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A Non-Parabolic Six Moments Model for the Simulation of Sub-100 nm Semiconductor Devices

TIBOR GRASSER AND ROBERT KOSIK
Christian Doppler Laboratory for TCAD in Microelectronics at the Institute for Microelectronics
grasser@iue.tuwien.ac.at

CHRISTOPH JUNGEMANN AND BERND MEINERZHAGEN
NST, TU Braunschweig, Hans-Sommer-Str. 66, D-38106 Braunschweig, Germany

HANS KOSINA AND SIEGFRIED SELBERHERR
Institute for Microelectronics, TU Vienna, Gusshausstr. 27–29, A-1040 Vienna, Austria

Abstract. Macroscopic transport models derived from Boltzmann's equation by using the method of moments are often used to efficiently evaluate the electrical behavior of semiconductor devices. The most commonly used model is the drift-diffusion model which comprises the first two moments of Boltzmann's equation. In this model the carrier gas is assumed to be in equilibrium with the lattice, an assumption severely violated in submicron semiconductor devices. Hydrodynamic and energy-transport models have therefore been proposed to overcome this limitation. However, these extended models have never been widely accepted as a viable substitute, because for small devices they often do not deliver the expected improved accuracy. Here we present a non-parabolic six moments model which predicts considerably more accurate currents than the energy-transport model down to gate-lengths as small as 40 nm.

Keywords: device simulation, Boltzmann's equation, moments method, macroscopic transport models, energy-transport model, six moments model

1. Introduction

Macroscopic transport models based on the first six moments of Boltzmann's equation [1] are a natural extension to the well known drift-diffusion (DD) model (two moments) and the various hydrodynamic and energy-transport models (three or four moments) [2]. In addition to the solution variables of the energy-transport (ET) model, which are the carrier concentration $n = \langle 1 \rangle$ and the average energy $w_1 = \langle \mathcal{E} \rangle / n$, the six moments (SM) model includes $w_2 = \langle \mathcal{E}^2 \rangle / n$. The quantity $\beta = (3/5) w_2 / w_1^2$ is the kurtosis of the distribution function and indicates the deviation from a heated Maxwellian distribution for which $\beta = 1$ holds (for parabolic bands). The knowledge of β allows to model non-equilibrium processes like hot carrier tunneling [3] and impact ionization [4] with improved accuracy compared to DD and ET models. Due to numerical stability problems of the implemention, previously published results were mainly obtained by applying these models to Monte Carlo data in post-processing steps. The closure relation for the highest order moment $w_3 = \langle \mathcal{E}^3 \rangle / n$ was identified as one of the crucial factors determining the numerical stability. We summarize our efforts and propose a refined closure relation. Another important issue is the modeling of the mobilities, relaxation times, and the non-parabolicity corrections to the streaming terms. To avoid uncertainties related to possibly inaccurate analytical mobility and relaxation time models we use tabulated bulk Monte Carlo data [5].

Finally, we present results of numerical solutions of consistent DD, ET, and SM models and compare them to self-consistent Monte Carlo (MC) simulation results, both with analytic [6] and full-band structures [7].

2. The Non-Parabolic Six Moments Model

The non-parabolic stationary balance and flux equations of the macroscopic moment models are [8]

$$\nabla \cdot n\mathbf{V}_i - i\mathbf{F} \cdot n\mathbf{V}_{i-1} = -n\frac{w_i - w_{i,\mathrm{eq}}}{\tau_i}, \quad (1)$$

$$\mathrm{q}n\mathbf{V}_i = -\mu_i \frac{2}{3} H_{i+1}(\nabla(nw_{i+1}) + \mathrm{q}n\mathbf{E}w_i h_i), \quad (2)$$

$$h_i = \frac{3 + 2i\ H_i}{2H_{i+1}}, \quad (3)$$

with $i = 0, 1, 2$. The mobilities μ_i, the relaxation times τ_i, and the non-parabolicity factors H_i were taken from tabulated bulk data of respective Monte Carlo simulations and modeled as a function of the average energy w_1 only, in analogy to [5].

