An Analytic Expression of Thermal Diffusion Coefficient for the Hydrodynamic Simulation of Semiconductor Devices

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A new analytical expression of thermal diffusion coefficient D^T is derived. To the first-order approximation, it is given by $(1+\eta)^{-1}(D/T_n)$ rather than $(1-\eta)(D/T_n)$ where $\eta = -(T_n/\mu^*)(\partial\mu^*/\partial T_n)$ and μ^* represents the temperature-dependent bulk mobility. This new transport coefficient is implemented in our 2-D hydrodynamic device simulator and it seems to produce more reasonable results.

Keywords: Hydrodynamic simulation; Thermal diffusion coefficient; Effective carrier energy; Non-local mobility model

1. INTRODUCTION

Since the original derivation of hot-carrier transport model by Stratton [1], there has been controversy about what the proper transport coefficient of the thermal diffusion current density is [2–5]. In the hydrodynamic (HD) transport model, in addition to the diffusion current due to the carrier density gradient, there is also a thermal diffusion current driven by the carrier temperature (or energy) gradient. In most semiconductor devices, the thermal diffusion current is often in opposite direction to the carrier diffusion current. Therefore, improper use of the thermal diffusion coefficient in the HD transport model often affects

the outcome of device simulation result. The purpose of this paper is to provide an analytical expression for the thermal diffusion coefficient which is more consistent with Monte Carlo (MC) simulation data.

2. TWO FORMULATIONS OF TRANSPORT MODEL

In general, there are two different formulations of the HD transport model [6]. Stratton's original formulation of the current density is given by [1]

$$\vec{J}_n = qn\mu^*\vec{E} + q\nabla(nD). \quad (1)$$

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Assuming that the Einstein relation $D = \mu^* k_B T_n / q$ is valid and the bulk (homogeneous) mobility $\mu^*(T_n)$ is a known function of the electron temperature T_n , Eq. (1) becomes

$$\vec{j}_n = qn\mu^*\vec{E} + \mu^*k_B T_n \nabla n + n\mu^* \left(1 + \frac{T_n}{\mu^*} \frac{\partial \mu^*}{\partial T_n}\right) k_B \nabla T_n. \quad (2)$$

We may cast the diffusion current density into the form

$$\vec{j}_{\text{diff}} = qD\nabla n + qnD^T \nabla T_n \quad (3)$$

where D^T represent the thermal diffusion coefficient. Then, Stratton's formulation gives

$$D^T = \frac{D}{T_n} \left(1 + \frac{T_n}{\mu^*} \frac{\partial \mu^*}{\partial T_n}\right). \quad (4)$$

In our earlier work which is based on moments of the Boltzmann transport equation [7], we proposed a current density of the form [8],

$$\vec{j}_n = \mu^* [qn\vec{E} + U\nabla n + (1 - \lambda_p)n\nabla U] \quad (5)$$

where $U = \langle \vec{v} \hbar \vec{k} \rangle \cdot \vec{1}$ and λ_p is a dimensionless parameter extractable from the MC simulation. The origin of λ_p comes from the modeling of the momentum collision moment $\vec{C}_p = \langle \hbar \vec{k} (\delta f / \delta t)_{\text{coll}} \rangle$ as

$$\vec{C}_p = -\frac{q\vec{V}}{\mu^*} + \lambda_p \nabla U. \quad (6)$$

It should be noted that Eq. (5) becomes Eq. (2) if $\lambda_p = -(T_n / \mu^*) (\partial \mu^* / \partial T_n)$. However, the MC simulation data does not quite agree with this relation [9]. In the following, we shall present an analytical expression of λ_p which is more consistent with the MC data.

3. DERIVATION OF TRANSPORT PARAMETER λ_p

Based on a series of MC simulations of $n^+ - n - n^+$ structures [8], we have discovered

that to capture the non-local effect, the carrier mobility is best described by an effective carrier energy (or temperature) defined by [10, 11]

$$W_{\text{eff}} = -\frac{q \vec{j}_\epsilon \cdot \vec{j}_n}{\delta_\epsilon |\vec{j}_n|^2}, \quad (7)$$

where the simplified energy flux density $\vec{j}_\epsilon$ is given by [11, 12]

$$\vec{j}_\epsilon = -\delta_\epsilon \left(\frac{\vec{j}_n}{q} \right) W - \Delta_\epsilon \frac{\mu^* n W}{q} \nabla W, \quad (8)$$

and $W \approx (3/2)k_B T_n$ represents the average electron energy (see Fig. 1). The thermal conductivity coefficient Δ_ϵ and Peltier coefficient δ_ϵ are related to each other through [12]

$$\Delta_\epsilon = \delta_\epsilon \left[(1 - \lambda_{\epsilon p}) \frac{1}{(W + U)} \frac{\partial R}{\partial W} - (1 - \lambda_p) \frac{\partial U}{\partial W} \right] \quad (9)$$

where $R = \langle \epsilon \vec{v} \hbar \vec{k} \rangle \cdot \vec{1}$, and $\lambda_{\epsilon p}$ is another dimensionless parameter extractable from the MC simulation. In the following, we assume first that $\lambda_p \approx \lambda_{\epsilon p}$ which is supported by the MC data [8], and second, for simplicity, $R = (10/9)W^2 \approx (5/2)(k_B T_n)^2$ and $U = (2/3)W \approx k_B T_n$. These two approximations lead to a simplified relation

FIGURE 1 Comparison of the MC extracted mobility $\mu(\text{MC})$, $\mu(W)$, and $\mu(W_{\text{eff}})$ for device B in Ref. [8]. $\mu(W_{\text{eff}})$ fits better with $\mu(\text{MC})$.

between Δ_ϵ and δ_ϵ :

$$\Delta_\epsilon \approx (2/3)\delta_\epsilon(1 - \lambda_p). \quad (10)$$

Equation (10) implies that the thermal diffusion coefficient Δ_ϵ of $\vec{j}_\epsilon$ is related to the thermal diffusion coefficient D^T of $\vec{j}_n$ through the factor $(1 - \lambda_p)$.

