Exact and moment equation modeling of electron transport in submicron structures

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We compare I - V characteristics of a semiconducting submicron n^+nn^+ diode as predicted by extended moment equation approximations to those obtained from the solution of the corresponding Boltzmann equation. All lower order models fail in the predominantly ballistic regime. Moreover, the conductance is inadequately predicted by these models, even in nonballistic cases due to the high build-in electric fields.

The ongoing size reduction of semiconductor devices prompts the need for descriptions extending the drift-diffusion approach.¹ We compare I - V characteristics of semiconducting submicron structures obtained from a systematic hierarchy of extended moment equations to those predicted by the corresponding Boltzmann equation.² Transport of electrons in such structures is characterized by both hot and ballistic electrons as well as large gradients in e.g., the electron density and the electric field.³⁻⁵ Further reduction of typical sizes and the use of high-mobility materials cause these effects to become even more pronounced. We study a GaAs-based n^+nn^+ diode numerically and show that all lower order moment models give inadequate predictions of e.g., the diode conductance, particularly in the ballistic regime. For precise results one has to resort to solving the full Boltzmann equation, either by the method of characteristics^{5,6} or through direct Monte Carlo simulations.⁷ Increasing the truncation order of the moment models does not lead to a significant extension of the parameter region in which these models can be usefully applied. *It is not possible to treat ballistic transport phenomena with a low order system of moment equations.*

First, we introduce the systematic hierarchy of moment models and describe the procedure to obtain the closing relations.^{3,4} Then the predicted I - V characteristics are compared with the Boltzmann equation results as a function of what we call the "ballisticity" in the system. We define this quantity as $B \equiv (\tau v_{d,\max})/d$, where τ is the relaxation time of the collision process, $v_{d,\max}$ the maximal drift velocity, as predicted by the moment models, in the diode, and d the width of the n region in the diode.

The stationary Boltzmann equation governs the electron distribution function $f(r, v)$ and in one spatial and velocity dimension reads⁵

$$[v\partial_r - E(r)\partial_v] f(r, v) = -\frac{1}{\tau} [f(r, v) - f_0(r, v)], \quad (1)$$

where we adopt the parabolic band approximation and assume a constant relaxation time approximation for the collision term. We use scaled variables; position r and velocity

v are measured in units r_0 (the Debye length) and v_0 (the thermal velocity), respectively, where

$$r_0 = \left(\frac{\epsilon k_B T_0}{e^2 M_{\text{ref}}} \right)^{1/2}; \quad m^* v_0^2 = k_B T_0 \quad (2)$$

in which k_B is Boltzmann's constant, T_0 the lattice temperature, ϵ the permittivity, e the unit of charge, m^* the effective mass, and M_{ref} a reference particle density in the system. f_0 is the distribution function describing local equilibrium, and both f and f_0 are in units M_{ref}/v_0 . The electric field E is measured in units $E_0 \equiv (m^* v_0^2)/(e r_0)$, and is determined by Poisson's equation which can be expressed in the above notation as:

$$\partial_r \Psi(r) = M_0(r) - C(r); \quad E = -\partial_r \Psi, \quad (3)$$

where $C(r)$ describes the doping profile and M_0 the particle density, in units M_{ref} . An n^+nn^+ diode is represented by a doping profile $C(r) = C_-$ in the n region and $C_+ (=M_{\text{ref}})$ in the n^+ regions (typically $C_- \ll C_+$).

Physically relevant information is usually expressed in terms of velocity moments of the distribution function; the m th moment M_m is defined as $M_m \equiv \langle v^m \rangle$. The set of moments $\{M_m(r)\}$ obeys

$$d_r M_{m+1} + m E M_m = -\frac{1}{\tau} \{M_m - M_{m,0}\}. \quad (4)$$

We use the local equilibrium distribution

$$f_0(r, v) \equiv \frac{M_0(r)}{\sqrt{2\pi}} \exp\left(-\frac{v^2}{2}\right) \quad (5)$$

for which the reference moments $\{M_{m,0}\}$ can readily be evaluated. The evolution of the m th moment is governed in part by the spatial derivative of the $(m+1)$ th moment. A closing relation must be postulated expressing a higher order moment in terms of lower order moments thus rendering the Eqs. (4) finite and open for numerical treatment.

A systematic class of closing relations is generated by truncating an expansion of the distribution function f . Consider the following expansion of f :^{2,4}

$$f(r, v) = \frac{e^{-\xi^2/2}}{\sqrt{2\pi}} \sum_{j=0}^{\infty} f_j(r) \text{he}_j(\xi), \quad (6)$$

where $\{\text{he}_j\}$ are Hermite polynomials and $\xi \equiv (v - v_1(r))/v_2(r)$. Thus, we expand f around a "Max-

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FIG. 1. Comparison of I - V characteristics as predicted by the Boltzmann equation (full lines), drift diffusion (dotted lines), and four moment model (dashed lines) for a structure with a total length of 4.4×10^{-6} m and a width of the n region of 0.4×10^{-6} m. Results are shown for $\tau = 5 \times 10^{-14}$ s (case a); $\tau = 1 \times 10^{-13}$ s (case b); $\tau = 2.9 \times 10^{-13}$ s (case c) and $\tau = 5 \times 10^{-13}$ s (case d). We used a lattice temperature $T_0 = 300$ K, a permittivity $\epsilon_r = 12.5$, and an effective mass $m^* = 0.069 m_e$ (m_e the electron rest mass). Finally, we used doping parameters $C_+ = 10^{24} \text{ m}^{-3}$ and $C_- = 2 \times 10^{21} \text{ m}^{-3}$.

