Failure of Moments-Based Transport Models in Nanoscale Devices Near Equilibrium

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***Abstract*—It is shown that the conductance in nanoscale devices near equilibrium strongly depends on the choice of the transport model. Errors larger than a factor of two can be encountered, if the drift-diffusion (DD) model is used instead of a model based on the full Boltzmann equation. This effect is due to a fundamental difference in carrier heating between bulk systems and devices. Although carrier heating is included in hydrodynamic models, this effect is captured only partially by these models due to the model inherent approximations. A direct consequence of the failure of the DD approximation is that the usual method for inversion layer mobility extraction from measurements in the linear regime becomes inaccurate for short gate lengths and the extracted mobilities might be too small. This error has also an impact on the modeling accuracy at strong nonequilibrium. In the case of the DD model, the overestimation of the conductivity in the linear regime can partly compensate the underestimation of the current at high bias, and the model accidentally appears to be more accurate than expected.**

***Index Terms*—Boltzmann equation (BE), drift-diffusion (DD), equilibrium, hydrodynamic, small-signal.**

I. Introduction

THE shrinking of the device dimensions below 100 nm is pushing the classical TCAD tools like the drift-diffusion (DD) or hydrodynamic (HD) models to their limits. While the impact of the shrinking on the accuracy of the classical simulators has been investigated extensively for strong nonequilibrium (e.g., [1]–[3]), this is not the case for linear transport. In [4] it has been shown that even under equilibrium conditions device results of the moments-based models might deviate from the exact solution of the Boltzmann equation (BE) due to built-in fields. This phenomenon is especially pronounced in nanoscale devices because of the small feature size and steep junctions, which result in huge built-in fields. This failure of the macroscopic transport models is explained in this work for the first time based on a thorough theoretical discussion and the accuracy of the DD and HD models near equilibrium is assessed for nanoscale devices.

II. Theory

For the sake of brevity only the stationary nondegenerate unipolar 1-D case for electrons in relaxed silicon is discussed in this section and generation/recombination processes are neglected. Electron transport is described with the model developed by the Modena group [5], which is based on an analytical nonparabolic band structure with six elliptical valleys. Impurity scattering is modeled by a modified Brooks–Herring transition rate [6]. The BE is given in this case by

$$-qE(x)\frac{\partial f^\nu(x,\vec{k})}{\partial \hbar k_x}+v_x^\nu(\vec{k})\frac{\partial f^\nu(x,\vec{k})}{\partial x} = \frac{\Omega}{(2\pi)^3}\sum_{\nu'=1}^{6}\int W^{\nu,\nu'}(x;\vec{k}|\vec{k}')f^{\nu'}(x,\vec{k}') - W^{\nu',\nu}(x;\vec{k}'|\vec{k})f^\nu(x,\vec{k})d^3k' \quad (1)$$

where q is the positive electron charge, $E=-\partial\Psi/\partial x$ the electric field in x direction, Ψ the electrostatic potential, $\hbar$ Planck's constant divided by 2π, x the x coordinate in real space, $\vec{k}$ the wave vector relative to the center of the νth valley, $f^\nu(x,\vec{k})$ the distribution function, $v_x^\nu(\vec{k})$ the group velocity in x direction, Ω the system volume, and $W^{\nu',\nu}(x;\vec{k}'|\vec{k})$ the transition rate [7].

Balance equations are obtained by multiplication of the BE with a microscopic quantity $X^\nu(\vec{k})$ and integration over $\vec{k}$-space [6], [8]

$$n\left\langle\frac{\partial qX}{\partial\hbar k_x}\right\rangle E+\frac{\partial n\langle Xv_x\rangle}{\partial x}-n\left\langle v_x\frac{\partial X}{\partial x}\right\rangle=-n\left\langle\hat{S}\{X\}\right\rangle \quad (2)$$

with

$$n\langle X\rangle=\frac{2}{(2\pi)^3}\sum_{\nu=1}^{6}\int X^\nu(\vec{k})f^\nu(x,\vec{k})d^3k \quad (3)$$

where n is the particle density and the scattering term is given by

$$\hat{S}\{X\}=\frac{\Omega}{(2\pi)^3}\sum_{\nu'=1}^{6}\int W^{\nu',\nu}(x,\vec{k}'|\vec{k})\left[X^\nu(\vec{k})-X^{\nu'}(\vec{k}')\right]d^3k'. \quad (4)$$

