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Numerical Simulation of Semiconductor Devices: Energy-transport and Quantum Hydrodynamic Modeling

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1. Introduction

Submicron semiconductor devices that incorporate hot electron effects or quantum tunneling are playing an increasingly important role in advanced microelectronic applications. For the simulation of such devices, fluiddynamical equations are used as a reasonable compromise between computational efficiency and an accurate description of the underlying device physics. In this paper, we are concerned with two modern semiconductor models: the energy-transport and the quantum hydrodynamic equations.

The energy-transport models consist of the conservation laws for mass and energy for the electrons, coupled self-consistently to the Poisson equation. They are derived from the semiconductor Boltzmann equation. More precisely, from the Boltzmann equation, the so-called spherical harmonic expansion (SHE) model is obtained in the diffusion limit and then, through a diffusion limit, respectively making electron-electron or phonon scattering large, the energy-transport equations are derived from the SHE model [1]. We present numerical simulations of energy-transport models, incorporating non-parabolic band diagrams. The structure of the current equations allows to rewrite the stationary problem in a drift-diffusion formulation, which is discretized by using the exponential fitting mixed finite-element method. Numerical simulations of a one-dimensional ballistic silicon diode are performed, and the influence of the non-parabolicity parameter on the spuriuos velocity overshoot peak is shown.

The quantum hydrodynamic equations consist of the conservation laws for mass, momentum and energy, including the Poisson equation. The momentum and energy equations contain quantum correction terms, which account for the quantum effects. They are equivalent to a mixed-state Schrödinger-Poisson system, under the conditions of vanishing relaxation terms and assuming an appropriate closure condition in the energy equation [6]. The one-dimensional stationary equations are discretized by means of finite differences, and numerical simulations of a resonant tunneling diode are performed. The numerical results show negative differential resistance effects.

2. Energy-transport Models

The stationary energy-transport equations in one space dimension read as follows [1]:

$$\begin{aligned}
-J_{1,x} &= 0, && (1)\\
-J_{2,x} &= -J_1 V_x + W(n,T), && (2)\\
J_1 &= L_{11}\Big(\big(\frac{q\mu}{k_BT}\big)_x - \frac{qV_x}{k_BT}\Big) - L_{12}\Big(\frac{1}{k_BT}\Big)_x, && (3)\\
qJ_2 &= L_{21}\Big(\big(\frac{q\mu}{k_BT}\big)_x - \frac{qV_x}{k_BT}\Big) - L_{22}\Big(\frac{1}{k_BT}\Big)_x, && (4)\\
\varepsilon_s V_{xx} &= q(n-C). && (5)
\end{aligned}$$

The variables are the chemical potential μ, the electron temperature T, and the electric potential V. Furthermore, J_1, J_2 are the particle and energy current densities, respectively. The physical constants are the elementary charge q, the Boltzmann constant k_B, and the semiconductor permittivity ε_s. The electron density n depends on μ and T. The space dependent function $C = C(x)$ is the doping profile, $L_{ij} = L_{ij}(n,T)$ are the diffusion coefficients, and $W = W(n,T)$ is the energy relaxation term. These equations hold in the (bounded) semiconductor domain $\Omega = (0,\ell)$, and they are complemented by the boundary conditions

$$n(0) = C(0), \quad n(\ell) = C(\ell), \quad T(0) = T(\ell) = T_0,$$
$$V(0) = 0, \quad V(\ell) = U,$$

where T_0 is the lattice temperature and U the applied potential.

An important observation is that the current densities can be written in the drift-diffusion form

$$J_i = g_i(n,T)_x - g_i(n,T)\frac{V_x}{T}, \quad i = 1,2, \qquad (6)$$

with $g_1 = L_{11}$ and $g_2 = L_{21}$. This formulation is valid for *any* current densities coming from a SHE model (see [3]).