A critical issue is the modeling of the closure relation for the highest-order moment w_3. In [1] we proposed to use a generalized Maxwellian closure

$$w_3 = (35/6)w_1^3\beta^c, \quad (4)$$

with c an integer in the range $[0 \ldots 3]$. Stable implementations were only obtained for $c = 3$, the values $c \leq 2$ showed pronounced oscillations in the solution. However, the results obtained from $c = 2$, though often unstable, appeared to better reproduce the Monte Carlo results. We now take a somewhat different approach: by requiring consistency with bulk Monte Carlo simulations we obtain c from a best match of w_3 to w_3^{MC}, which gives $c = 2.7$. Other closure relations derived from theoretical considerations based on the maximum entropy principle [9,10] and relations derived from the cumulants of the distribution function [11] which results in

$$w_3 = (35/6)w_1^3(3\beta - 2) \quad (5)$$

have been compared as well (cf. Fig. 1). Note that Eq. (5) is also obtained from Grad's method [12]. However, only the generalized Maxwellian closure delivers satisfactory results and a numerically stable implementation (cf. Fig. 2).

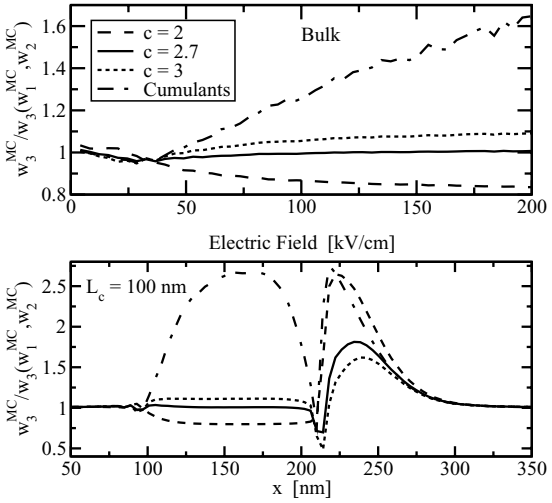

Figure 1. Ratio of the closure relations obtained by a Monte Carlo post-processing step with the exact result. The top figure shows the silicon bulk result for a doping concentration of $N_{\mathrm{D}} = 10^{18}\,\mathrm{cm}^{-3}$ while the bottom figure shows the result for a 100 nm n^+-n-n^+ structure. The generalized Maxwellian closure with $c = 2.7$ gives the best results.

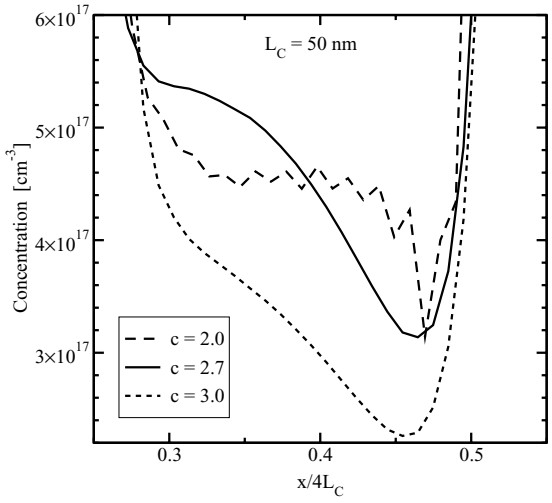

Figure 2. Comparison of the carrier concentrations obtained from various closure parameters c for the 50 nm n^+-n-n^+ structure. The instabilities arising from $c = 2$ are clearly visible.

In addition to the SM model we consider the corresponding ET model, where the equation for w_2 is kept but the equation for the energy-flux $\mathbf{V}_1$ is closed with $w_2 = (5/3)w_1^2$, corresponding to a heated Maxwellian distribution. The equation for w_2 is therefore decoupled from the lower order equations and provides an estimate for w_2 and thus β [1,13].

It is important to note that since all model parameters are obtained from bulk Monte Carlo simulations the transport model is fit-parameter free. The model parameters can therefore not be tuned to obtain a desired result. This approach therefore removes a critical uncertainty often found in moment based models.