Balance equations for the particle and current densities can be derived from the BE without any approximations [6], [8]. The continuity equation is obtained with $X=1$

$$\frac{\partial j}{\partial x}=0 \quad (5)$$

where $j=n\langle v_x\rangle$ is the particle current density in x direction. $X=\tau v_x$ yields the constitutive equation of the current density [8]

$$j=-n\mu E-D\frac{\partial n}{\partial x}-n\left(\frac{\partial D}{\partial x}-F\right) \quad (6)$$

Manuscript received April 25, 2005. The review of this paper was arranged by Editor C. McAndrew.

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Digital Object Identifier 10.1109/TED.2005.857184

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where the scattering term is solved exactly due to the definition of the microscopic relaxation time $\tau^{\nu}(\vec{k})$ [8], [9]

$$\hat{S}\{\tau v_x\} = v_x. \tag{7}$$

The mobility reads in this case [6], [10]

$$\mu = \left\langle \frac{\partial q \tau v_x}{\partial \hbar k_x} \right\rangle \tag{8}$$

the diffusion coefficient

$$D = \left\langle \tau v_x^2 \right\rangle \tag{9}$$

and

$$F = \left\langle \frac{\partial \tau}{\partial x} v_x^2 \right\rangle. \tag{10}$$

Since (6) is derived from the BE without any approximations, it is exact. However, it cannot be used without the full solution of the BE, because the transport parameters depend on the distribution function, which in general can be obtained only by solving the BE. In order to use (6) in a macroscopic transport model, approximations are required (e.g., [8], [11]), which will not be discussed.

With the particle gas temperature T^{BE} defined by a generalized Einstein relation

$$D = \mu U^{\mathrm{BE}} = \mu \frac{k_{\mathrm{B}} T^{\mathrm{BE}}}{q} \tag{11}$$

(6) can be brought into a form more appropriate for the discussion of macroscopic transport models

$$j = -n\mu \left[E + \frac{U^{\mathrm{BE}}}{n} \frac{\partial n}{\partial x} + \frac{\partial U^{\mathrm{BE}}}{\partial x} + K \right] \tag{12}$$

where K is an abbreviation for

$$K = \frac{1}{\mu} \left(U^{\mathrm{BE}} \frac{\partial \mu}{\partial x} - F \right). \tag{13}$$

The first term in the square brackets on the RHS of (12), the electric field, is the force of the drift current, the second term drives particle diffusion, the third term results in thermodiffusion, and the last term covers all other diffusion forces neglected in most macroscopic models.

By introducing the quasi-Fermi potential Φ with a nonlinear transformation [12]

$$n = n_i \exp\left(\frac{\Psi - \Phi}{U^{\mathrm{BE}}} \right) \tag{14}$$

where n_i denotes the intrinsic particle concentration, (12) can be rearranged to

$$j = n\mu \left[\frac{\partial \Phi}{\partial x} + \frac{\Psi - \Phi - U^{\mathrm{BE}}}{U^{\mathrm{BE}}} \frac{\partial U^{\mathrm{BE}}}{\partial x} - K \right] \tag{15}$$

where all terms in the square brackets vanish for equilibrium.

In order to investigate ohmic transport, (5) and (15) are linearized around equilibrium resulting in

$$\frac{\partial \delta j}{\partial x} = 0 \tag{16}$$

and

$$\delta j = n_0 \mu_0 \left[\frac{\partial \delta \Phi}{\partial x} + \frac{\Psi_0 - \Phi_0 - U_0}{U_0} \frac{\partial \delta U^{\mathrm{BE}}}{\partial x} - \delta K \right]. \tag{17}$$

The subscript $_0$ denotes an equilibrium quantity and δ a small-signal variable (i.e., the linear deviation from the equilibrium value).