In order to give analytical expressions for the diffusion coefficients and the energy relaxation term, in the variables n and T, we have to impose some physical assumptions: *(i)* The energy band ε of the semiconductor crystal

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is spherical symmetric and a monotone function of the modulus $k = |\vec{k}|$ of the wave vector $\vec{k}$; *(ii)* a momentum relaxation time $\tau(\varepsilon)$ can be defined by $\tau^{-1} = \phi_0 \varepsilon^\beta N(\varepsilon)$, where $\phi_0 > 0$, $\beta > -1$, and $N(\varepsilon) = 4\pi k^2/|\varepsilon'(k)|$ is the density of states of energy $\varepsilon = \varepsilon(k)$; *(iii)* the electron density is given by Boltzmann statistics; *(iv)* the energy band diagram is defined by Kane's relation: $\varepsilon(1+\alpha\varepsilon) = \hbar^2 k^2/2m$, where $\alpha > 0$ is the non-parabolicity parameter, $\hbar$ the reduced Planck constant, and m the effective electron mass; *(v)* $\alpha k_B T \ll 1$.

The condition (ii) is used, for parabolic bands, in Lyumkis *et al.* [7] with $\beta = 1/2$ and in Chen *et al.* [2] with $\beta = 0$. The corresponding energy-transport models are referred to as the *Lyumkis model* and the *Chen model*, respectively. The assumption (iii) is valid for semiconductor devices with doping concentrations below $10^{19}\,\mathrm{cm}^{-3}$. The fifth hypothesis is valid for silicon devices, in which $\alpha = 0.5\,(\mathrm{eV})^{-1}$ and T is of the order 10^3 K.

Under the assumptions (i)-(v) and up to second order terms in $\alpha k_B T$, the functions g_1 and g_2 are given by [3]

$$g_i(n,T) = qn\mu_i^{\alpha,\beta}(k_B T)^i, \quad i = 1,2, \tag{7}$$

where the mobility $\mu_i^{\alpha,\beta}$ is defined by

$$\begin{aligned} \mu_1^{\alpha,\beta} &= \mu_0 \frac{1-3(2-\beta)\alpha k_B T}{1+15\alpha k_B T/4}\left(\frac{T}{T_0}\right)^{-1/2-\beta}, \\ \mu_2^{\alpha,\beta} &= (2-\beta)\mu_0 \frac{1-3(3-\beta)\alpha k_B T}{1+15\alpha k_B T/4}\left(\frac{T}{T_0}\right)^{-1/2-\beta}, \end{aligned}$$

and μ_0 is the (low-field) mobility constant. The energy relaxation term can be computed as

$$\begin{aligned} W(n,T) &= \frac{3}{2}\frac{nk_B(T_0-T)}{\tau(T)}, \\ \tau(T) &= \tau_0 (k_B T)^{\beta-1/2}\frac{\Gamma(\beta+1)+5\Gamma(\beta+2)\alpha k_B T}{1+15\alpha k_B T/4}, \end{aligned}$$

where Γ is the Γ-function. Notice that in the parabolic band case $\alpha = 0$, we obtain the same current densities and energy relaxation terms as in [7] (with $\beta = 1/2$) and in [2] (with $\beta = 0$).

The continuity equations are discretized by using the mixed finite element method. This method can be sketched as follows: *(i)* First, we transform the problem by means of the Slotboom variable to a symmetric form. Since in the present case a Slotboom variable does not exist, we approximate T in the current relation (6) by a piecewise constant function and transform the approximate equation by *local* Slotboom variables such that this equation can be written in symmetric form. *(ii)* Then, the corresponding continuity equations can be discretized with mixed finite elements. *(iii)* Finally, by a suitable discrete change of variable the discrete equations are rewritten in terms of the original variables g_1, g_2, respectively. The final result can be interpreted as a non-linear Scharfetter-Gummel discretization (see [3] for details).

In order to solve the resulting coupled system of algebraic equations, we employ a variant of the Gummel method. The Poisson equation is solved by means of a P_1 non-conforming finite element method. The temperature T is computed in terms of g_1 and g_2 by inverting appropriately the relations (7). The Gummel-type iteration scheme is coupled to a continuation in the applied bias.

