DUAL ENERGY TRANSPORT MODEL FOR ADVANCED DEVICE SIMULATION

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Abstract

Dual energy transport (DUET) model in semiconductor devices including heterostructures has been developed to simulate the distribution of carrier and lattice temperatures in addition to profiles of the electrostatic potential and carrier concentrations. The modeling approach is in consistency with the conventional drift-diffusion (DD) model, making it easy to implement in the existing code. Carrier energy dependent mobility and impact ionization models have been examined and are used for simulation of various velocity overshoot and hot electron effects. Two simulation examples, one for the submicron MOSFET and another for the deep-submicron SOI, are presented through comparison with measurement data to demonstrate the improvement of the new model over DD model in predicting the device characteristics for modern (submicron) structures.

I INTRODUCTION

As the feature size of semiconductor devices shrinks to the quarter-micron regime, nonlocal effects such as hot electrons and velocity overshoot become important in determining the device characteristics. The conventional drift-diffusion transport model has been and continuously been used in industry and academia for design and analysis of IC devices largely because its auxiliary physical models such as the field-dependent mobility model and impact ionization model are well calibrated. But it fails to predict those device characteristics which becomes critical in sub- and deep sub-micron devices. A notable example is the substrate current in MOSFET. Neither can DD model provide such vital information as to the average kinetic energy of carriers in the device. On the other hand, Monte Carlo (MC) method can provide very detailed information about the carrier distribution in real and momentum spaces. But in addition to the excessive CPU time requirement and complexity of model parameters, most present MC codes can only simulate one-carrier device behavior, thus are not yet suitable for the design of practical devices. Through tracing back to the origin of DD model from Boltzmann Transport Equation (BTE) and by relieving the constraints of constant effective mass and temperature, we were able to develop a more complete transport model in semiconductors, which reveals not only the carrier concentration and current density (essentially a measure of carrier average velocity) but also the carrier energy density. Assuming Fermi-Dirac (FD) statistics as the basis for the distribution function and applying the perturbation theory, the average kinetic energy can be linked to the temperature parameter used in FD statistics in the same formulation as for an ideal gas in classical thermodynamics, thus correctly identifying the

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concept of carrier temperature. Moreover, the lattice temperature can easily be incorporated in the model by considering the energy exchange among the carrier subsystems and lattice. We thus proposed a dual (carrier and lattice) energy transport model (DUET) for semiconductor devices, and have successfully implemented the model in Stanford's device simulation code, PISCES, as version 2ET. Since the code was up to work we have conducted several tests and results obtained from the simulation are encouraging. Recently, we also extend the capabilities of the code to cover the electrical simulation of heterostructures such as light emitter diodes (LEDs) and surface emitting diodes (SELs).

In the following we first introduce the complete formulation of the DUET model, and describe the energy dependent physical models as implemented in PISCES-2ET code. Finally, examples are given and future work is discussed.

II DUET MODEL FORMULATION

DUET model uses six state variables – potential (ψ), electron and hole concentrations and temperatures (n, p, T_n, and T_p), and lattice temperature (T_L) to describe the status of a semiconductor device. All governing equations for these variables are derived from the conservation or balance principle for matter and energy. Except of the Poisson's equation for ψ, this conservation principle can be expressed in the following equation using Fick's second law:

$$\frac{\partial u}{\partial t} = -\nabla \cdot \mathbf{F} + g - r \tag{1}$$

where u represents the concerned physical quantity, $\mathbf{F}$ is the flux of u, and g and r are generation and recombination rates of u, respectively. The key issue in the modeling is thus to find expressions for $\mathbf{F}$, g, and r in terms of u. It is well known that in DD model, the carrier flux consists of the diffusion and drift terms, or by introducing the quasi-Fermi level E_F, is proportional to the gradient of E_F. The fundamentals behind the DD model lie actually in BTE, which itself is a representation of the continuity principle,

$$\frac{d}{dt} f(\mathbf{r}, \mathbf{k}, t) = \left.\frac{\partial f}{\partial t}\right|_{coll} \tag{2}$$

where $\mathbf{k}$ is the wavenumber vector, and the way of constructing the distribution function of f. Following Stratton's approach [1], in the existence of the electric field by applying the perturbation theory and relaxation time approximation (RTA) the distribution function at any instant can be expressed as

$$f(\mathbf{r}, \mathbf{k}) = f_0(\mathbf{r}, E) - \tau(\mathbf{r}, \epsilon)\frac{\hbar}{m^*}\left(\mathbf{k} \cdot \nabla_{\mathbf{r}} f_0 - q\frac{\partial f_0}{\partial \epsilon}\mathcal{E} \cdot \mathbf{k}\right) \tag{3}$$

