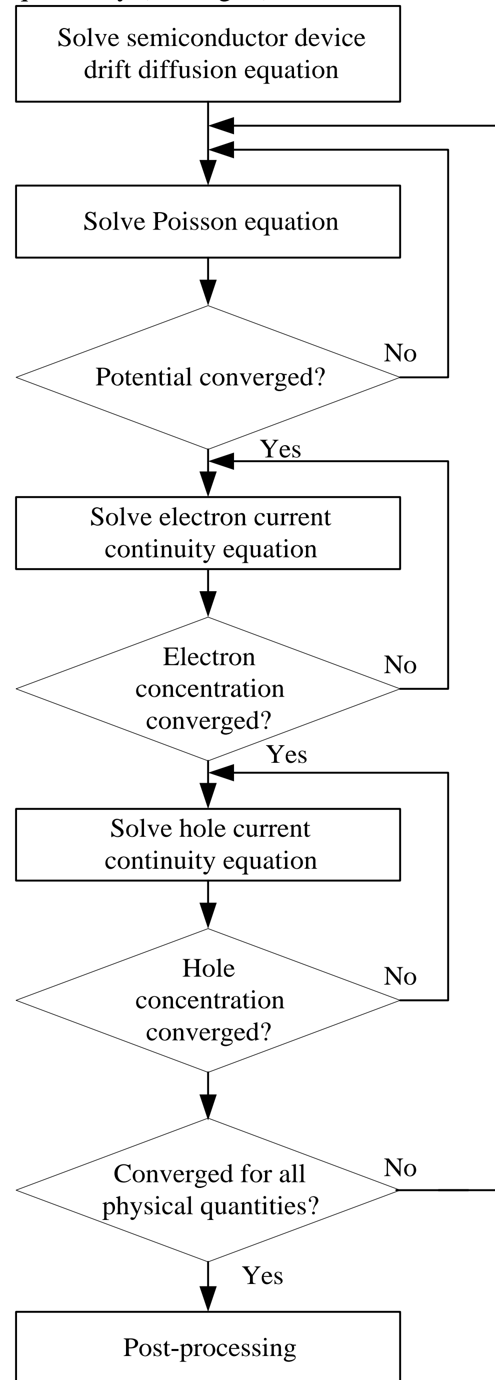

Fig. 3. Gummel's decoupling algorithm for the DD model simulation.

For the numerical solution of semiconductor device DD model, Poisson's equation is solved for $\boldsymbol{f}^{(g+1)}$ given the previous states $u^{(g)}$ and $v^{(g)}$. The electron current continuity equation is solved for $u^{(g+1)}$ given $\boldsymbol{f}^{(g)}$ and $v^{(g)}$. The hole current continuity equation is

solved for $v^{(g+1)}$ given $\boldsymbol{f}^{(g)}$ and $u^{(g)}$. The superscript index g denotes the Gummel's iteration loops. Each decoupled PDE is solved with our adaptive computing algorithm, as shown in Fig. 4.

Decoupled equation is discretized with finite volume method. The corresponding nonlinear system is solved with monotone iterative algorithm. When converged solution is computed, we perform error estimation of the results for all elements. If the solution does not satisfy the specified stopping criterion (TOL), we will run the mesh refinement and repeat the computation. The results obtained from DD model are used as the input data for the numerical solutions of the carrier balance equations.

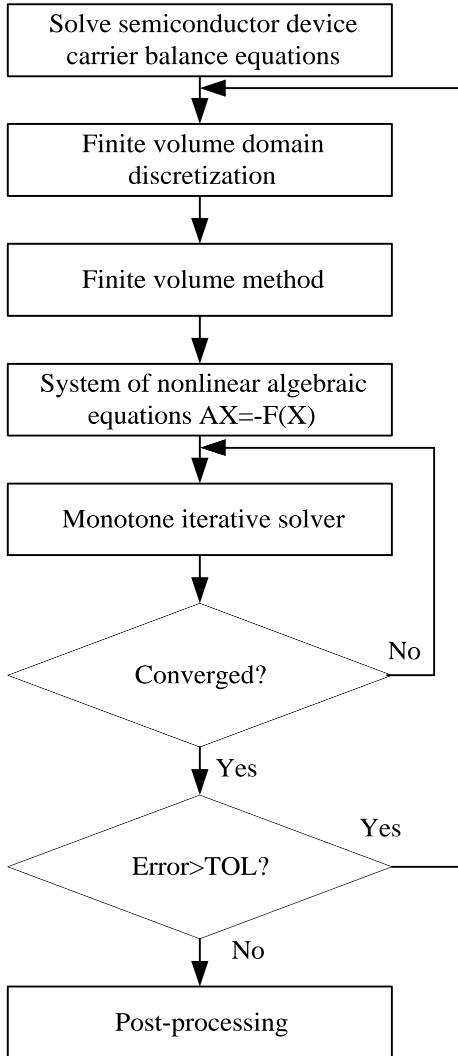

Fig. 4. Adaptive finite volume solution algorithm for each Gummel decoupled DD equations.