wellian" distribution with the option to include a suitably transformed velocity, viz. the introduction of v_1 and v_2 . With a judicious choice of v_1 and v_2 the expansion functions f_1 and/or f_2 can be made zero and the accuracy of a truncating approximant to f improved without increasing the truncation order. The expansion functions $\{f_j(r)\}$ can be expressed as linear combinations of the moments $\{M_m\}$; $m = 0, 1, \dots, j$ and the functions v_1 and v_2 . Hence, truncating this expansion at order n by putting $f_n = 0$ renders a closing relation between M_n and $\{M_j\}$; $j = 0, 1, \dots, n-1$. We consider moment models with order $n = 4$.

Putting $v_1 = 0$ and $v_2 = 1$ implies expanding f around a pure Maxwellian distribution and results in the linear closing relation $M_4 = 6M_2 - 3M_0$. Taking $v_1 = M_1/M_0$ renders $f_1 = 0$ and corresponds to an expansion of f around a "drifted Maxwellian," where the velocity is corrected with the drift velocity of the electrons. The closing relation is now nonlinear and can be written as

$$M_4 = 4v_1M_3 + 6(v_2^2 - v_1^2)M_2 - 3[2v_2^4 - (v_2^2 - v_1^2)^2]M_0. \quad (7)$$

The function v_2 can in addition be used to render $f_2 = 0$ by taking v_2 equal to the root of the electron temperature relative to the lattice temperature. This corresponds to expanding f around a "scaled and drifted Maxwellian," i.e., the velocity is corrected with the drift velocity and scaled with the local temperature. In case $n = 2$, corresponding to the drift-diffusion model, expansion around a pure Maxwellian yields $M_2 = M_0$ whereas an expansion around a drifted Maxwellian gives the nonlinear closing relation $M_2 = (v_1^2 + 1)M_0$.

In Fig. 1 we show the I - V characteristics of the moment models and the corresponding Boltzmann equation results for a typical n^+nn^+ -diode. Results are shown for

FIG. 2. Plot of I_B/I_m as a function of the "ballisticity" parameter B for the same parameters as in Fig. 1. Here case (b) is represented by "diamonds"; case (c) by "plusses" and case (d) by "crosses". At each τ value two curves are shown; the lower presents the drift-diffusion results and the upper corresponds to the four moment results.

the drift diffusion and four moment models with linear closing relations; see also Ref. 2. In regions where τ is small, i.e., in the nonballistic regime, all models give almost equally good results for the current as well as for the conductance of the diode, whereas in strong ballistic situations all models yield diode conductances and currents that deviate considerably from the Boltzmann results. Increasing the truncation order from two (drift diffusion) to four extends the τ region in which the deviations are less than (say) 10%. However, the conductance in the strongly ballistic regime is never adequately calculated from the moment equations. The I - V predictions of the "linear" and "nonlinear" moment models turn out to agree quite well with each other in the entire parameter region studied and hence the later results are not shown here. The hydrodynamic model⁸ was also studied. It gives adequate results for relatively low relaxation times and applied voltages. At higher relaxation times it fails to give any predictions due to instabilities related to drift velocity approaching the thermal velocity.^{9,10}

In order to further elucidate the effects of the "ballisticity" (B) in the structure we have plotted the ratio between the Boltzmann current (I_B) and the corresponding moment current (I_m) as a function of B in Fig. 2. An increase in τ and/or a decrease in d favors ballistic effects. The choice of B to measure "ballisticity" in the system clearly reflects this. As B is increased, i.e., ballistic effects are amplified, the agreement between the moment models and the Boltzmann model becomes less. Figure 2 shows that also the relative error in the current increases with B and τ . Moreover, all models give such relative error even when the applied voltage tends to zero due to the high built-in potential found in these structures. Large electric fields generated near doping steps cause locally far from equilibrium situations to be reached already at small applied voltages. Finally, we observe that at high ballisticity ($I_B/I_m \sim \log(B)$), for all moment models.

Our evaluations for the n^+nn^+ diode indicate that strong ballistic effects cannot be adequately described with any low-order moment model. Of course, the use of the relaxation time approximation for the collision integral in the Boltzmann equation, implies an exaggeration of ballistic effects.^{5,11} However, we anticipate that even when using more realistic scattering terms, the same sort of discrepancies will be found in predominantly ballistic situations. In essence, the distribution function develops a sharp high-velocity ballistic peak in far from equilibrium situations, next to a “bell”-shaped near equilibrium distribution at lower velocities within the structure.^{5,6,11} This intricate structure can no longer be represented by any small number of moments, e.g., a single typical velocity and temperature. Conversely, in the nonballistic regime such a high-velocity peak is absent and the essential structure of the distribution function can quite well be captured with a small number of typical scales/moments.

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