where E is the carrier energy and ϵ is the kinetic part of E, f_0 is the even part of f in k–space and is dependent on the carrier kinetic energy only. The relaxation time τ is assumed to depend on ϵ only too. $\mathcal{E}$ is the electric field. All other symbols have conventional meanings. If f_0 is taken as the Fermi-Dirac distribution function, one can readily obtain the expression for the carrier density and flux by definition as follows:

$$n = N_C F_{1/2}\left(\frac{E_{Fn} - E_C}{k_B T_n}\right) \tag{4}$$

$$\mathrm{j}_n = n\mu_n \nabla E_{Fn} + qn\mu_n Q_n \nabla T_n \tag{5}$$

where N_C is the effective density for the conduction band and E_C is the energy level for the conduction band edge, $F_{1/2}$ is the Fermi integral of order one half. Coefficients μ_n and Q_n in

Eq. (5) are electron mobility and thermopower, respectively, and are related to each other. It is obvious that when T_n is constant the above expression for the current is reduced to the conventional DD model.

To find the governing equation for carrier temperature, we start from the balance equation for the kinetic energy. For electrons, we have

$$\frac{\partial w_n}{\partial t} = -\nabla \cdot \mathbf{s}_n + \mathbf{j}_n \cdot \mathcal{E}_n - u_{wn} \tag{6}$$

where w_n is the electron kinetic energy density, $\mathbf{s}_n$ is the energy flux, and u_{wn} is the net energy loss rate. The Joule heat term of $\mathbf{j}_n \cdot \mathcal{E}_n$ represents the conversion from the potential to kinetic energy and the subscript n in $\mathcal{E}_n$ indicates the fact that for heterostructures, the electric field might be different for electrons and holes. Again using Eq. (3) and by definition w_n and $\mathbf{s}_n$ are computed as follows:

$$w_n = \frac{3}{2} n k_B T_n \gamma_n \tag{7}$$

$$\mathbf{s}_n = -P_n T_n \mathbf{j}_n - \kappa_n \nabla T_n \tag{8}$$

where γ_n is the degeneracy factor which equals unity when Boltzmann statistics is used, P_n and κ_n are thermoelectric power and thermal conductivity for electrons, respectively. From Eq. (7) and taking $\gamma_n = 1$, we can identify that T_n indeed has the meaning of temperature for a classical electron gas.

The remaining task in completing the model formulation is to find the carrier and its energy exchange among sub-systems. For carrier exchange, i.e., recombination and generation, we include the Shockley-Read-Hall (SRH), Auger, and radiative recombinations, and impact ionization. All these carrier exchanges are accompanied by the energy exchange. In addition, we also include the energy exchange between carriers and lattice through phonon scattering modeled using energy relaxation times, τ_{wn} and τ_{wp}.

We thus arrive at the following set of equations:

Poisson's equation

$$\nabla \cdot (-\epsilon \nabla \psi) = q(p - n + N_D^+ - N_A^-) \tag{9}$$

Carrier continuity equations:

$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot \mathbf{j}_n - u \tag{10}$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q} \nabla \cdot \mathbf{j}_p - u \tag{11}$$

Energy balance equations for carriers:

$$\frac{\partial w_n}{\partial t} = -\nabla \cdot \mathbf{s}_n + \mathbf{j}_n \cdot \mathcal{E}_n - u_{wn}$$

$$\frac{\partial w_p}{\partial t} = -\nabla \cdot \mathbf{s}_p + \mathbf{j}_p \cdot \mathcal{E}_p - u_{wp}$$

where

$$\begin{aligned} u_{wn} = {} & (u_{srh} + u_{rad}) \frac{3}{2} k_B T_n - (u_{n,Auger} - g_{n,imp}) \left[E_g(T_L) + \frac{3}{2} k_B T_p \right] \\ & - g_{p,imp} \frac{3}{2} k_B T_n + \frac{w_n(T_n) - w_n(T_L)}{\tau_{wn}} \end{aligned} \tag{12}$$

$$u_{wp} = (u_{srh} + u_{rad})\frac{3}{2}k_B T_p - (u_{p,Auger} - g_{p,imp})\left[E_g(T_L) + \frac{3}{2}k_B T_n\right] - g_{n,imp}\frac{3}{2}k_B T_p + \frac{w_p(T_p) - w_p(T_L)}{\tau_{wp}} \quad (13)$$

Thermal diffusion equation for lattice:

$$c_L\frac{\partial T_L}{\partial t} = \nabla\cdot(\kappa_L\nabla T_L) + u_{srh}\left[\frac{3}{2}k_B T_n + E_g(T_L) + \frac{3}{2}k_B T_p\right] + \frac{w_n(T_n) - w_n(T_L)}{\tau_{wn}} + \frac{w_p(T_p) - w_p(T_L)}{\tau_{wp}} \quad (14)$$

