Failure of Macroscopic Transport Models in Nanoscale Devices near Equilibrium

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ABSTRACT

It is shown that the conductance in nanoscale devices depends already at equilibrium strongly 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 transport equation (BTE). This effect is captured only partially by hydrodynamic (HD) models, because the longitudinal diffusion constant of those models is usually smaller than the one of the BTE. Since the macroscopic models overestimate the conductivity near equilibrium, the DD and HD approximations might not be sufficiently accurate for reverse engineering or compact modeling of nanoscale devices in the linear regime.

Keywords: drift-diffusion, hydrodynamic, Boltzmann transport equation, small-signal, equilibrium

1 Introduction

The shrinking of the device dimensions below 100 nm is pushing the classical TCAD tools like the DD or 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 Ref. [4] it is shown that even under equilibrium conditions device results of the momentum-based models might deviate from the exact solution of the BTE due to built–in fields. This phenomenon is especially strong in nanoscale devices because of the small feature size and huge built–in fields. The impact of this effect on the accuracy of the DD and HD models is investigated for the first time in this work for nanoscale devices.

2 Theory

The balance equations of the particle and current densities can be derived from the Boltzmann transport equation **without** any approximations [5, 6]. For the sake of brevity only the stationary nondegenerate unipolar 1D case for electrons in silicon is discussed and generation/recombination processes are neglected. The continuity equation reads in this case

$$\frac{\partial j}{\partial x} = 0 \ , \tag{1}$$

where j is the particle current density in x-direction. The constitutive equation of the current density is given by

$$j = -n\mu E - D\frac{\partial n}{\partial x} - n\left(\frac{\partial D}{\partial x} - F\right) \ . \tag{2}$$

n is the particle density, $E = -\partial\Psi/\partial x$ the electric field, and Ψ the electrostatic potential. The transport parameters are expectations of the distribution function in k-space. The mobility reads: $\mu = q\langle\partial\tau v_x/\partial\hbar k_x\rangle$, the diffusion constant: $D = \langle\tau v_x^2\rangle$, and $F = \langle v_x^2\partial\tau/\partial x\rangle$, where τ is the microscopic relaxation time, $\hbar k_x$ the quasi-momentum, and v_x the group velocity in x-direction [6–8].

The quasi-Fermi potential Φ is obtained by a nonlinear transformation: $n = n_i \exp\left((\Psi-\Phi)/U^{\mathrm{BTE}}\right)$, where n_i denotes the intrinsic particle concentration, $U^{\mathrm{BTE}} = k_{\mathrm{B}}T^{\mathrm{BTE}}/q$ the thermal voltage, and T^{BTE} the particle gas temperature, which is defined by the Einstein relation $U^{\mathrm{BTE}} = D/\mu$. Eq. (2) now reads

$$j = n\mu\left[\frac{\partial\Phi}{\partial x} + \frac{\Psi-\Phi}{U^{\mathrm{BTE}}}\frac{\partial U^{\mathrm{BTE}}}{\partial x} - \frac{1}{\mu}\left(\frac{\partial D}{\partial x} - F\right)\right] \ , \tag{3}$$

where all three terms in the square brackets vanish for equilibrium. In order to investigate ohmic transport, Eqs. (1) and (3) are linearized for equilibrium resulting in

$$\frac{\partial\delta j}{\partial x} = 0 \ , \tag{4}$$

and

$$\delta j = n_0\mu_0\left[\frac{\partial\delta\Phi}{\partial x} + \frac{\Psi_0-\Phi_0}{U_0}\frac{\partial\delta U^{\mathrm{BTE}}}{\partial x} - \frac{1}{\mu_0}\left(\frac{\partial\delta D}{\partial x} - \delta F\right)\right] \ . \tag{5}$$

The subscript $_0$ denotes an equilibrium quantity and δ a small-signal variable. Due to Eq. (4) the current density

is position independent and

$$\int_0^L \frac{\delta j \mathrm{d}x}{n_0\mu_0} = qA\delta j \int_0^L \frac{\mathrm{d}x}{qAn_0\mu_0} = \frac{\delta I}{G_0^{\mathrm{DD}}} =$$

$$\int_0^L \frac{\partial \delta\Phi}{\partial x} + \frac{\Psi_0 - \Phi_0}{U_0}\frac{\partial \delta U^{\mathrm{BTE}}}{\partial x} - \frac{1}{\mu_0}\left(\frac{\partial \delta D}{\partial x} - \delta F\right)\mathrm{d}x \ , \tag{6}$$

with L being the length of the 1D device, A its cross section, $\delta I = qA\delta j$ the terminal current, and $G_0^{\mathrm{DD}} = qA/\int_0^L \mathrm{d}x/n_0\mu_0$ the small-signal conductance at equilibrium based on the DD approximation.