As a numerical example we present the simulation of an n^+nn^+ ballistic silicon diode. In the n^+-regions the maximal doping concentration is $5 \cdot 10^{17}\,\mathrm{cm}^{-3}$; in the n-channel the minimal doping profile equals $2 \cdot 10^{15}\,\mathrm{cm}^{-3}$. The length of the n^+-regions is $0.1\,\mu$m, whereas the length of the channel region equals $0.4\,\mu$m. The mobility constant is taken to be $\mu_0 = 1500\,\mathrm{cm}^2/\mathrm{Vs}$ and the energy relaxation time equals $\tau_0 = 0.4 \cdot 10^{-12}$ s. The applied potential is $U = 1.5$ V. We have chosen the data such that our results can be compared to the numerical results of the literature (see, e.g., [2]).

We perform numerical results for a uniform mesh of 500 nodes. In Figure 1 the electron mean velocity $u = J_1/(qn)$ for two different values of the non-parabolicity parameter α using Lyumkis' model is shown. The spurious velocity overshoot peak at the left junction becomes smaller for non-vanishing non-parabolicity parameter. The same effect can be observed using Chen's model (see Figure 2), where the spuriuos velocity overshoot spike almost vanishes for $\alpha = 0.5\,(\mathrm{eV})^{-1}$. In Figure 3 we present the current-voltage characteristics for the different models in double-logarithmic scale. The particle current density J_1 is always smaller in non-parabolic band situations. Its dependence on the applied voltage U is approximately sublinear, i.e. $J_1 \sim U^\gamma$, where γ is between 0.83 and 0.88 depending on the model [3].

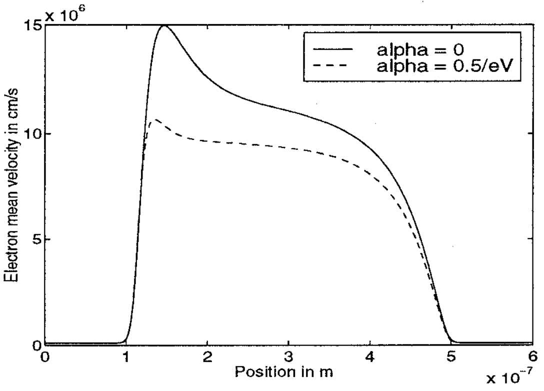

Figure 1: *Electron mean velocity versus position in a ballistic diode using Lyumkis' model.*

3. Quantum Hydrodynamic Models

The one-dimensional stationary quantum hydrodynamic equations are written as follows:

$$J_x = 0, \tag{8}$$

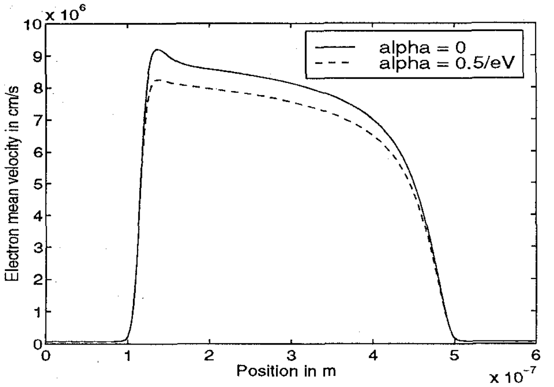

Figure 2: *Electron mean velocity versus position in a ballistic diode using Chen's model.*