First, the case of the DD approximation is discussed, for which the term in the square brackets of (17) is approximated by

$$\frac{\partial \delta \Phi}{\partial x} + \frac{\Psi_0 - \Phi_0 - U_0}{U_0} \frac{\partial \delta U^{\mathrm{BE}}}{\partial x} - \delta K \approx \frac{\partial \delta \Phi}{\partial x} \tag{18}$$

and

$$\delta j = n_0 \mu_0 \frac{\partial \delta \Phi}{\partial x} \tag{19}$$

due to the assumption that the electron distribution function is given by the equilibrium distribution [13]. Division of (19) by $n_0\mu_0$ and integration over real space yields together with (16)

$$\begin{aligned} \int_0^L \frac{\delta j}{n_0 \mu_0} dx &= \delta I \int_0^L \frac{1}{q A n_0 \mu_0} dx \\ &= \int_0^L \frac{\partial \delta \Phi}{\partial x} dx \\ &= \delta \Phi(L) - \delta \Phi(0) \\ &= \delta V \end{aligned} \tag{20}$$

where L is the length of the one–dimensional (1-D) structure, A its cross section, δV the small-signal terminal bias, and $\delta I = qA\delta j$ the terminal current. The resultant DD conductance at equilibrium is given by the well-known result

$$\frac{\delta I}{\delta V} = \frac{\partial I}{\partial V} = G_0^{\mathrm{DD}} = \frac{qA}{\int_0^L \frac{1}{n_0 \mu_0} dx}. \tag{21}$$

In the same way the conductance can be calculated based on the BE and all terms on the RHS of (17) are considered

$$\frac{\delta I}{G_0^{\mathrm{DD}}} = \int_0^L \left(\frac{\partial \delta \Phi}{\partial x} + \frac{\Psi_0 - \Phi_0 - U_0}{U_0} \frac{\partial \delta U^{\mathrm{BE}}}{\partial x} - \delta K \right) dx. \tag{22}$$

Rearrangement of the RHS and integration by parts yields

$$\frac{G_0^{\mathrm{BE}}}{G_0^{\mathrm{DD}}} = 1 + \int_0^L \left(\frac{1}{U_0} \frac{\partial U^{\mathrm{BE}}}{\partial V} E_0 - \frac{\partial K}{\partial V} \right) dx \tag{23}$$

where it has been assumed that the electron temperature is given at the contacts by the lattice temperature in accordance with the usual boundary conditions. The second summand under the integral is rather small and vanishes exactly for highly doped contacts and a position-independent microscopic relaxation time. This means that only particle drift and diffusion have an impact on the conductance at equilibrium, whereas the other diffusion forces including thermodiffusion are negligible. There-

fore, the small-signal conductance derived from the BE reads at equilibrium

$$\frac{G_0^{\mathrm{BE}}}{G_0^{\mathrm{DD}}} \approx 1 + \int_0^L \frac{1}{T_0}\frac{\partial T^{\mathrm{BE}}}{\partial V} E_0 dx. \tag{24}$$

Thus, the difference in the conductances is proportional to the strength of the electric field at zero bias (i.e., built-in fields).

The integral on the RHS of (24) yields negative values, because the source of a change in the particle gas temperature is the Joule term [14], which is proportional to the electric field, and a positive electric field leads to a decrease in temperature for current flow in the negative x direction caused by a positive voltage applied to the RHS terminal of the 1-D device. Thus, in the case of nonzero built-in fields the conductance at equilibrium calculated with the BE is smaller than the DD result.

