Transport in Nanostructures: A Comparative Analysis Using Monte Carlo Simulation, the Spherical Harmonic Method, and Higher Moments Models

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Abstract. With the modern transistor size shrinking below 45 nm the classical drift-diffusion model to describe transport in the conducting channel is loosing its validity. In short-channel devices carriers get accelerated by the driving field and do not thermalize before they reach the drain contact. Thus, the assumption underlying the classical transport model, that the driving electric field produces a weak perturbation of the local equilibrium distribution function, is violated.

Several generalizations of the classical drift-diffusion model are possible. The most common approach in the TCAD community is to introduce higher moments of the distribution function. Another approach is to use a spherical harmonic expansion of the distribution function.

We perform a comprehensive analysis of the validity of the higher-moments transport models with the model based on spherical harmonic expansion by rigorously comparing their results with results of the Monte Carlo solution of the Boltzmann transport equation.

1 Introduction

The success of microelectronics technology has been partly enabled and supported by sophisticated Technology Computer-Aided Design (TCAD) tools which are used to assist in IC development and engineering at practically all stages from process definition to circuit optimization. At this moment, the TCAD related research and development cost reduction amounts to 35% and is expected to increase to 40% in the near future [1].

Most TCAD tools are based on semi-classical macroscopic transport models. From an engineering point of view, semi-classical models, such as the drift-diffusion transport model, have enjoyed an amazing success due to their relative simplicity, numerical robustness, and the ability to perform two- and three-dimensional simulations on large unstructured meshes [9]. However, with device size dramatically reduced the TCAD tools based on a semi-classical transport description begin to show shortcomings. With downscaling the devices' channel length the driving field and its gradient increase dramatically in the short

I. Lirkov, S. Margenov, and J. Waśniewski (Eds.): LSSC 2009, LNCS 5910, pp. 443–450, 2010.

channel. As a result the carrier distribution along the channel can no longer be described by the shifted and heated Maxwellian distribution, and the solution of the Boltzmann transport equation is needed to determine sufficiently accurate the distribution function.

The Monte Carlo method is a well-established numerical technique to solve the Boltzmann transport equation. Traditionally, the so called forward Monte Carlo method [7] is used to find the distribution function. For realistic structures, however, a direct numerical solution of this equation by discretization of the phase space is computationally too expensive. TCAD tools, however, do not usually solve the Boltzmann equation and are based on simplified transport models. Approximate solutions can be obtained by the method of moments. Defining the moments of the distribution function $f(\mathbf{r}, \mathbf{k}, t)$, one consecutively obtains the drift-diffusion model [4], the hydrodynamic model [2], the energy-transport models [10], or the six moments model [3]. Transport models based on the moments of the Boltzmann equation are well accepted in TCAD. Another way of generalizing the classical drift-diffusion model is to use a spherical harmonic expansion of the distribution function.

In this work we perform a comprehensive analysis of the validity of the higher-moments transport models with the model based on spherical harmonic expansion by rigorously comparing their results with results of the Monte Carlo solution of the Boltzmann transport equation. The analytical conduction band model with the non-parabolicity parameter $\alpha = 0.5\,\mathrm{eV}^{-1}$ is assumed in all the methods.

2 Simulation Methods

2.1 Monte Carlo Solution of the Boltzmann Equation

The Monte Carlo methods have been applied to a variety of materials [6,11]. Within this approach, particles are moving on classical trajectories interrupted by scattering processes with phonons and impurities. Although solving the Boltzmann equation with a Monte Carlo technique is computationally very expensive, it is necessary to obtain accurate closure relations, expressing higher moments via the moments of lower order, to introduce and control scattering mechanisms at the microscopic level and, most importantly, to incorporate the peculiarities of the semiconductor band structure. Thus, different Monte Carlo algorithms are conveniently used for the calibration of TCAD tools [7].

