An Efficient Approach to Solving The Boltzmann Transport Equation in Ultra-fast Transient Situations

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Abstract

A previously developed hydro-kinetic concept based on evolution of the distribution function is used to arrive at an efficient approach to solving the Boltzmann transport equation (BTE) in ultra-fast transient situations. The solution can properly account for effects of extreme non-equilibrium phenomena. The approach is applied to study the temporal evolution of the electron distribution in n-type *Si*. Results from the Monte Carlo method are also included to verify the accuracy of the proposed approach.

1. Introduction

Performance and reliability of the submicron devices have been found to be strongly influenced by the hot-electron behavior which, for example, might result in leakage gate current and device degradation [1,2]. To study these hot-electron effects, the carrier distribution function in the device needs to be determined. Therefore, in addition to non-stationary transport parameters including density n, mean energy $\overline{\epsilon}$, and average velocity $\overline{v}$, knowledge of the non-stationary and/or hot-electron distribution function also becomes crucial in small devices.

Various approaches to the distribution function have been used to study non-stationary or hot-electron phenomena in devices. Among these, the efficient approaches using the displaced Maxwellian [3], Legendre polynomial [4], and the energy-dependent distribution [5,6] are commonly used. However, these methods all have some severe limitations in highly non-stationary and/or hot-electron situations [6]. To more accurately determine the distribution function, the Monte Carlo simulation is usually used although it demands a large CPU time. In this study, an efficient approach to the hydro-kinetic distribution evolving at the velocity relaxation scale is proposed. This approach is applied to study the fast temporal evolution of the distribution function related to relaxation of the transport parameters of electrons in *Si*.

2. Theoretical Background - The Hydro-kinetic Transport Concept

The hydro-kinetic concept [6] is presented in Fig. 1 where the axis represents the time scale of the distribution function. The exact solution of the BTE is given by the kinetic distribution function $f(\boldsymbol{k})$ where $\boldsymbol{k}$ is the wave vector. The BTE is only valid for the time scales greater than the collision duration time, τ_c. The **hydro-kinetic** concept is based on the fact that, when use the moments (**hydrodynamic** parameters) to describe the **kinetic** distribution function, it requires an infinite set of moments, namely $f(\boldsymbol{k}) = f(\boldsymbol{k}, n, \overline{\boldsymbol{k}}, \overline{\epsilon}, \overline{\boldsymbol{k}^3}, \overline{\boldsymbol{k}^4}, \ldots)$. Therefore, relaxation times of the moments can be used to characterize $f(\boldsymbol{k})$.

In general, $\tau_n > \tau_\epsilon > \tau_m$ (the carrier density, energy, and momentum relaxation times, respectively) in semiconductors, and relaxation times of higher order moments are assumed to be less than τ_m. As illustrated in Fig. 1, after a sudden change in field, information described by the higher-order moments will vanish faster than that described by n, $\bar{\epsilon}$ and $\bar{k}$. As a consequence, after a sufficient time, $f(k)$ will evolve into a τ_m-scale hydro-kinetic distribution $f_m(k,n,\bar{\epsilon},\bar{k})$ which takes into account temporal/spatial variations through the changes in n, $\bar{\epsilon}$ and $\bar{k}$. f_m thus varies as fast as $\bar{k}$ and is valid for the scale of interest on the order of τ_m. To determine $f_m(k,n,\bar{\epsilon},\bar{k})$, n, $\bar{\epsilon}$, and $\bar{k}$ have to be solved from the hydrodynamic equations which are written as

$$\frac{\partial n}{\partial t} + \nabla\cdot(n\bar{\upsilon}) = -\frac{n}{\tau_n}, \tag{1a}$$

$$\frac{\partial n\bar{\epsilon}}{\partial t} + \nabla\cdot\langle \epsilon\upsilon\rangle = qnE\cdot\bar{\upsilon} - \frac{n(\bar{\epsilon}-\epsilon_o)}{\tau_\epsilon}, \tag{1b}$$

$$\frac{\partial n\bar{p}}{\partial t} + \nabla\langle p\cdot\upsilon\rangle = qnE - \frac{n\bar{p}}{\tau_m} \tag{1c}$$

where $\bar{p}$ is the average momentum, and the relaxation times are defined in terms of integrals of the distribution function and transition rates over $\bar{k}$ space. [7] At the scale near τ_m, f_m is used to evaluate the relaxation times which therefore becomes $\bar{\epsilon}$ and $\bar{k}$ dependent, as illustrated in Fig. 1.