In the transport expressions for the current density and energy flux, there are four coefficients, μ, Q, P, and κ, and they are all related to each other through the relaxation time, τ. This is one of the advantages of the DUET model. Once one of them is known, the others can be deduced from the known parameter. In reality, however, these coefficients can be treated as empirical parameters or obtained from experiment. For example, knowing the dependence of μ on the carrier temperature, thermopower Q can be obtained for electrons:

$$Q_n = \frac{k_B}{qn}\left[1 + T_n\frac{\partial}{\partial T_n}\ln\mu_n(\mathrm{r}, T_n)\right] \quad (15)$$

Finally, we list the energy dependent mobility and impact ionization models as used in PISCES-2ET:

$$\mu(N, T_L, E_\perp, T_c) = \frac{\mu_0(N, T_L, E_\perp)}{1 + \gamma(N, T_L, E_\perp)[w(T_c) - w(T_L)]} \quad (16)$$

where the subscript c for n or p, and $\gamma(N, T_L, E_\perp) = \mu_0(N, T_L, E_\perp)/[q\tau_w v_{sat}^2(T_L)]$ [2]. And the impact ionization rate, α,

$$\alpha = A\exp[-(b/\mathcal{E}_{eff})^m] \quad \text{with} \quad \mathcal{E}_{eff} = \frac{3}{2}\frac{k_B}{q}\frac{T_c - T_L}{\tau_w v_{sat}} \quad (17)$$

III SIMULATION EXAMPLES

We present two examples which show that the DD model is no longer accurate in predicting $I - V$ characteristics for submicron devices when the non-stationary phenomena such as the velocity overshoot and nonlocal field dependence of physical parameters such as the impact ionization rate become important. While both DD and DUET models provide good simulation results compared to the measurement for devices with relatively long channel length, DD model starts to break for output characteristics of SOI at $L_{eff} = 0.12\,\mu$m (Fig. 1) and substrate current of MOSFET at $L_{eff} = 0.8\,\mu$m (Fig. 2). On the other hand DUET can consistently model the device characteristics well even when the device size is scaled down to the deep submicron range.

IV CONCLUSION

DUET model follows the same moment approach as DD model does but has two obvious advantages. Firstly, it closes the system in a more consistent way and resolves the conflict intrinsic to DD model, i.e., the field dependent mobility model as commonly used in device simulators employing DD model vs. the constant temperature assumption leading to the DD current expression. Secondly, it is able

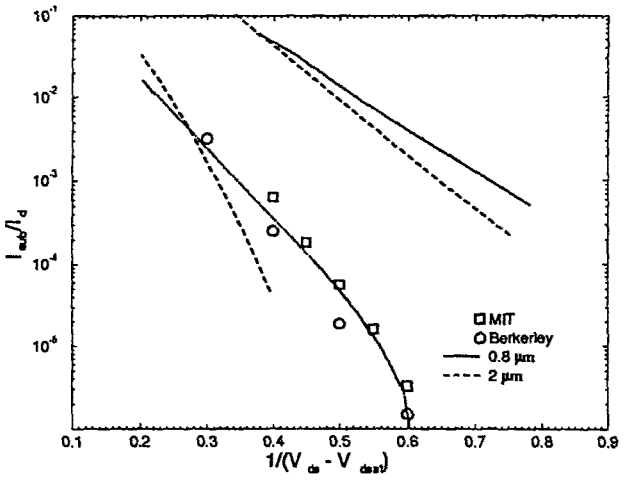

Figure 1: Simulation results for the substrate current in MOSFET with two different channel length (2 and 0.8 μm) and the comparison is made for 0.8 μm case between the ET-simulated and measured results (from MIT and UC Berkeley, respectively). The upper curves are simulated using DD model while the lower curves are obtained from ET simulation.

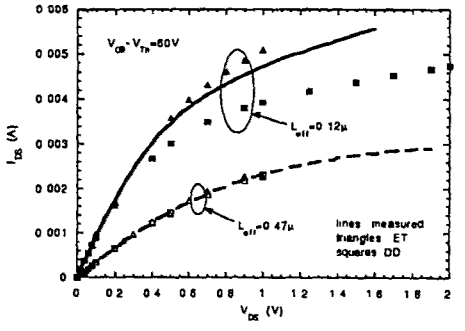

Figure 2: Simulated and measured data for SOI structure with different channel length.

to provide information regarding the carrier kinetic energy. However, there is still a need to carefully calibrate the transport coefficients and to develop more reliable energy-dependent physical models. Especially for the impact ionization and breakdown simulation, since these phenomena are basically determined by the high energy tail of the carrier distribution, the dependency on the average energy has to be elaborated and verified through experiments.

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