3. Comparison

To investigate the accuracy of the SM model and its corresponding ET model we consider a series of one-dimensional n^+-n-n^+ structures with doping concentrations of $5 \times 10^{19}\,\mathrm{cm}^{-3}$ and $10^{17}\,\mathrm{cm}^{-3}$. The channel length was varied from 1000 nm down to 40 nm while maintaining a maximum electric field of approximately 300 kV/cm. A comparison of the average velocity $\mathbf{V}_0$ and the kurtosis β obtained from the macroscopic models with the analytic-band Monte Carlo simulation is shown in Figs. 3 and 4 for three devices. The spurious velocity overshoot is significantly reduced in the SM model, consistent with previous results [14], while the kurtosis produced by the decoupled SM (ET) model is only a poor approximation to the Monte Carlo results for shorter channel lengths. An accurate kurtosis, however, is a prerequisite for modeling hot carrier effects.

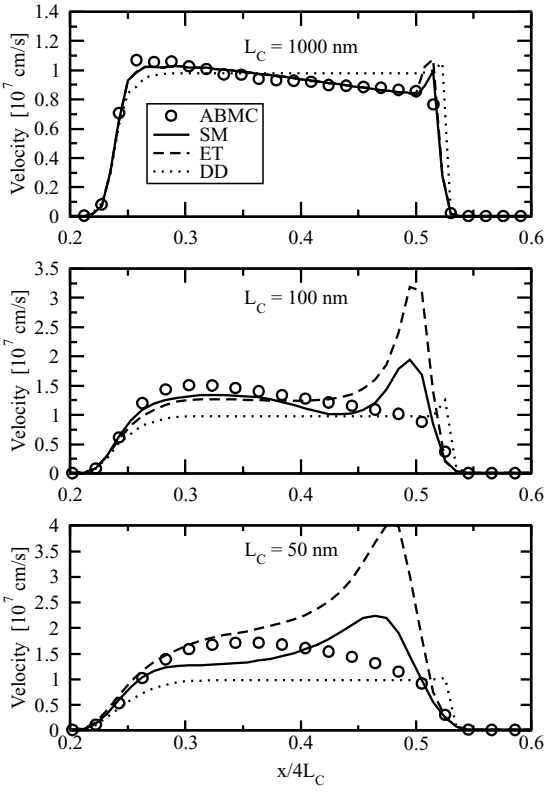

Figure 3. Comparison of the average velocity obtained from the macroscopic models with self-consistent analytic-band Monte Carlo (ABMC) simulations for three n^+-n-n^+ structures.

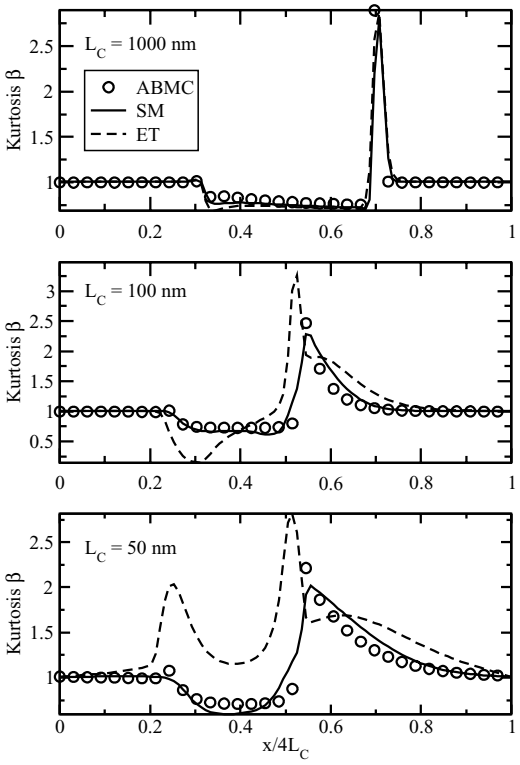

Figure 4. Comparison of the kurtosis obtained from the macroscopic models with self-consistent analytic-band Monte Carlo (ABMC) simulations for three n^+-n-n^+ structures.

The terminal currents as a function of the channel length are shown in Fig. 5, where the ET model shows the well known overestimation of the currents for $L_c \leq 100\,\mathrm{nm}$ while the DD model underestimates them for $L_c \leq 500\,\mathrm{nm}$. The SM model stays close to the Monte Carlo results down to $L_c = 40\,\mathrm{nm}$.

