Monte Carlo and hydrodynamic simulation of a one dimensional $n^+ - n - n^+$ silicon diode

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An improved closure relation - based on the entropy principle - is implemented in a Hydrodynamic model for electron transport. Steady-state electron transport in the "benchmark" n^+- n - n^+ submicron silicon diode is simulated and the quality of the model is assessed by comparison with Monte Carlo results.

1. INTRODUCTION

Electronic transport in semiconductors can be described by hydrodynamic models (hereafter HM), obtained by taking the first few moments of the Boltzmann transport equation (BTE). The two main problems one must tackle are 1. how to "close" the resulting infinite hierarchy of equations and, 2. how to model the right-hand-side of the moment equations (*i.e.*, the "collision" or "production" terms). Baccarani and Wordeman [1] (hereafter BW) introduced a HM in which the closure is obtained by using the Fourier law with the Wiedemann-Franz expression for the heat conductivity. This choice leads to some theoretical difficulties, due to the *ad hoc* solution of the closure problem as well as to the approximations made in modeling the collision terms.

Anile and Pennisi [2] (hereafter AP) and Anile and Muscato [3] proposed a HM in which the closure is obtained by exploiting the entropy principle. This model, which is a hyperbolic system consisting of 13 scalar equations, is free from the above difficulties and completely determines the description of the heat flow.

A computationally simpler system can be obtained by the well known Maxwellian iteration procedure which amounts at expanding the equations for the heat flux and for the viscous stresses around the state of partial thermal equilibrium (assuming that the velocity, the heat flux, the viscous stresses and their gradients as well as the temperature and the velocity gradients are first order quantities). In order to test this system, we simulate the stationary electron flow in the one dimensional $n^+ - n - n^+$ submicron diode, which mimics the channel of a MOSFET [4]. Relaxation times for energy, momentum, energy flow, and shear (appearing in the collision terms) are determined by using the Monte Carlo code *DAMOCLES*[TM] [5]. The Monte Carlo (hereafter MC) simulations are obtained in the case of parabolic spherical band approximation, in order to be consistent with the AP model, obtained under these restrictions.

2. THE HYDRODYNAMIC MODEL

The system of equations we consider are :

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_j}(nu_j) = 0 \qquad (1)$$

$$\frac{\partial(nu_i)}{\partial t} + \frac{\partial}{\partial x_j}\left(nu_iu_j + \frac{nk_BT}{m^*}\delta_{ij}\right) + \frac{nqE_i}{m^*} = Q_i \qquad (2)$$

$$\frac{\partial}{\partial t}\left(\frac{1}{2}nm^*u^2 + \frac{3}{2}nk_BT\right)$$
$$+ \frac{\partial}{\partial x_i}\left[\left(\frac{1}{2}nm^*u^2 + \frac{5}{2}nk_BT\right)u_i + h_i + m^*u_j\widehat{\Theta}_{<ij>}\right]$$
$$+ nqE_iu_i = Q_w \qquad (3)$$

$$h_i = -\frac{5}{2}\frac{\tau_q}{m^*}nk_BT\frac{\partial(k_BT)}{\partial x_i} + \frac{5}{2}nk_BTu_i(\frac{1}{\tau_p} - \frac{1}{\tau_q})\tau_q \qquad (4)$$

$$\widehat{\Theta}_{<ij>} = 0 \qquad (5)$$

where τ_w, τ_p, τ_q are the relaxation times for energy, momentum and energy-flux, which are functions of temperature and doping. Comparing eq.(4) to the Wiedemann-Franz law, adopted in the BW model, we see an extra convective term. Moreover, the heat conductivity (at variance with the BW model) is fully determined by τ_q.

3. SIMULATION OF THE $n^+ - n - n^+$ SILICON DIODE

The $n^+ - n - n^+$ diode consists of two n^+ regions 0.1 μm-long doped to a density of N = 10^{18} cm^{-3}, while the central n region is 0.4 μm wide, with a doping density of $N = 10^{16}$ cm^{-3}. We consider Ohmic boundary conditions, $T_0 = 300K$, and 1 V of applied bias. The AP model is discretized by using finite differences and 1-D box method. The solution of the resulting nonlinear system is obtained by Newton's method with the Bank and Rose damping. The relaxation times for energy, momentum and heat flow are obtained with MC simulation of the diode. The values of the relaxation times are fitted to the expression of the form (E being the normalized energy in eV/k_BT_0):

$$\tau(E) = a + b * (E - 1) + c * e^{-d*(E-1)} \qquad (6)$$

according to Table I. Gnudi *et al.* [6] have integrated the BW model for the benchmark under consideration. They obtained values for τ_p and τ_w from homo-