The integral over the first term on the RHS yields $\int_0^L \partial\delta\Phi/\partial x \mathrm{d}x = \delta\Phi(L) - \delta\Phi(0) = \delta V$, where δV is the small-signal terminal bias. Rearrangement of the RHS (e.g. $\delta U^{\mathrm{BTE}}/\delta V = \partial U^{\mathrm{BTE}}/\partial V$) and integration by parts yields

$$\frac{\delta I}{G_0^{\mathrm{DD}}} =$$

$$\left(1 + \int_0^L \frac{1}{U_0}\frac{\partial U^{\mathrm{BTE}}}{\partial V}E_0 - \frac{1}{\mu_0}\left(\frac{\partial^2 D}{\partial V \partial x} - \frac{\partial F}{\partial V}\right)\mathrm{d}x\right)\delta V$$

$$\approx \left(1 + \int_0^L \frac{1}{U_0}\frac{\partial U^{\mathrm{BTE}}}{\partial V}E_0 \mathrm{d}x\right)\delta V \ , \tag{7}$$

where the approximation holds exactly for highly doped contacts and a position-independent microscopic relaxation time. The small-signal conductance derived from the BTE reads therefore at equilibrium

$$\frac{G_0^{\mathrm{BTE}}}{G_0^{\mathrm{DD}}} \approx 1 + \int_0^L \frac{1}{T_0}\frac{\partial T^{\mathrm{BTE}}}{\partial V}E_0 \mathrm{d}x \ . \tag{8}$$

The integral yields negative values, because the source of a change in the particle gas temperature is the Joule term, which is proportional to the electric field and a positive electric fields leads to a decrease in temperature for current flow in the positive x-direction. Thus, in the case of nonzero built-in fields the conductance at equilibrium calculated with the BTE is smaller than the DD result.

A similar effect is found in the case of HD models. The Einstein relation of the generalized HD model reads $D = \mu f U^{\mathrm{HD}}$, where $T^{\mathrm{HD}} = qU^{\mathrm{HD}}/k_{\mathrm{B}}$ is the dynamic temperature and $f = \tau_j/\tau_j^*$ [9]. The diffusion term of Eq. (2) is approximated by

$$D\frac{\partial n}{\partial x} + n\left(\frac{\partial D}{\partial x} - F\right) \approx \mu f \frac{\partial n U^{\mathrm{HD}}}{\partial x} \ . \tag{9}$$

This yields for the conductance

$$\frac{G_0^{\mathrm{HD}}}{G_0^{\mathrm{DD}}} = 1 + \int_0^L \left(1 + T_0\frac{\partial f}{\partial T^{\mathrm{HD}}}\right)\frac{1}{T_0}\frac{\partial T^{\mathrm{HD}}}{\partial V}E_0 \mathrm{d}x$$

$$\approx 1 + \int_0^L \frac{1}{T_0}\frac{\partial T^{\mathrm{HD}}}{\partial V}E_0 \mathrm{d}x \ , \tag{10}$$

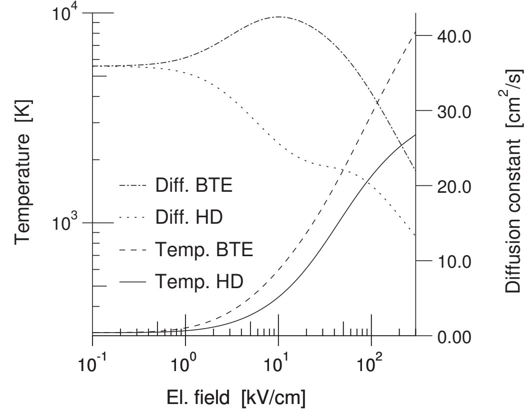

Figure 1: Electron gas temperatures T^{BTE}, T^{HD} and longitudinal diffusion constants for bulk silicon with a donor concentration of $10^{15}/\mathrm{cm}^3$ at room temperature.

where the approximation holds due to $T_0\partial f/\partial T^{\mathrm{HD}} \ll 1$ for the HD model.

Although Eqs. (8) and (10) look similar, they do not yield the same results, because they are based on very different definitions of the temperature

$$T^{\mathrm{HD}} = \frac{m^*}{3k_{\mathrm{B}}}\langle v^2\rangle \ , \tag{11}$$

$$T^{\mathrm{BTE}} = \frac{qD}{k_{\mathrm{B}}\mu} \ , \tag{12}$$

where $1/m^*$ is the expected value of the inverse mass at equilibrium [9]. Both definitions yield at equilibrium the lattice temperature. In the case of the BTE the temperature is defined by the Einstein relation, whereas in the HD case the Einstein relation is used to calculated the diffusion constant for a given dynamic temperature. Therefore, the diffusion constants of the BTE and HD models differ.

3 Results

The two temperatures $T^{\mathrm{BTE}}, T^{\mathrm{HD}}$ are shown in Fig. 1 for lowly doped bulk silicon based on the electron model of Ref. [10] and T^{BTE} is always larger than T^{HD}. This means that the exact diffusion constant of the BTE is much larger than the one of the HD model at high driving fields. Consequently, one can expect that $\partial T^{\mathrm{BTE}}/\partial V$ will be larger than $\partial T^{\mathrm{HD}}/\partial V$ and $G_0^{\mathrm{BTE}} < G_0^{\mathrm{HD}} < G_0^{\mathrm{DD}}$.

