Re-examination of the Hot-Carrier Transport Model Using Spherical Harmonic Expansion of the Boltzmann Transport Equation

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ABSTRACT

The transport coefficients μ, μ_ε, D and D_ε are extracted from the spherical harmonic expansion (SHE) of the electron distribution function. The truncation effect of the higher-order term in the SHE on these transport coefficients is studied. The Einstein relation is also examined for hot-carrier transport. Comparison with Monte Carlo (MC) data shows that the modeling of $\mu, \mu_\varepsilon, D/\mu$ and $D_\varepsilon/\mu_\varepsilon$ in terms of local variables N_d and W alone may not be sufficient.

1. Introduction

Historically, there are two different approaches to the derivation of hydrodynamic (HD) transport models. Stratton's approach [1] is based on the relaxation time approximation (RTA) for Boltzmann's collision integral while Bløtekjaer's [2] is based on the moments of the Boltzmann Transport Equation (BTE). The BTE can be rigorously expanded into spherical harmonics (SH) [3]. However, Stratton derived the constitutive equations for the current density and the energy flux density by using only the first two terms of SH [1]. In today's submicron devices,carrier and energy transports are carried out under conditions far from thermal equilibrium and the neglect of the higher-order terms in the SHE may introduce substantial errors.

In this paper, the definition of transport coefficients appearing in the energy transport model is re-examined and an empirical expression is obtained by using the SHE of electron distribution function extracted from the bulk MC data.

2. Derivation of Transport Coefficients

SHE of the BTE

For simplicity, we only consider the 1-D problem here. The SHE is then reduced to Legendre polynomial expansion (LPE). We expand the distribution function as follows:

$$f(x,\vec{k}) = \sum_{n=0}^{\infty} f_n(x,\varepsilon) P_n(cos\theta), \tag{1}$$

where θ is the angle between $\vec{k}$ and the x-axis and $P_n(cos\theta)$ are the Legendre polynomials. From Liang et al. [3], the first-order component of the BTE leads to

$$v(\varepsilon)(\frac{\partial}{\partial x} - qE_x\frac{\partial}{\partial x})\frac{f_0}{3} + v(\varepsilon)[\frac{\partial}{\partial x} - qE_x(\frac{\partial}{\partial x} + \frac{3\gamma'}{2\gamma})]\frac{2}{3}(\frac{f_2}{5}) = -\frac{1}{\tau_1}\frac{f_1}{3}, \tag{2}$$

where $\gamma(\varepsilon)$ is the dispersion relation, $v(\varepsilon) = \sqrt{2m^*\gamma(\varepsilon)}/m^*\gamma'(\varepsilon)$, $\gamma'(\varepsilon) = d\gamma(\varepsilon)/d\varepsilon$, E_x is the electric field in the x-direction, and τ_1 is the collision relaxation time associated with $P_1(cos\theta)$. Thus $f_1(x,\varepsilon)$ is related to spatial and energy derivatives of $f_0(x,\varepsilon)$ and $f_2(x,\varepsilon)$.

If (2) is multiplied by $\Phi(\vec{k}) = \hbar\vec{k}$ and integrated over the entire energy range, we obtain the conservation equation for the momentum. This is the approach taken by Bløtekjaer [2] and by Tang et al. [4]. However, if both sides of (2) are multiplied by $\tau_1 qv$ and then integrated over the energy, we obtain the constitutive equation for the current density j. This is basically the approach taken by Stratton [1] and by many others [5]. In this paper, we follow Stratton's approach.