In order to obtain an analytical expression of λ_p , we expand the reciprocal of the (inhomogeneous) mobility around the bulk (homogeneous) mobility and treat the difference between W_{eff} and W as a small perturbation. From Eq. (6) we have

$$\frac{1}{\mu} = -\frac{\vec{V} \cdot \vec{C}_p}{qV^2} = \frac{1}{\mu^*} - \lambda_p \frac{\vec{V} \cdot \nabla U}{qV^2}. \quad (11)$$

Substitution of Eq. (8) into Eq. (7) gives

$$W_{\text{eff}} - W = -\frac{\Delta_\epsilon}{\delta_\epsilon} \frac{W\mu^*}{qV^2} \vec{V} \cdot \nabla W. \quad (12)$$

Expanding $1/\mu$ around $1/\mu^*$ and treating $(W_{\text{eff}} - W)$ as a small perturbation, we obtain

$$\frac{1}{\mu} = \frac{1}{\mu^*} + \frac{\partial}{\partial W} \left(\frac{1}{\mu^*} \right) \cdot \left(-\frac{\Delta_\epsilon}{\delta_\epsilon} \frac{W\mu^*}{qV^2} \vec{V} \cdot \nabla W \right) \quad (13)$$

Comparing Eq. (11) and Eq. (13) and substituting Eq. (10) into Eq. (13) with the approximation $U \approx (2/3)W$, we finally arrive at

$$\lambda_p = W\mu^* \frac{\partial}{\partial W} \left(\frac{1}{\mu^*} \right) (1 - \lambda_p) = \eta(1 - \lambda_p)$$

where

$$\eta = -\frac{W}{\mu^*} \frac{\partial \mu^*}{\partial W} \approx -\frac{T_n}{\mu^*} \frac{\partial \mu^*}{\partial T_n}.$$

Hence,

$$\lambda_p = \eta/(1 + \eta). \quad (14)$$

The physical meaning of Eq. (13) is clear. The energy-dependent mobility μ^* is strictly for bulk semiconductors only. However, if W is replaced by

FIGURE 2 $1/\mu$ vs. W and W_{eff} for devices A, B, and C.

W_{eff} in μ^* , this energy-dependent bulk mobility can also be extended to the case of inhomogeneous field, with a negligible “hysteresis” loop [11] (see Fig. 2). The second term on the r.h.s. of Eq. (13) represents a non-local correction to the bulk mobility.

An interesting feature of the result (14) is that the value of λ_p never exceeds unity and therefore the positive definiteness of D^T in Eq. (3) is guaranteed. This is not the case for $\lambda_p = \eta$ which is Stratton’s model. Depending on what kind of the bulk mobility model $\mu^*(N_i, T_n)$ is used, if we assume $\lambda_p = \eta$, the value of λ_p sometimes may exceed unity resulting in a negative D^T . Besides being unphysical, a negative D^T often causes numerical instability.

4. SIMULATING RESULTS

We have implemented this new analytical expression of λ_p in our 2-D HD simulator. A $0.1 \mu\text{m}$ partially-depleted SOI-MOSFET given in Figure 2 of Ref. [12] is simulated. Figure 3 indicates a substantial spread in the I_D - V_D characteristic curve among different models. In general, the model $\lambda_p = 1$ ($D^T = 0$) and the model $\lambda_p = \eta$ overestimate the drain current density because of $D^T \approx 0$. This result is due to the suppression of the thermal back diffusion in the hot-carrier region. On the other hand, the model $\lambda_p = \eta/(1 + \eta)$ predicts slightly

FIGURE 3 I_{ds} - V_{ds} characteristics of the partially-depleted SOI-MOSFET at $V_g = 1.5$ V for different λ_p 's.

larger current density than the conventional HD model ($\lambda_p = 0$). It is interesting to note that in the hot-carrier regime, η has typically a value ≈ 1 and thus our new analytical model predicts $D^T \approx (1/2)(D/T_n)$ rather than $D^T \approx 0$.

5. CONCLUSION

We have derived a new analytical expression for the coefficient of the thermal diffusion current density D^T . This derivation is based on an observation that a local energy-dependant bulk mobility can capture the non-local effect if the average electron energy is replaced by an effective average electron energy which is proportional to the ratio between the energy flux density and the charge flux density. To the first-order approximation, this leads to a simple expression $D^T = (1 + \eta)^{-1}(D/T_n)$ rather than $D^T = (1 - \eta)(D/T_n)$, the result of Stratton's formulation. We have implemented this new analytical model in the 2-D simulation of a partially depleted SOI MOSFET. The simulation results indicate that I-V characteristic curves are sensitive to the choice of the transport coefficient D^T .

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