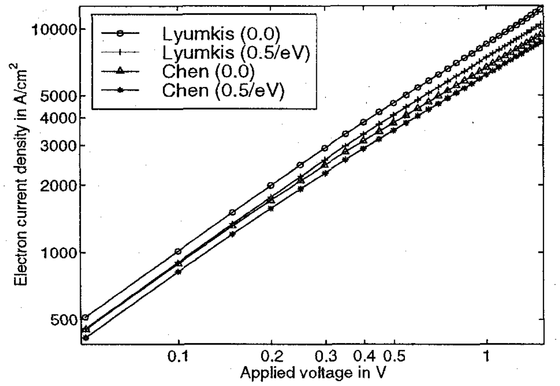

Figure 3: *Current-voltage characteristics for a ballistic diode.*

$$\begin{aligned}\left(\frac{m}{q}\frac{J^2}{n} + qnk_BT\right)_x - q^2n(V_{\text{ext}}+V)_x & \qquad (9)\\ -\frac{q\hbar^2}{4m}\left(n(\ln n)_{xx}\right)_x &= -R_J(J,T),\\ \frac{m}{q}\left(\frac{J}{n}E + Jk_BT\right)_x - mJ(V_{\text{ext}}+V)_x & \qquad (10)\\ -\frac{\hbar^2}{4q}\frac{J}{n}\left(n(\ln n)_{xx}\right)_x + Q_x &= -R_E(n,T),\\ \varepsilon_s V_{xx} &= q(n-C).(11)\end{aligned}$$

These equations are satisfied in the semiconductor domain $\Omega = (0, \ell)$. The variables are the electron density n, the particle current density J, the electron temperature T, and the electric potential V. The energy density is defined by $E = \frac{3}{2}nk_BT + \frac{1}{2}mJ^2/q^2n$, and Q is the heat flux. The functions R_J and R_E are the momentum and the energy relaxation terms, respectively, and they are given by modified Baccarani-Wordeman models:

$$R_J(J,T) = \frac{mJ}{\tau_p}\frac{T}{T_0},$$

$$R_E(n,T) = \left(E - \frac{3}{2}nk_BT_0\right)\frac{mT}{T_0(1+zT)\tau_w},$$

where τ_p and τ_w are relaxation times, T_0 is the lattice temperature, and $z > 0$ is a parameter. The external potential V_{ext} models interior quantum barriers. The term $\hbar^2\left(n(\ln n)_{xx}\right)_x$, coming from the Bohm potential, is a dispersive quantum correction.

The quantum hydrodynamic equations without relaxation terms can be derived from a mixed-state Schrödinger-Poisson system [6]. More precisely, from the Schrödinger-Poisson system one obtains the equations (8)-(11) with $R_J = R_E = 0$, but the heat flux cannot in general be expressed in terms of n, J, and T only. In analogy to classical fluiddynamics, a closure condition has to be added in order to obtain a closed set of equations. We choose to specify Q by the Fourier law $Q = -\kappa(k_BT)_x$ and define κ by the Wiedemann-Franz formula $\kappa = \kappa_0(\mu_0 mk_BT_0/q)n$, where κ_0 is a constant. Another choice could be to neglect the heat flux or to assume constant electron temperature (and hence to neglect the energy equation). The quantum hydrodynamic model can also be obtained from the quantum Boltzmann equation by means of a moment method [4]. Recently, a quantum hydrodynamic model with "smooth" quantum potential has been derived from the Bloch equation [5].

The advantage of the quantum hydrodynamic equations is that macroscopic boundary conditions can be easily prescribed:

$$n(0) = C(0), \;\; n(\ell) = C(\ell), \;\; n_x(0) = 0, \;\; n_x(\ell) = 0,$$
$$V(0) = 0, \;\; V(\ell) = U, \;\; T(0) = T_0, \;\; T(\ell) = T_0.$$

The primary application of the quantum hydrodynamic models is the simulation of quantum devices that depend on particle tunneling through potential barriers, like resonant tunneling diodes. For the numerical simulations, we first write the energy equation (10) as a second order equation in T, by using (9). Then the modified system of equations is discretized by finite differences on an equidistant grid. In order to avoid artificial numerical viscosity, central finite differences are used to approximate the third-order term in (9). The resulting algebraic system is solved on a grid of 1000 nodes employing a damped Newton scheme, which is coupled to a adaptive continuation in the applied bias (see [8] for details).

The device is defined as follows. The diode has an n^+nn^+ structure with a doping concentration of $C_{\max} = c_1$ in the n^+-regions and $C_{\min} = c_0$ in the n-region. The channel length is 250 Å, and the material of the symmetric diode is GaAs. In the n-region, there are two $\text{Al}_x\text{Ga}_{x-1}\text{As}$ barriers, which are modeled by the external potential V_{ext}. The barrier and well widths and the space layers between the barriers and the junctions are equal to 50 Å. The barrier heigth is denoted by V_0. For τ_w, τ_p, μ_0 and z we use the same values as in [4].