Transport Coefficients as Functions of the SHE Coefficients

Using the notation of [5] except for the energy, the current density j and the energy flux density s are defined as:

$$j = -q\int_0^\infty v\frac{f_1}{3}g(\varepsilon)d\varepsilon, \tag{3}$$

$$s = \int_0^\infty \varepsilon v\frac{f_1}{3}g(\varepsilon)d\varepsilon, \tag{4}$$

where

$$g(\varepsilon) = \frac{1}{2\pi^2}(\frac{2m^*}{\hbar})^{3/2}\gamma^{1/2}\gamma'$$

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is the density of states. Substituting (2) into (3) and (4), the following two constitutive equations are obtained:

$$j = q\mu E_x n + q\frac{d'}{dx}(Dn), \quad (5)$$

$$s = -\mu_\varepsilon E_x n W - \frac{d'}{dx}(D_\varepsilon n W), \quad (6)$$

where

$$W = \frac{1}{n}\int_0^\infty \varepsilon f_0 g(\varepsilon) d\varepsilon$$

is the average energy and the prime on the derivative denotes that the derivative does not apply to the impurity concentration. The transport coefficients μ, μ_ε, D and D_ε are defined as:

$$\begin{pmatrix} \mu \\ \mu_\varepsilon \end{pmatrix} = \frac{-q\int_0^\infty \begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} \tau_1 v^2 [\frac{1}{3}\frac{\partial f_0}{\partial \varepsilon} + (\frac{2}{3}\frac{\partial}{\partial \varepsilon} + \frac{\gamma'}{\gamma})\frac{f_2}{5}] g(\varepsilon) d\varepsilon}{\int_0^\infty \begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} f_0 g(\varepsilon) d\varepsilon} \quad (7)$$

and

$$\begin{pmatrix} D \\ D_\varepsilon \end{pmatrix} = \frac{\int_0^\infty \begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} \tau_1 v^2 [\frac{1}{3} f_0 + \frac{2}{3}(\frac{f_2}{5})] g(\varepsilon) d\varepsilon}{\int_0^\infty \begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} f_0 g(\varepsilon) d\varepsilon}. \quad (8)$$

According to (7) and (8), these transport coefficients are precisely defined through energy integrals involving f_0, f_2 and $\tau_1(N_i, \varepsilon)$.

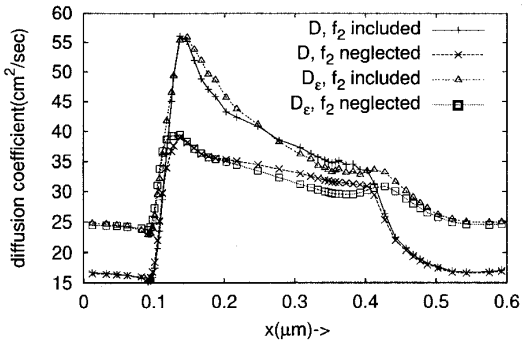

Fig. 1 Effect of neglecting f_2 on D and D_ε.

Using the inhomogeneous MC data of $n^+ - n - n^+$ structures [4], we have compared μ, μ_ε, D and D_ε with and without the term involving f_2. We have found that although the difference between the two for μ and μ_ε is small because the energy derivatives of f_0, f_2 are involved in the definition of μ and μ_ε, it is not negligible for D and D_ε as shown in Fig. 1. This is because the condition $f_0 \gg f_2$ is not satisfied, particularly in the region where the average energy W is increasing. Figs. 2 and 3 show the result of the LPE of electron distribution function at two locations, one at increasing energy ($\frac{dW}{dx} > 0$) and the other at decreasing energy ($\frac{dW}{dx} < 0$), but both having about the same W. It is seen that on the increasing energy (heating) side, the condition $f_0 \gg f_1 \gg f_2 \ldots, etc.$ is hardly satisfied. This indicates that the distribution function is highly anisotropic and that the assumption of equi-partition of energy is invalid. On the decreasing energy (cooling) side, the magnitude of $f_1, f_2, \ldots, etc.$ diminish rapidly; however, the shape of f_0 is far from Maxwellian. This reflects the fact that the high-energy tail of electron distribution is relaxing very slowly towards the Maxwellian form.