geneous **full-band** MC simulation and a tuning was made on the heat conductivity. These simulations fit well the MC data by definition. The BW model has been obtained from the BTE by suitable (and sometime unjustified) approximations, assuming parabolic bands. Therefore, in order to be consistent, it must be compared with parabolic MC simulations, in which the electron effective mass is $m^* = 0.32$ m_e (in order to reproduce the correct density of states). The AP model differs from the BW because: i) more moment equations are taken into account and a rigorous closure is obtained; ii) there are no free parameters; iii) we compare our results with the same **parabolic MC simulations**. The simulation shows that [7], at the drain junction, the heat flow evaluated with our HM overestimates the MC one and that, as consequence, the hydrodynamic energy is lower than the corresponding quantity evaluated with the MC model and the velocity obtained by the HM exhibits the well-known "spurious" peak We ascribe this discrepancy to the limitations of the Maxwellian iterative approximation. This can be overcome by: a) including viscous effects; b) employing a flux-limiter heat equation which can be obtained rigorously from the full system [8]. In this article we investigate the first route by extending the previous system to incorporate Navier-Stokes like viscous effects

$$\widehat{\Theta}_{<ij>} = -\frac{nk_BT}{m^*}\tau_\sigma\left(\frac{\partial u_i}{\partial x_i} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right) \qquad (7)$$

where τ_σ is the relaxation time for shear. The results are shown in Fig. 1,2,3,4. We notice that also in this case the heat flow is overestimated by the HM, when compared to the MC results. We are currently investigating the other route, and these results will be published elsewhere.

TABLE I Relaxation times (ps), channel 0.4μm

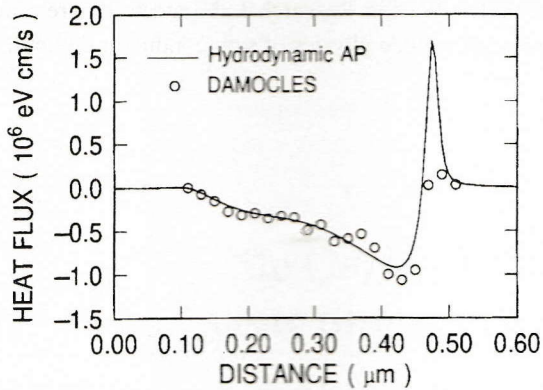|	a	b	c	d
τ_w	0.1731	0.0313	0.2382	0.5167
τ_p	0.0681	-0.0023	0.2056	0.9547
τ_q	0.0471	-0.0007	0.1330	0.6911
τ_σ	0.0093	0.0027	0.0904	0.5640

FIGURE 1 Heat-flux vs. distance computed using the hydrodynamic AP model with viscosity compared to Monte Carlo results
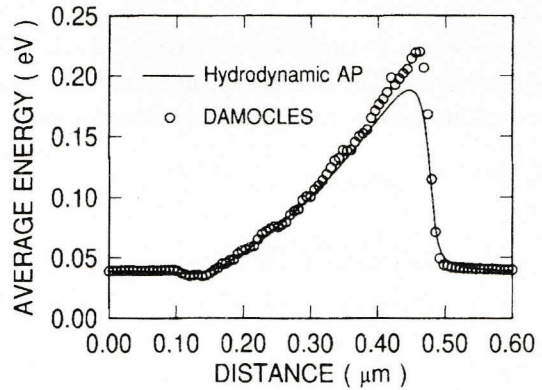
FIGURE 2 Average electron energy vs. distance computed using the hydrodynamic AP model with viscosity compared to Monte Carlo results
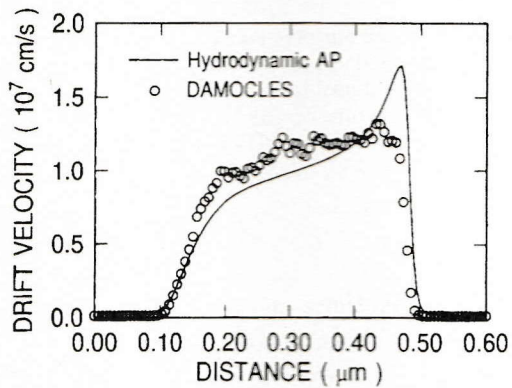
FIGURE 3 Average drift velocity vs. distance computed using the hydrodynamic AP model with viscosity compared to Monte Carlo results
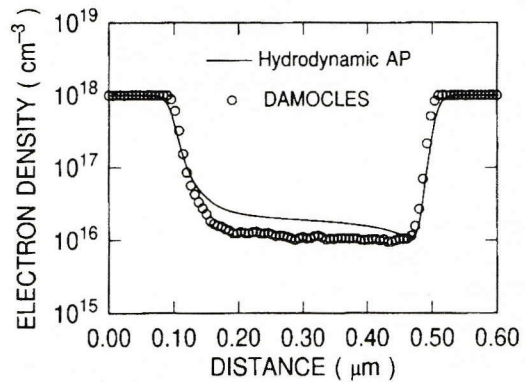
FIGURE 4 Electron density vs. distance computed using the hydrodynamic AP model with viscosity compared to Monte Carlo results

Acknowledgements

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