In the first test we use the following values: $c_0 = 10^{16}\,\text{cm}^{-3}$, $c_1 = 2 \cdot 10^{18}\,\text{cm}^{-3}$, $V_0 = 0.05\,\text{eV}$, $\ell = 625\,\text{Å}$,

$\kappa_0 = 0.1$. In Figure 4 the current-voltage characteristics for two different lattice temperatures are compared. As expected, there is a region of negative differential resistance (NDR) with a peak-to-valley ratio which is decreasing for increasing temperatures. The electron temperature for various applied voltages is presented in Figure 5 using a lattice temperature of 300 K. The temperature in the drain region is increasing for higher biases, due to the retarding of the electrons at the beginning of the drain region, because of the higher doping.

In the region of NDR, the electron density is expected to accumulate in the quantum well. To illustrate this effect we have performed a second test with the data: $c_0 = 10^{16}\,\mathrm{cm}^{-3}$, $c_1 = 10^{18}\,\mathrm{cm}^{-3}$, $V_0 = 0.27\,\mathrm{eV}$, $\ell = 833\,\text{Å}$, $\kappa_0 = 0.05$. In Figure 6 we see an accumulation of electrons in the quantum well for $0.6\,\mathrm{V} < U < 0.7\,\mathrm{V}$, the region of NDR. There is also a distinct decrease of electrons in the barriers for these applied voltages.

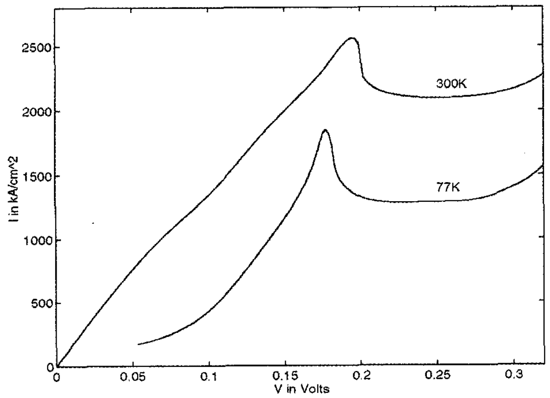

Figure 4: *Current-voltage characteristics for a tunneling diode.*

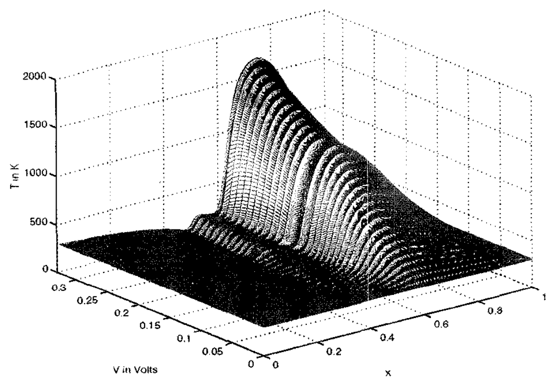

Figure 5: *Electron temperature versus position and applied voltage.*

Acknowledgements

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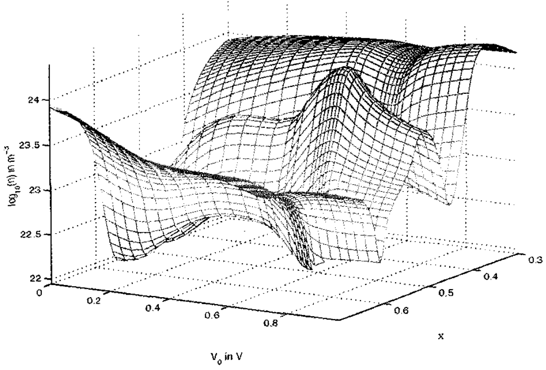

Figure 6: *Electron density versus position and applied voltage.*

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