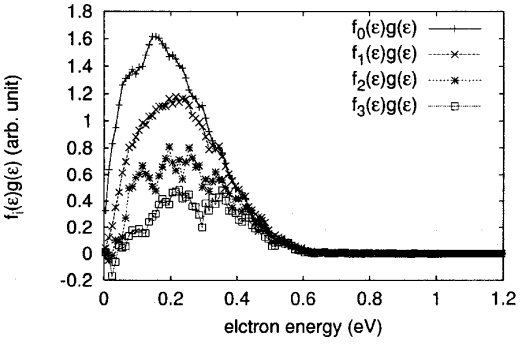

Fig. 2 The LPE of electron distribution function at $x = 0.248\mu m$, where $\frac{dW}{dx} > 0$ and $W = 0.209eV$.

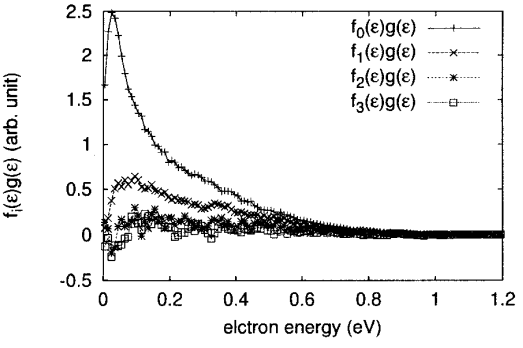

Fig. 3 The LPE of electron distribution function at $x = 0.412\mu m$, where $\frac{dW}{dx} < 0$ and $W = 0.222eV$.

3. Examination of the Einstein Relation

We have also examined the Einstein relations D/μ and $D_\varepsilon/\mu_\varepsilon$ which are shown in Fig. 4. While $D_\varepsilon/\mu_\varepsilon$ is approximately equal to $2W/3q(\approx k_B T_e/q)$, D/μ is not. This is related to the non-equipartition of energy, signified by the presence of f_2. The ratios D_ε/D and μ_ε/μ are

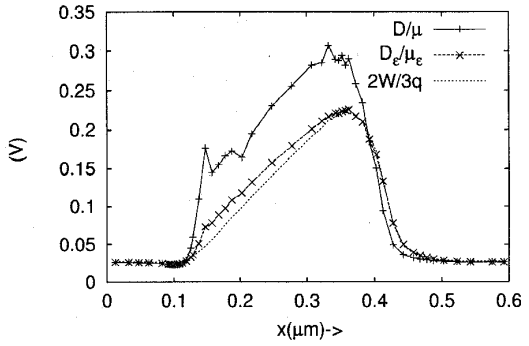

Fig. 4 Plots of D/μ and $D_\varepsilon/\mu_\varepsilon$ vs. distance compared to $2W(x)/3q$.

often given in the literature as

$$\frac{D_\varepsilon}{D} \approx \frac{\mu_\varepsilon}{\mu} = \frac{5}{3} + \frac{2}{3}\frac{W}{\mu}\frac{\partial \mu}{\partial W} = \xi(W). \tag{9}$$

This simple ratio is based on two assumptions: (i) f_2 is negligible compared to f_0, and (ii) f_0 is proportional to $e^{-\frac{\varepsilon}{k_B T_e}}$. As can be seen from Fig. 5 in which these ratios are compared to the MC data, these two ratios are quite different under the non-equilibrium condition.

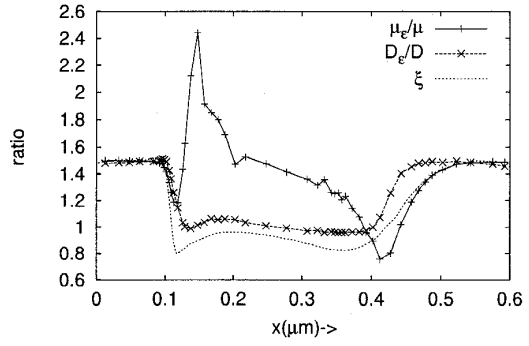

Fig. 5 Comparison of D_ε/D, μ_ε/μ and $\xi(W)$ vs. distance.