2.2 Higher Moments Models

From an engineering point of view, the advantages of the drift-diffusion model are its efficiency and numerical robustness. These properties make two- and three-dimensional numerical studies of fairly complex device structures feasible. However, hot-carrier effects are difficult to estimate correctly and non-local effects such as velocity overshoot are completely neglected. Higher-order transport models such as the hydrodynamic transport [2] and the energy transport [10]

models are designed to overcome some of the shortcomings of the drift-diffusion model. The energy-transport model additionally takes into account the carrier energy balance. However, it typically tends to overestimate the non-local effects and thus the on-current of a device motivating the development of transport models including higher order moments. Some time ago a six moments transport model has been proposed [3]. Such a model, while computationally more efficient than the Monte Carlo method, provides additional information on the shape of the distribution function.

2.3 Spherical Harmonic Expansion

The steady state Boltzmann equation can conveniently be solved by expanding the angular dependence of the distribution function $f(\mathbf{r}, \mathbf{k})$ on $\mathbf{k}$ using a complete set of spherical harmonics $Y_{lm}(\theta, \phi)$:

$$f(\mathbf{r}, \mathbf{k}) = \sum_{lm} f_{lm}(\mathbf{r}, k) Y_{lm}(\theta, \phi), \tag{1}$$

where the θ and ϕ are the polar angles between the electric field $\mathbf{E}$ and $\mathbf{k}$. In the low-field limit one can truncate the expansion (1) after the terms with $l = 1$, which in case of parabolic isotropic bands and randomizing elastic scattering results in a drift-diffusion transport model with low-field mobility. As is shown in [5], in case of elastic scattering this approximation gives good results for silicon where the valleys are not isotropic. For general scattering processes and realistic band structures as well as at higher driving fields more terms in the expansion (1) are needed [8].

3 Results

In order to investigate the validity of macroscopic transport models we have carried out extensive Monte Carlo simulations of transport through a silicon n*in* structure. The length of the two heavily doped contacts ($N_D = 10^{20}$ cm^{-3}) is kept constant, while the length of the intrinsic channel ($N_A = 10^{16}$ cm^{-3}) varies. The band structure of silicon is approximated by six valleys with parabolic dispersion relation. Electron scattering with acoustic and optical phonons as well as with ionized impurities is taken into account.

The average velocity determines carrier transport in the structure. The average velocity as a moment of the distribution function can be computed along the device and is thus a more sensitive measure of validity for a particular transport model than any integral characteristic of a device like the total current. A typical result for the average velocity of carriers along an n*in* structure with an intrinsic region length of 40 nm computed with the Monte Carlo method is shown in Fig. 1. The solution of the Boltzmann equation by spherical harmonic expansion, with different number of terms in the series (1) is also displayed in Fig. 1. In such a short device the series (1) truncated at $l = 1$ gives only a poor approximation for the velocity profile. At the same time it is demonstrated that

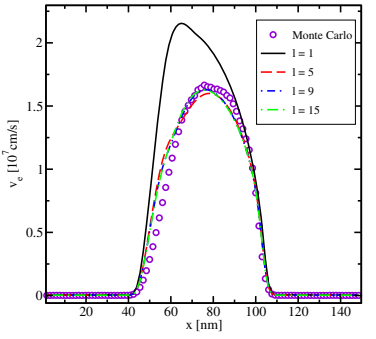

Fig. 1. Average velocity along the n*in* structure computed by solving the Boltzmann transport equation with the Monte Carlo method and using the spherical harmonic expansion method, with different numbers of terms included in the series (1). It is demonstrated that even in a short-channel structure the series expansion with terms only up to $l = 9$ included provides excellent results as compared to the more time consuming Monte Carlo data.

the spherical harmonic expansion (1) including terms up to $l = 9$ gives a perfect result. The inclusion of terms with $l > 9$ into (1) does not change the velocity profile confirming the rapid convergence of the series (1). Therefore, the spherical harmonic expansion method gives excellent results with only a few terms included into (1) even for short-channel devices. For this reason the method is much less time consuming than the Monte Carlo solution of the Boltzmann equation. However, Monte Carlo data are needed in order to validate the applicability of the spherical expansion method to describe transport in short-channel devices.