A similar effect is found in the case of HD models. This is shown for the generalized HD model published in [15]. The Einstein relation of this HD model reads

$$D = \mu\frac{m^*}{m_0^*}U^{\mathrm{HD}} = \mu\frac{m^*}{m_0^*}\frac{k_{\mathrm{B}}T^{\mathrm{HD}}}{q} \tag{25}$$

where

$$T^{\mathrm{HD}} = \frac{m_0^*}{3k_{\mathrm{B}}}\langle \vec{v}^2 \rangle \tag{26}$$

is the dynamic temperature and $1/m^*$ the trace of the expectation of the inverse mass tensor divided by three. The diffusion term of (6) is approximated by

$$\frac{\partial nD}{\partial x} - nF \approx n\mu\frac{m^*}{m_0^*}\left(\frac{U^{\mathrm{HD}}}{n}\frac{\partial n}{\partial x} + \frac{\partial U^{\mathrm{HD}}}{\partial x}\right). \tag{27}$$

This yields for the conductance

$$\frac{G_0^{\mathrm{HD}}}{G_0^{\mathrm{DD}}} = 1 + \int_0^L \left(1 + \frac{T_0}{m_0^*}\frac{\partial m^*}{\partial T^{\mathrm{HD}}}\right)\frac{1}{T_0}\frac{\partial T^{\mathrm{HD}}}{\partial V} E_0 dx. \tag{28}$$

Similar to the case of the BE, thermodiffusion has no impact on the conductivity at equilibrium. For the analytical band structure given in [5] the factor in the brackets in (28) is close to one and (28) can be approximated as

$$\frac{G_0^{\mathrm{HD}}}{G_0^{\mathrm{DD}}} \approx 1 + \int_0^L \frac{1}{T_0}\frac{\partial T^{\mathrm{HD}}}{\partial V} E_0 dx. \tag{29}$$

Although (24) and (29) look similar, they do not give the same result, because they are based on very different definitions of the temperature (26), (11) and the temperatures are calculated in very different ways. While (11) is evaluated based on the full solution of the BE, (26) is the result of the less accurate HD model. Only at equilibrium both temperatures are equal and given by the lattice temperature.

III. Results

Under homogeneous bulk conditions and in the case of the 1-D N^+NN^+-structure the BE is solved by a newly developed spherical harmonics solver, where the spherical harmonics expansion is truncated at an order for which the errors in the quantities of interest are negligible. The spherical harmonics expansion has the advantage over the Monte Carlo method that the small-signal analysis can be performed without excessive CPU times [16]. In the case of the 2-D double gate (DG)-NMOSFET the Monte Carlo method is used to solve the BE [6]. The transport parameters of the drift-diffusion (DD) and hydrodynamic models are calculated under homogeneous bulk conditions based on full solutions of the BE and parameterized with the driving force and electron temperature, respectively [15].

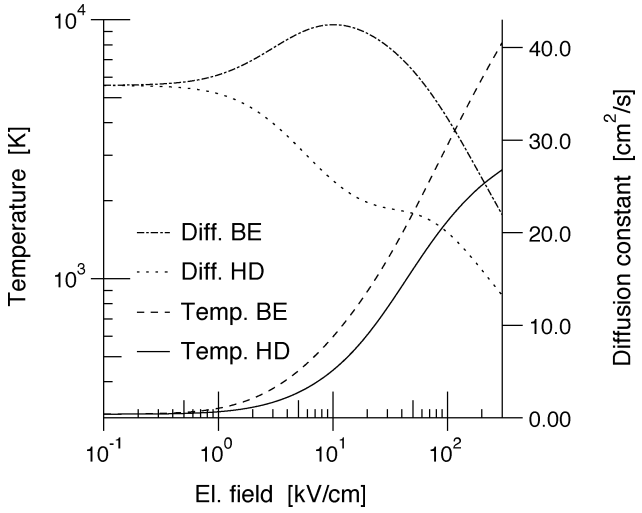

Fig. 1. Electron gas temperatures T^{BE}, T^{HD}, and longitudinal diffusion coefficients for bulk silicon doped with $10^{15}/\mathrm{cm}^3$ at room temperature.