4. Non-local Effect of Carrier Transport

From the device simulation point of view, the task now is to model the transport coefficients μ, μ_ε, D and D_ε in terms of the state variables such as $n, \vec{V}$ and W. It is always desirable if these transport coefficients can be expressed as a single-valued function of W only. The local energy-dependent model which is based on the *homogeneous* MC data, accurate over the energy range $0.04eV \leq W \leq 0.5eV$, can be expressed empirically as:

$$\frac{1}{\mu^*} = \frac{1}{1.34}\left[\sqrt{1+\frac{N_d(\frac{W_0}{W})}{1.1\times 10^{17}+0.05N_d}}\right] + \rho, \tag{10}$$

$$\frac{1}{\mu^*_\varepsilon} = 0.5\left[\sqrt{1+\frac{N_d(\frac{W_0}{W})}{1.6\times 10^{17}+0.08N_d}}\right] + \rho_\varepsilon, \tag{11}$$

$$\frac{D^*}{\mu^*} = \frac{1}{q}[\frac{2}{3}W + f(W)\rho_u], \tag{12}$$

$$\frac{D^*_\varepsilon}{\mu^*_\varepsilon} = \frac{2W}{3q}, \tag{13}$$

where N_d is the total doping concentration in cm^{-3}, $W_0 = \frac{3}{2}k_B T_0$ is the equilibrium lattice energy in eV, μ^* and μ^*_ε are in $cm^2/mV\cdot s$, and ρ, ρ_ε and ρ_u are functions of W given by

$$\rho = \sum_{i=0}^{i=3}\rho_i(W-W_0)^i,$$

$$\rho_\varepsilon = \sum_{i=0}^{i=3}\rho_{\varepsilon i}(W-W_0)^i,$$

$$\rho_u = \sum_{i=0}^{i=3}\rho_{ui}(W-W_0)^i.$$

The coefficients ρ_i, $\rho_{\varepsilon i}$ and ρ_{ui} are listed in Table I. The function

$$f(W) = \begin{cases} 1-\exp[-4(\frac{W}{W_0}-1)] & \text{if } W > W_0 \\ 0 & \text{otherwise} \end{cases}$$

is inserted in (12) to assure that D^*/μ^* reduces to its equilibrium value of $2W_0/3q$ as W approaches W_0.

Table I: List of coefficients for the Einstein relation (D/μ), the mobility (μ^*), and the energy mobility (μ^*_ε).

Index	i=0	i=1	i=2	i=3
Units	(eV)		(eV^{-1})	(eV^{-2})
ρ_i	-3.83×10^{-2}	+24.37	-9.68	+47.03
$\rho_{\varepsilon i}$	$+1.01\times 10^{-1}$	+16.23	+13.16	+7.39
ρ_{ui}	-1.00×10^{-3}	+0.299	-0.546	+0.778

However, even these local MC-calibrated energy-dependent models do not predict the device performance accurately when they are applied to the actual inhomogeneous device simulation. The reason is that the non-local effect depends on the shape of the distribution function and the average energy alone can not fully characterize it. As an example of such non-local effects, Fig. 6 compares the difference between $(\frac{D}{\mu})_{local}$ using (12) and $(\frac{D}{\mu})_{MC}$ from the MC simulation.

Using the local model given by (10)-(13), the average electron velocity V and the energy flux density s are calculated from the HD equations and are compared to the

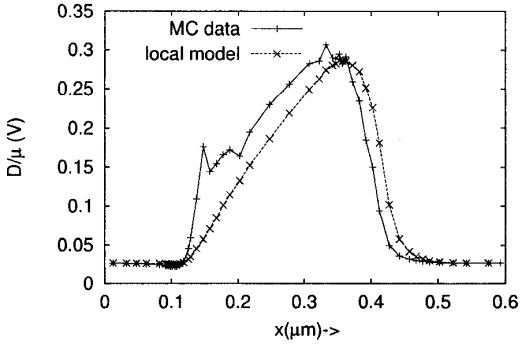

Fig. 6 Comparison of D/μ predicted by the local energy-dependent model with that of actual MC simulation data.