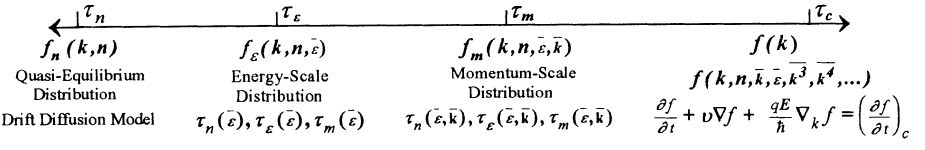

Fig. 1: Evolution of the distribution function

At a scale on the order greater than τ_m (i.e., near τ_ϵ), the $\bar{k}$ dependence becomes insignificant because generally $\tau_\epsilon \geq \tau_m$. The distribution therefore evolves into a τ_ϵ-scale hydro-kinetic distribution $f_\epsilon(k,n,\bar{\epsilon})$ that varies as fast as $\bar{\epsilon}$ and is only valid at scales on the order of τ_ϵ. At this scale, $f_\epsilon(k,n,\bar{\epsilon})$ is used to evaluate the relaxation times which thus becomes only energy dependent, as shown in Fig. 1. For a scale much greater than τ_ϵ, $\bar{\epsilon}$ and $\bar{k}$ are close to the steady state, and the carrier behavior can be described by the quasi-equilibrium distribution function, f_n.

3. τ_ϵ- and τ_m-Scale Hydro-kinetic Transport Models

The approach to the τ_ϵ-scale hydro-kinetic distribution f_ϵ has been introduced in a previous paper [6], In the current study, the evolution process of the distribution from f_m into f_ϵ is presented. The evolution due to scattering is assumed to be a relaxation process influenced by $\bar{\epsilon}$ and $\bar{p}$ relaxation and the change in field. The relaxation of the hydro-kinetic distribution function can be performed numerically with given f_ϵ:

$$f_m^{\ell+1}(\boldsymbol{k}) = f_\epsilon^{\ell+1}(\boldsymbol{k}) + \left[f_m^{\ell}(\boldsymbol{k}-\Delta\boldsymbol{k}_m^{\ell}) - f_\epsilon^{\ell}(\boldsymbol{k})\right]\exp\left(-\Delta t^{\ell}/\tau_h^{\ell+1/2}\right), \tag{2}$$

where $1/\tau_h$ is the relaxation rate for f_m evolving toward f_ϵ, and $\Delta t = t^{\ell+1} - t^{\ell}$. f_m^{ℓ} is taken

as an initial distribution to evaluate the next step distribution, $f_m^{\ell+1}$. The difference between f_m and f_ϵ at each time step tends to reduce and is, for a relaxation process, proportional to $exp(-\Delta t/\tau_h)$ due to the scattering process. On the other hand, Δk_m denotes the shifted amount in k space influenced by the electric field.

f_m at each step can be solved if Δk_m and τ_h are determined. The solution of Eqs. (1a)-(1c) can be used to assist in determining Δk_m and τ_h. The relaxation of $\overline{\epsilon}$ and $\overline{k}$ at each time step can be obtained by taking the moments of the Eq. (2). The solution of these relaxation equations for $\overline{\epsilon}$ and $\overline{k}$ must be consistent with that from Eqs. (1a)-(1c). This therefore determines Δk_m and τ_h at each time step, and then f_m is determined from Eq. (2). In this study, only the energy-dependent relaxation times are used in Eqs. (1a)-(1c) to calculate the hydrodynamic parameters. To include the momentum dependence in the relaxation times, the determined f_m, as discussed in Sec. 2, needs to be used to evaluate the relaxation times that are then used again to solve Eqs. (1a)-(1c) for the hydrodynamic parameters. The iteration will provide more accurate results for hydrodynamic parameters and f_m, and will be studied in the near future.

4. Application

Using the τ_ϵ- and τ_m-scale hydro-kinetic models, the response of a homogeneous concentration of electrons in n-type *Si* at 300K to a rapid increase in electric field is investigated. Results including the mean energy, average velocity, and the distribution function (f_ϵ and f_m) obtained from the hydro-kinetic models are examined and compared with those determined by the Monte Carlo simulation. It is assumed that no impact ionization is involved.

A step field increasing from 5 to 30 kV/cm within 0.1 psec is applied, and $\overline{\epsilon}$ and $\overline{v}$ responding to this field are given in Figs. 2a and 2b, respectively. It is shown that $\overline{\epsilon}$ and $\overline{v}$ calculated from Eqs. (1b) and (1c) are in very good agreement with the Monte Carlo results. An evident velocity overshoot is observed due to the drastic increase in field.