Conventional algorithm for the numerical solution of electrons and holes energy balance equation in semiconductor device simulation consists of: (i) applying finite volume method to discretize the equations, (ii) using Scharfetter-Gummel-Tang scheme, an exponential fitting liked algorithm, [10-13] for the electron and hole energy balance equations to construct system of nonlinear algebraic equations, (iii) solving the nonlinear system with Newton's iteration method, and (iv) repeating the step (iii) until the solution converged.

Our simulation algorithm, as shown in Fig. 5, replaces Newton's iteration by the monotone iterative method and the iterative scheme for the corresponding discretized nonlinear system is of the following form [3-9]:

$$(\mathbf{D}+\boldsymbol{l}\mathbf{I})\mathbf{Z}^{(m+1)}=(\mathbf{L}+\mathbf{U})^{(m)}-\mathbf{F}(\mathbf{Z}^{(m)})+\boldsymbol{l}\mathbf{I}\mathbf{Z}^{(m)}, \tag{7}$$

where $\mathbf{Z}$ is the unknown vector, $\mathbf{F}$ is the nonlinear vector form, and $\mathbf{D}$, $\mathbf{L}$, $\mathbf{U}$, and $\mathbf{I}$ are diagonal, lower triangular, upper triangular, and identity matrices, respectively. The monotone iterative parameter $\boldsymbol{l}$ is determined node-by-node depending on the device structure, doping concentration, bias condition, and nonlinear property of each decoupled equation.

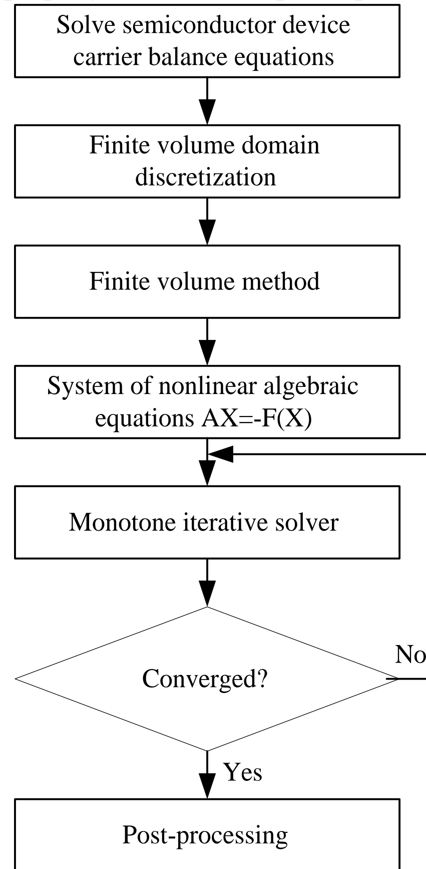

Fig. 5. Solution algorithm for the energy balance equations in carrier temperature calculation.

The monotone iterative method applies here for semiconductor device temperature simulation [10-15] is a global and constructive method in the sense that it

does not involve any Jacobian matrix. However, the Newton's iterative method not only has Jacobian matrix but also inherently requires a sufficiently accurate initial guess to begin with the solutions. Note that the Eq. (7) is highly parallel; consequently, the monotone iterative method is very cost effective in terms of both computational time and storage memory.

4 Simulation Results and Discussions

We present simulation results of the carrier temperature simulation for different submicron MOSFET devices. We only demonstrate electron temperature distribution for 0.25 μm conventional and LDD structures N-MOSFET at high bias conditions. Similarly, the hole temperature distribution can be calculated with the proposed method. The electron concentration, electrostatic potential, electric field, and electron current density are computed from drift diffusion model. Fig. 6, shows the simulated devices' doping profiles, the left Fig. 6(a) is a LDD MOSFET and the right one is conventional MOSFET structure. The gate oxide thickness for these two devices is equal to 70A°, the ratio of device width and channel W / L_{eff} equals to 40/0.25 and V_{BS} = 0V. The profiles have their maximum values $10^{20}/cm^3$ and are from SUPREME-4 semiconductor process simulator [].

Figs. 7 shows the simulated electrostatic potential functions for these different two devices at applied voltages $V_{DS} = V_{GS}$ = 3.0V, respectively. At this same bias condition, by comparing with Fig. 7(b), we find the electrostatic potential of LDD MOSFET, as shown in Fig. 7(a), has a slow variation near drain side than the result from conventional MOSFET structure.