Current-voltage characteristics computed with the Monte Carlo (identical to those computed with spherical harmonic expansion method) and using the macroscopic transport models based on the moments of the distribution function are shown in Fig. 2 and Fig. 3, for several channel lengths. It is demonstrated that for long devices (1000 nm) the drift-diffusion (DD), the energy transport (ET) model, and the six moments (SM) model give almost equivalent results which are in perfect agreement with the results of the spherical harmonic expansion method. For a device with $L_{ch} = 250$ nm the drift-diffusion model underestimates the current. Since the carrier temperature is constant, the drift-diffusion model does not account for any non-local effects and cannot capture the non-local transport inside short-channel devices. This causes the accuracy of the drift-diffusion model to decrease for gate lengths shorter than 250 nm, where the restriction of constant carrier temperature must be relaxed. Due to the temperature gradient, heat flow and thermal diffusion appear. The drift-diffusion transport model must be augmented with the energy flow, or the third moment equation. The energy-transport model takes into account the energy flux equation in addition to the carrier energy balance equation. The energy-transport

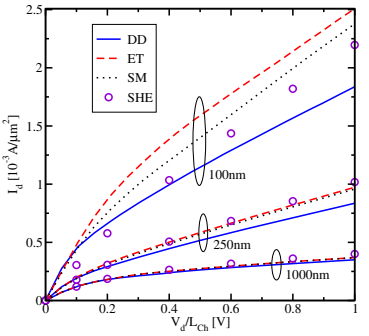

Fig. 2. Current-voltage characteristics for devices with different channel length computed with the spherical harmonic expansion method and using macroscopic transport models based on moments of the distribution function. Here DD stands for the drift-diffusion model, ET for energy-transport model, SM for the six moments model, and SHE for spherical harmonic expansion.

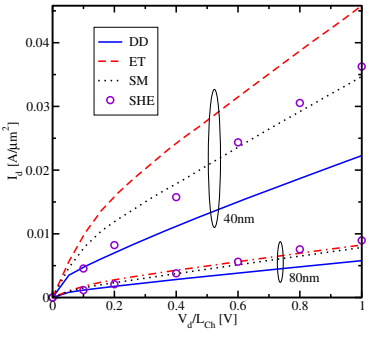

Fig. 3. The same as in Fig. 2 for shorter devices. The six moments model gives results closest to the results of Monte Carlo and the spherical Harmonic expansion methods.

model requires modeling of two mobilities for the current density and the energy flux for each carrier type, one relaxation time, and the non-parabilicity factor for non-parabolic bands. The simplified four-moments model is implemented in standard TCAD simulation tools and can be applied for a large set of semiconductor materials.

The energy-transport model overestimates the drive current. Fig. 4 illustrates the average velocity profile in a device with a 40 nm long channel. The drift-diffusion model underestimates the average velocity while the energy-transport model overestimates it. In order to reduce this spurious velocity overshoot effect the next moments should be included for devices with L_{ch} shorter than 100 nm, where the energy-transport model starts failing to predict the current accurately.

Going one step further in the model hierarchy one obtains a transport model of sixth order. A balance equation for the average squared energy and the related flux equation are added. To close the equation system, the moment of sixth

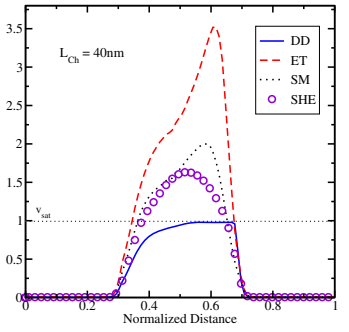

Fig. 4. Average velocity along the device with 40 nm channel length computed with the macroscopic transport models and with the spherical harmonic expansion method (equivalent to the Monte Carlo results). While the drift-diffusion model underestimates the velocity and current, the energy-transport model overestimates the velocity in short-channel devices. The six moments model improves the situation.

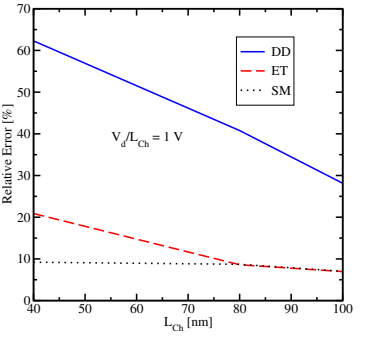

Fig. 5. Relative error of the current computed with macroscopic transport models. While the drift-diffusion and the energy-transport models are gradually losing their validity with the channel length reduced, the six moments model maintains its accuracy down to the channel length of 40 nm.

order has to be approximated using lower order moments. From Monte Carlo simulations serving as an accurate reference, an empirical closure relation has been proposed taking into account also the second order temperature. Compared to the energy-transport models, the six moments model requires two additional relaxation times for the second order temperature and the kurtosis flux. Having too many adjustable parameters is a particular inconvenience of the six moments model. A solution to this problem is based on tabulating some parameters of the model using Monte Carlo simulations. The parameter dependences on temperature, doping, and driving field are determined from the condition that the six moments transport model reproduces exactly all the six moments obtained from the Monte Carlo simulator under homogeneous conditions.