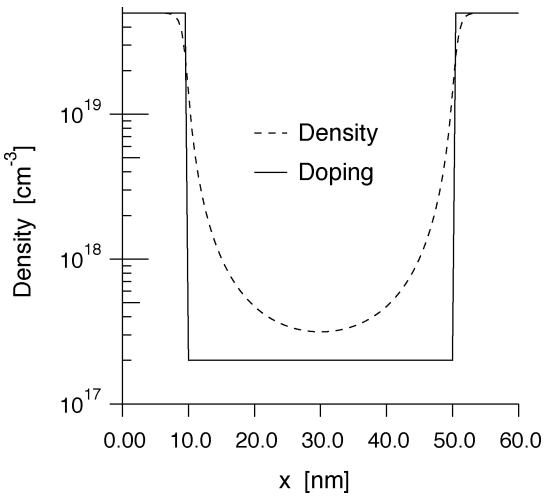

Fig. 2. Donor concentration and electron density at zero bias for the 40 nm N^+NN^+-structure.

The two temperatures T^{BE} and T^{HD} are shown in Fig. 1 for lowly doped bulk silicon and T^{BE} is always larger than T^{HD}. This means that the exact diffusion coefficient of the BE is much larger than the one of the HD model at high driving fields.

An N^+NN^+-structure with an N-region of 40 nm, which is doped with $2\cdot 10^{17}/\mathrm{cm}^3$ and to which at both ends 10-nm-long regions with a doping of $5\cdot 10^{19}/\mathrm{cm}^3$ are attached (Fig. 2), has been simulated with the DD, HD, and BE models. Due to the inhomogeneous doping, built-in fields form (Fig. 3) and a linear response of the temperature to the applied bias is observed. This

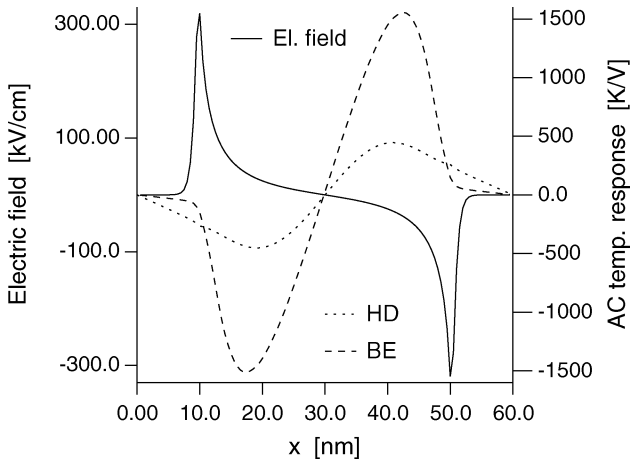

Fig. 3. Electric field and small-signal response of the temperature $(\partial T/\partial V)$ for the 40 nm N^+NN^+-structure at zero bias.

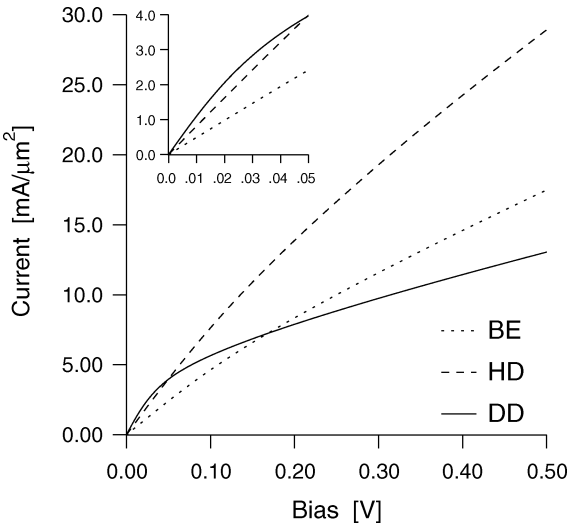

Fig. 4. Terminal current versus bias for the 40-nm N^+NN^+-structure at room temperature.