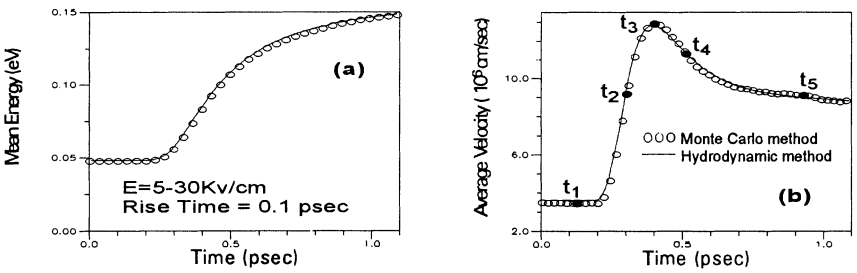

Fig. 2: Evolution of (a) mean energy (b) average velocity

The evolution of the distribution function under the influence of the step field is also shown in Figs. 3a-3e where f, f_ϵ, and f_m are illustrated at t_1-t_5. Figs. 3a-3e clearly show that the τ_ϵ-scale distribution f_ϵ evolves more slowly than f. This is because, as illustrated in Fig. 1, influenced of velocity relaxation is not properly accounted for in f_ϵ. As a result, f_ϵ starts to deviate from f when $\overline{v}$ increases rapidly due to the drastic increase in field. The discrepancy becomes significant during the overshoot interval as shown at t_2-t_4. On the contrary, f_m and f evolve closely over the simulation time since effects of velocity relaxation during the overshoot interval is properly included in f_m.

The maximum deviation between f_m and f is found at the time when $\overline{v}$ starts to decrease from the overshoot peak, as shown at t_4. However, the deviation is very small.

5. Conclusion

The study shows that the hydro-kinetic concept based on time scales of the hydrodynamic parameters can be used to characterize the evolution of the distribution function. The concept also leads to an accurate and efficient technique to solve the BTE. In the case of strong velocity overshoot, since f_m can include effects of velocity relaxation, f_m provides a much better description than f_ϵ. The CPU time required for solving the temporal evolution of the distribution and hydrodynamic parameters given in Figs. 2 and 3 is only about 10 seconds on a 486/33 PC. The approach to f_m might be an efficient method to study the phenomena associated with hot-electron effects in submicron devices.

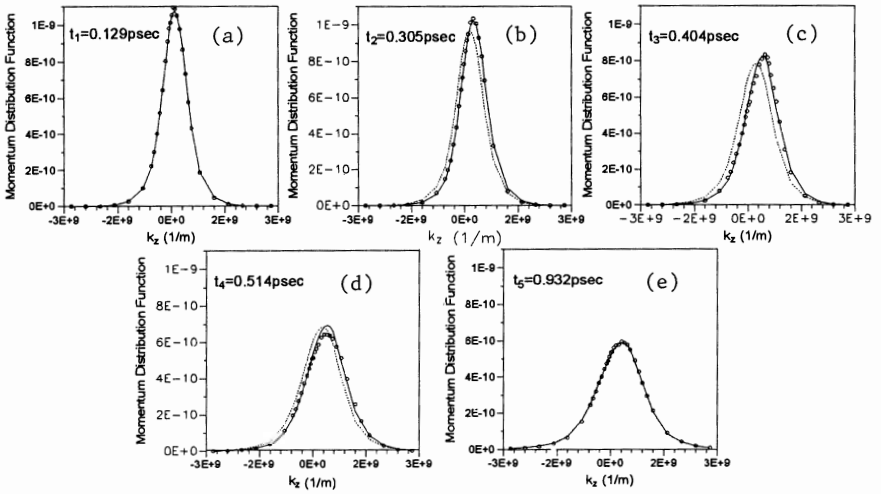

Fig. 3: Evolution of the distribution function. The times t_1-t_5 are indicated in Fig. 2. Symbols denote f calculated from the Monte Carlo method, solid lines represent f_m, and dots denote f_ϵ.

6. Acknowledgement

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References

[1] C. Fiegna, F. Venturi, M. Melanotte, E. Sangiorgi, and B. Ricco, IEEE Trans. Electron Dev., Vol. 38, p. 603, 1991.
[2] P. Roblin, A. Saman, and S. Bibyk, IEEE Trans. Electron. Dev., Vol. 35, p. 3229, 1988.
[3] K. F. Wu, M. P. Shaw, IEEE Trans. Electron Dev., Vol. 36, p. 603, 1989.
[4] N. Goldsman, L. Henrickson, and J. Frey, Solid-St. Electron. Vol. 34, 389 (1991).
[5] N. Goldaman and J. Frey, Solid State Electron., Vol. 31 p. 1089, 1988.
[6] Ming-C. Cheng and R. Chennupati, J. Phys. D., Vol. 28, pp. 160-173, 1995.
[7] Ming-C. Cheng and Lin Huang, J. Appl. Phys., Vol. 72, p. 3539, 1992.