The inclusion of higher moments improves the transport model significantly. The current-voltage characteristics are reproduced fairly well even in devices as short as 40 nm as demonstrated in Fig. 3, because of the more accurate results for the velocity (Fig. 4). The relative error of the current computed by the macroscopic transport models presented in Fig. 5 as function of the channel length clearly demonstrates the applicability of the six moments model to describe the output characteristics of devices with a channel as short as 40 nm.

4 Conclusion

Transport modeling for scientific computing applications has grown into a mature field of research. Models of different complexity, precision and accuracy are offered. Monte Carlo techniques are used to obtain solutions of the Boltzmann transport equation with arbitrary scattering mechanisms and general band structure. These methods require significant computing resources and are, therefore, relatively rarely used for industrial TCAD applications, where timely, but perhaps less accurate, results are of primary importance. For example, a typical time to get a single point at the output characteristic of a 100 nm long device on a 3 GHz AMD Opteron processor with a Monte Carlo method is 24 hours, while it is only 30 minutes with the spherical harmonic expansion method, in which terms up to ninth order are included. It is demonstrated that the spherical harmonic expansion method provides accurate results for structures with the channel length as short as 50 nm. At the same time, with the channel length decreased, the drift-diffusion and even the energy-transport models gradually lose their validity, and higher moments must be included into the model. We demonstrate that the six moments transport model, which needs only 60 seconds of CPU for a single IV point, provides accurate results for devices with the gate as short as 40 nm by a comprehensive comparison of the simulation results with the data obtained with the spherical harmonics expansion method and results of Monte Carlo simulations.

Acknowledgments

We gratefully acknowledge financial support from the Austrian Science Fund FWF, project P19997-N14.

References

1. International Technology Roadmap for Semiconductors: 2005 Edition (2005), `http://www.itrs.net/Common/2005ITRS/Home2005.htm`
2. Blotekjaer, K.: Transport equations for electrons in two-valley semiconductors. IEEE Trans. Electron Devices 17, 38–47 (1970)
3. Grasser, T., Kosina, H., Gritsch, M., Selberherr, S.: Using six moments of Boltzmann's transport equation for device simulation. J. Appl. Phys. 90, 2389–2396 (2001)

4. Gummel, H.: A self-consistent iterative scheme for one-dimensional steady state transistor calculations. IEEE Trans. Electron Devices ED-11, 455–465 (1964)
5. Herring, C., Vogt, E.: Transport and deformation-potential theory for many-valley semiconductors with anisotropic scattering. Physical Review 101, 944–961 (1956)
6. Jacoboni, C., Reggiani, L.: The Monte Carlo method for the solution of charge transport in semiconductors with applications to covalent materials. Reviews of Modern Physics 55, 645–705 (1983)
7. Kosina, H., Nedjalkov, M., Selberherr, S.: Theory of the Monte Carlo method for semiconductor device simulation. IEEE Trans. Electron Devices 47, 1899–1908 (2000)
8. Pham, A., Jungemann, C., Meinerzhagen, B.: Deterministic multisubband device simulations for strained double gate PMOSFETs including magnetotransport. IEDM Techn. Dig., 895–898 (2008)
9. Selberherr, S.: Analysis and Simulation of Semiconductor Devices. Springer, Heidelberg (1984)
10. Stratton, R.: Diffusion of hot and cold electrons in semiconductor barriers. Physical Review 126, 2002–2014 (1962)
11. Sverdlov, V., Ungersboeck, E., Kosina, H., Selberherr, S.: Current transport models for nanoscale semiconductor devices. Materials Science and Engineering R 58, 228–270 (2008)