In Fig. 2 the electron density and mobility at zero bias is shown for a Si N^+NN^+-structure, where the N-region is 400 nm long and doped with $2\times10^{15}/\mathrm{cm}^3$. At both ends of the N-region 100 nm long regions with a doping of $5\times10^{17}/\mathrm{cm}^3$ are attached. Due to the inhomogeneous doping built-in fields form (Fig. 3) and a linear response of the temperature with the applied bias is observed. This is only possible in the case of built-in fields. Otherwise the response at equilibrium would

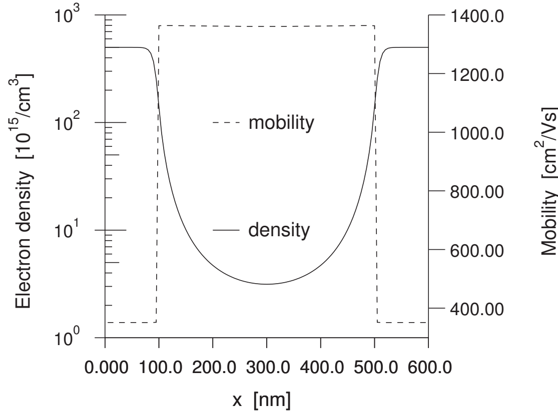

Figure 2: Electron density and mobility for the 400 nm Si N^+NN^+-structure at zero bias and room temperature.

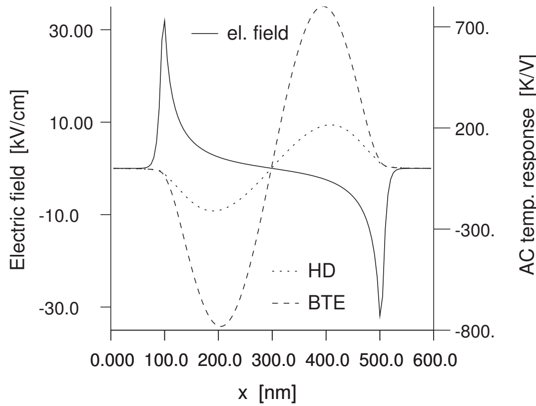

Figure 3: Electric field and small-signal response of the temperature $(\partial T/\partial V)$ for the device shown in Fig. 2 at zero bias.

be quadratic with bias and the conductance would be the same for the DD, HD, and BTE models. The value of the conductance at equilibrium relative to the DD model is for the HD case 92.8% and the BTE 80.0%. The large differences between the HD and BTE results are due to the weaker response of the HD temperature (Fig. 3). These differences increase in smaller devices. If the length of the N^+NN^+-structure is reduced by a factor of 10 and the doping increased by 100, G_0^{HD} is 71% of G_0^{DD} and G_0^{BTE} only 43%. This effect has also a strong impact on the nonequilibrium transport. In Fig. 4 the I-V curve for the scaled N^+NN^+-structure with a 40 nm long lowly doped region is shown. The crossover of the DD and HD currents is at 49 mV and BTE and DD at 173 mV. The overestimated conductance at zero bias is the reason why the overall accuracy of the DD model compared to BTE 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

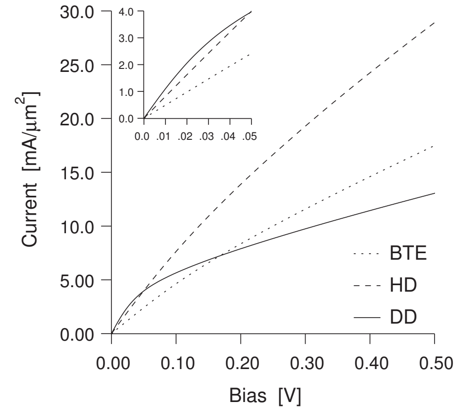

Figure 4: Terminal current versus bias for the 40 nm N^+NN^+-structure at room temperature.

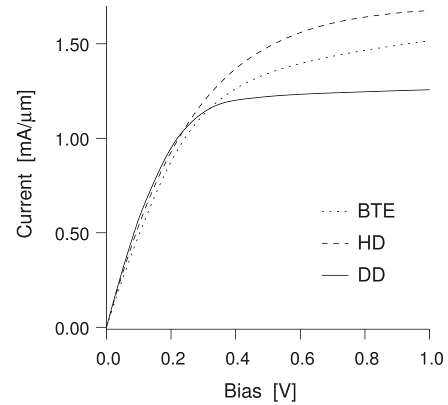

Figure 5: Drain current of a 50 nm DG-NMOSFET for a gate bias of 1.0V and room temperature.

the surface mobility models were turned off because of differences in their formulation.

4 Conclusions

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 definition of the temperature and the corresponding Einstein relation. 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 (e.g. inverse modeling, compact models) appears to be problematic for such devices.

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