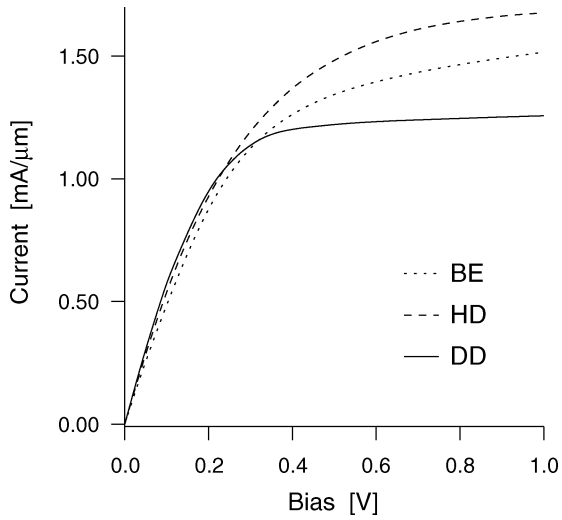

Fig. 5. Drain current of a 50-nm DG-NMOSFET for a gate bias of 1.0 V and room temperature.

is only possible in the case of built-in fields. Without built-in fields the temperature near equilibrium grows quadratically with bias and the conductance is the same for the DD, HD, and BE models. The value of the conductance at equilibrium relative to the DD model is for the HD case 72.4% and the BE 44.9%. The large differences between the HD and BE results are caused by the weaker response of the HD temperature (Fig. 3). This weaker response of the HD temperature is not only due to the definition of the temperature, but also due to the HD approximation. Simply changing the definition of the temperature is not sufficient to solve this problem. In HD models the temperature is the result of a second order differential equation [17], and the HD temperature is therefore smoother than the result of the BE. This leads to problems at steep junctions [18] and the linear temperature response of the HD model has a much smaller second derivative with respect to position at the junctions than the BE result (Fig. 3). Another reason for the failure of the HD approximation is that the distribution function strongly deviates from a drifted and heated Maxwellian [11], [19]. This is already the case in the linear regime. While under homogeneous bulk conditions the linear response of the electron distribution function near equilibrium can be described exactly by a spherical harmonics expansion up to the first order [9], this is no longer possible in a device with large built-in fields. In this case an expansion up to much higher orders is required and for the 40-nm N^+NN^+-structure a ninth order expansion was used. Consequently, the calculation of the HD transport parameters under homogeneous bulk conditions and parameterization solely with the temperature fails in such devices.

This effect has also a strong impact on nonequilibrium transport. In Fig. 4 the current–voltage (*I–V*) curve for the N^+NN^+-structure is shown. At small bias the DD model yields the largest current. Above 49 mV the HD current is the largest and above 173 mV the DD result is the smallest. The overestimated conductance at zero bias is the reason why the overall accuracy of the DD model appears to be better than the HD model. A similar behavior is found in the case of a 50-nm DG-MOSFET (Fig. 5) [3], where the surface mobility models of the particle and moments-based simulators were turned off because of differences in their formulation.

These results show that it might not be advisable to extract parameters of a surface scattering model by matching DD simulations to measurements of nanoscale devices in the linear regime (e.g., [20]), because the failure of the DD approximation in these devices might lead to a systematic bias in the results. By the same token inverse modeling based on the DD model in the linear regime might yield erroneous results. Even the usual methods for inversion layer mobility extraction from measurements are becoming critical for short channel MOSFETs, because the analytical formulas used to relate the mobility and drain current in the linear regime are based on the DD approximation (e.g., [21]).

IV. Conclusion

We have shown that the conductance of nanoscale devices depends at zero bias strongly on the choice of the transport model. This is due to the differences in the modeling of the diffusion term and nonlocal transport due to the built-in fields. It turns

out that part of the error in the terminal current due to the DD approximation at high bias is compensated by the overestimation at low bias. The overall accuracy of the DD approximation for the terminal current is therefore accidentally better than expected. Nevertheless, the application of the DD model in the linear regime, as often done during inverse modeling or in compact models, appears to be problematic for such devices.

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