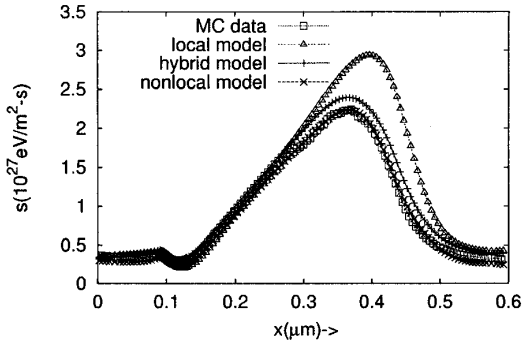

Fig. 8 Comparison of s predicted by the local model, the hybrid model and the non-local model with that of MC data.

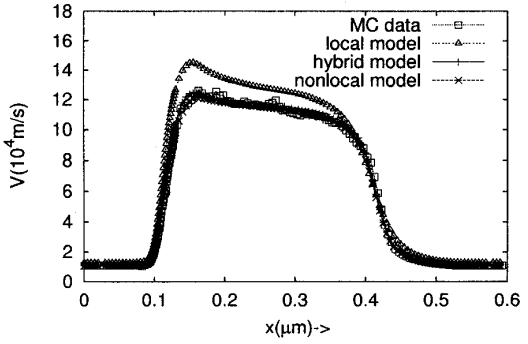

Fig. 7 Comparison of V predicted by the local model, the hybrid model and the non-local model with that of MC data.

MC results in Figs. 7 and 8, respectively. Also shown in these figures are results obtained by using the method of the moments of the BTE with expressions for j and s different from (5) and (6). In those expressions, μ^*, μ_s^*, U and R are modeled as functions of W as well as ∇W and a nonlinear term involving velocity and momentum is also included [4]. This model is labeled as the non-local model. Although this model reproduces the MC result quite well, often a steep price needs to be paid for numerical convergence. It is also possible to use the expression (6) with the transport model (11) and (13) for s and the non-local transport model for j from [4]. The result is labeled as the hybrid model in the figures.

5. Conclusion

Using the SHE of the distribution function and casting the current density and the energy flux density in the form of (5) and (6) respectively, the transport coefficients μ, μ_ε, D and D_ε can be rigorously defined through the expansion coefficients f_0, f_2 and their energy derivatives. We have found that D/μ deviates substantially from $2W/3q$ for the non-equilibrium transport. Moreover, most of these transport coefficients exhibit a strong non-local effect typically signified by the presence of the non-negligible component f_2. As a result, the local energy-dependent model of these transport coefficients often introduces substantial errors when it is applied to inhomogeneous device simulations. The same problem exists if an alternative approach of the moments of the BTE is used [4]. However, from the numerical implementation point of view the moment approach has a slight advantage over Stratton's formulation, because the mobility coefficients always appear outside of the gradient operator and the non-local correction is easier to implement. How to improve the non-local correction in the modeling without resorting to complicated transport equations and thus assuring numerical stability is still a challenge for the HD device simulation.

References

1. R. Stratton, *Phy. Rev.*, vol. 126, pp. 2002-2014, June 1962.

2. K. Bløtekjaer, *IEEE Trans. Electron Devices*, vol. 17, p. 38, 1970.

3. W. Liang et al. *IEEE Trans. Electron Devices*, vol. 44, pp. 257-267, Feb. 1997.

4. T.-w. Tang et al. *IEEE Trans. Electron Devices*, vol. 40, pp. 1469-1477, Aug. 1993.

5. D. Widiger et al. *IEEE Trans. Electron Devices*, vol. 32, p. 1092, June 1985.