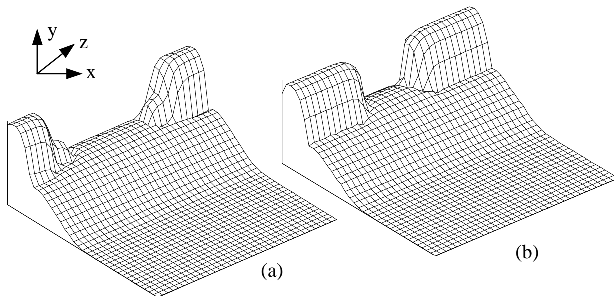

Fig. 6. Doping profiles for simulated N-MOSFET devices: (a) LDD, (b) conventional structure.

Furthermore, Fig. 8 presents the electron temperature distributions for different MOSFET devices' doping profiles. Fig. 8(a) demonstrates a lower electron temperature peak than the temperature peak of conventional MOSFET device at the drain side. It is no surprise because the LDD MOSFET has a slow variation in its potential (see Fig. 7(a)) and hence its electric field is small than conventional result. This results clarify the LDD structure can significantly reduce device hot carrier effects.

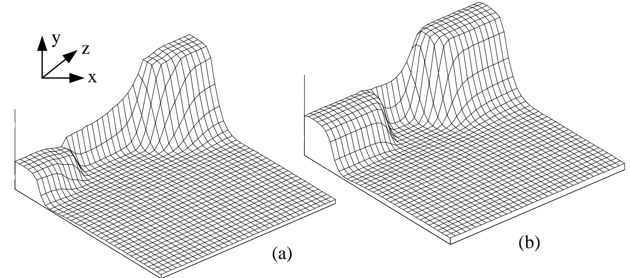

Fig. 7. Surface plots of the electrostatic potential for 0.25μm N-MOSFET devices with V_{DS} = 3.0V

With the developed carrier temperature simulator, we have calculated the electron temperature for LDD N-MOSFET is equals to 4940k and for conventional N-MOSFET structure it is to 6133k at V_{DS} = 3.0V and V_{GS} = 3.0V. The higher electron temperature is due to the high electric field at the drain side.

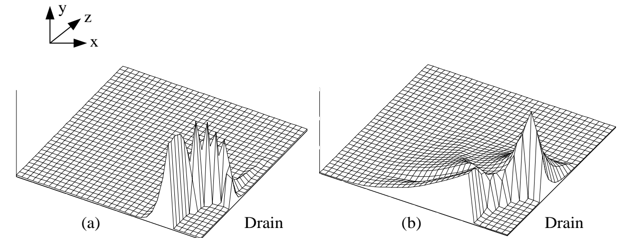

Fig. 8. Surface plot of electron temperature profiles for LDD and conventional N-MOSFET devices at V_{DS} = 3.0V and V_{GS} = 3.0V.

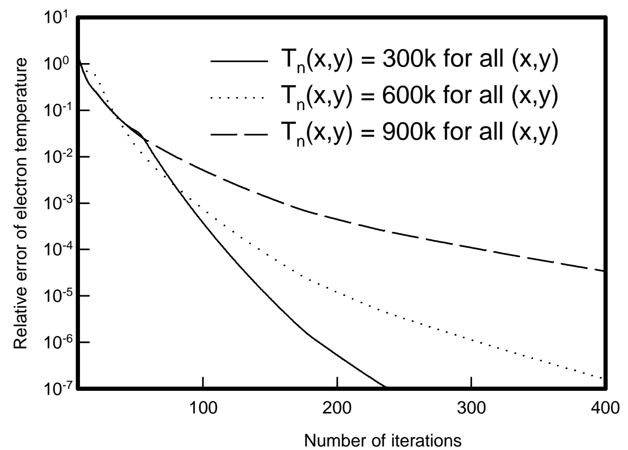

Fig. 9. Convergence behavior for unknowns T_n in the monotone iteration loop.

As shown in Fig. 9, we present the convergence of the monotone iterative algorithm for the numerical

solution of energy balance equation in deep submicron semiconductor device carrier temperature simulation. This figure suggests the monotone iterative algorithm in the numerical solution of energy balance equations has a global convergence property for various initial guesses.

5 Conclusions

In this paper, we have successfully generalized our proposed earlier monotone iterative computing methodology for carrier temperature calculation in deep submicron MOSFET device simulation. This approach mainly relies on finite volume and monotone iterative methods. Numerical results and convergent behavior for submicron N-MOSFET devices are also presented to show the robustness and efficiency of the method. In the future work, we extend this computing method in semiconductor advanced hydrodynamic model and Boltzmann transport equation simulation.

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