In addition we simulated the 50 nm double-gate MOSFET from [15] and compared the results to self-consistent full-band Monte Carlo results. To avoid empirical surface scattering models, where consistency between all models is difficult to obtain, we omit surface scattering altogether for the present comparative study. To avoid unrealistic mobility values, the channel doping was set to $N_A = 1.25 \times 10^{18}\,\mathrm{cm}^{-3}$, electrically compensated by a similarly large donor doping N_D.

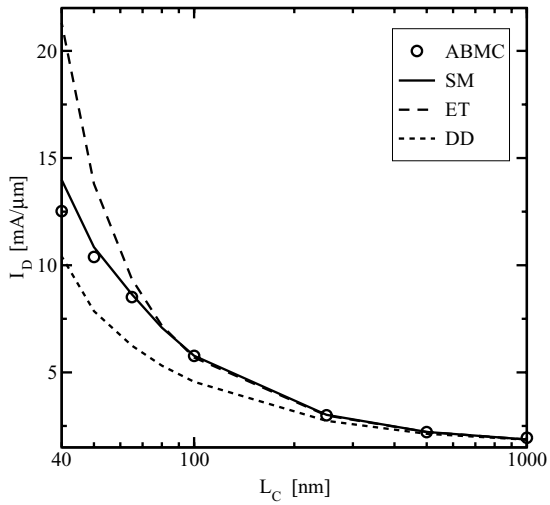

Figure 5. Comparison of the n^+-n-n^+ structure terminal currents obtained from the macroscopic models with self-consistent analytic-band Monte Carlo (ABMC) simulations for various gate lengths.

Even without surface scattering, the full-band channel mobilities were found to be different from the bulk case because of the mere presence of the interface not accounted for in the tabulated models. We introduced this effect by scaling all channel mobilities with a constant factor ($\approx$0.92) which was determined independently for each model from the simulation of a 250 nm MOSFET biased at $V_G = 1$ V and $V_D = 100$ mV. This

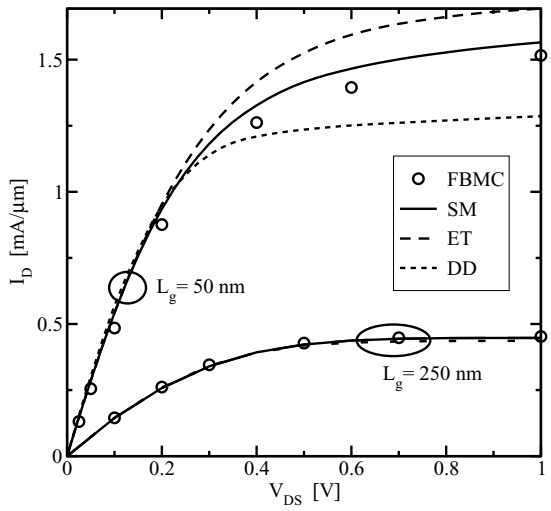

Figure 6. Comparison of the output characteristics obtained from the various models with self-consistent full-band Monte Carlo (FBMC) simulations for the 50 nm and 250 nm DG MOSFET.

effect is regularly calibrated together with the surface mobility model.

The simulation results in Fig. 6 show the same qualitative behavior as found in the n^+-n-n^+ structures. The observed differences in the near-equilibrium output conductance, which are in agreement with the results published in [16], indicate that surface scattering should not be calibrated using devices with such short channels, but rather their long-channel counterparts.

4. Conclusion

We have derived a six moments model from Boltzmann's transport equation where particular attention was given to the modeling of the highest-order moment. It was found that the heated-Maxwellian approximation commonly used to close forth-order energy-transport models is inaccurate for sub-100 nm devices. In particular it can be concluded that a fully self-consistent solution of the six moments model is important, because the kurtosis cannot be obtained in a post-processing step. Altogether it was found that the SM model stays much closer to the Monte Carlo results than the ET model, which makes the SM model a worthwhile choice for modeling such small devices.

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