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Testing Hydrodynamical Models on the Characteristics of a One-Dimensional Submicrometer Structure

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Recent advances in technology leads to increasing high speed performance of submicrometer electron devices by the scaling of both process and geometry. In order to aid the design of these devices it is necessary to utilize powerful numerical simulation tools. In an industrial environment the simulation codes based on the Drift-Diffusion models have been widely used. However the shrinking dimension of the devices causes the Drift-Diffusion based simulators to become less accurate. Then it is necessary to utilize more refined models (including higher order moments of the distribution function) in order to correctly predict the behaviour of these devices. Several hydrodynamical models have been considered as viable simulation tools. It is possible to discriminate among the several hydrodynamical models on the basis of their results on the output characteristics of the electron device which are measurable (I-V curves). We have analyzed two classes of hydrodynamical models: i) HFIELDS hydrodynamical models and HFIELDS drift-diffusion model; ii) self-consistent extended hydrodynamical models with relaxation times determined from Monte Carlo simulations.

1 INTRODUCTION

Recent advances in technology leads to increasing high speed performance of submicrometer electron devices by the scaling of both process and geometry. In order to aid the design of these devices it is necessary to utilize powerful numerical simulation tools. In an industrial environment the simulation codes based on the Drift-Diffusion models have been widely used. However the shrinking dimension of the devices causes the Drift-Diffusion based simulators to become less accurate. Then it is necessary to utilize more refined models (including higher order moments of the distribution function) in order to correctly predict the behaviour of these devices. Short of a direct Monte Carlo simulation (hereafter MC), which requires prohibitively large computational cost in an industrial setting, hydrodynamical models have been considered as viable simulation tools.

Several hydrodynamical models have been considered in the literature with various degrees of sophistication and completeness, since the pioneering work of Blotekjaer [1]. For a given device structure the various hydrodynamical models can give widely different results for the velocity and energy profiles according to the various assumptions made in the model (the crucial parameter seems to be the heat conductivity of the electron gas). However the different velocity or energy profiles are hardly accessible to experimental detection. Therefore it is mandatory to discriminate among the various hydrodynamical models on the basis of their results on the output characteristics of the electron device which are measurable (I-V curves).

We have analyzed two classes of hydrodynamical models:

- HFIELDS drift-diffusion model (hereafter HDD) and the HFIELDS hydrodynamical model based on the Blotekjaer, Baccarani and Wordeman model (here after BBW) [2]-[4]. HFIELDS is a general purpose two-dimensional device simulator developed at Bologna University which performs a wide range of tasks like steady-state, small-signal and transient analysis. It solves the semiconductor equations incorporating the most important physical effects using a wide range of models. Default parameters are used both in the drift-diffusion version and in the hydrodynamical version (τ_p, τ_w [5], heat conductivity) . The latter is phenomenologically represented by the Weidemann-Franz law with c = –2.1 (this choice has no physical justification and is motivated only by fitting the velocity and energy curve to MC simulations for the particular $n^+ - n - n^+$ device [6], which will be considered in sec.3).
- the Anile, Pennisi and Muscato model [7],[8],[9] (hereafter APM): this is a **self-consistent** extended hydrodynamical models with relaxation times determined from inhomogeneous Monte Carlo simulations. Heat conductivity is consistently represented by linear Fourier law plus a (dominant) convective term.

2 DESCRIPTION OF THE HYDRODYNAMICAL MODELS

The hydrodynamical models we consider can be derived from the moment equations of the BTE (semiclassical Boltzmann transport equation for charged carriers in semiconductors). Throughout the derivation spherical parabolic bands and the effective mass approximation have been assumed.

The models we consider can be described within the general framework of the following balance equations. For the electron component (neglecting electron-hole generation and recombination, which is inessential for the applications we shall present in the sequel) these equations comprise :

- the particle number balance equation

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\underline{u}) = 0, \tag{1}$$

- the momentum balance equation

$$\frac{\partial}{\partial t}(nu^i) + \frac{\partial}{\partial x^j}(nu^i u^j + \frac{nk_BT}{m^*}\delta^{ij}) + \frac{nqE^i}{m^*} = Q^i, \tag{2}$$

- the energy balance equation

$$\frac{\partial}{\partial t}(\tfrac{1}{2}nm^*\underline{u}^2 + \tfrac{3}{2}nk_BT) + \nabla \cdot [(\frac{1}{2}nm^*\underline{u}^2 + \frac{5}{2}nk_BT)\underline{u} + \underline{h}] + nq\underline{E}\cdot\underline{u} = Q_W, \tag{3}$$

- the Poisson equation

$$\nabla \cdot (\varepsilon \nabla \phi) = q(n - N_D^+). \tag{4}$$

Here m^* is the electron effective mass, n, u, T the electron density, average velocity and temperature, h is the heat flux, $\underline{E}$ is the electric field, $\underline{E} = -\nabla\phi$, ϕ the potential, q the absolute value of the electric charge, N_D^+ the ionized donors density and $\in$ the lattice dielectric constant. Finally Q, Q_w. are the momentum and energy productions due to collisions.

Notice that in the balance equations (1-3) we have neglected any anisotropic terms in the pressure tensor. This can be justified because these terms, for the applications we shall consider, are rather small [6]. The various hydrodynamical models we investigate differ on choices about :

i. the closure problem, i.e. a constitutive law for the heat flux $\underline{h}$,
ii. modeling the production terms Q, Qw.

As stated in the Introduction we have examined the BBW model and the recent APM.

2.1 The BBW model

i) The closure problem

Without any justification it is assumed that the heat flux vector obeys Fourier's law

$$\underline{h} = -k\nabla T, \tag{5}$$

and the heat conductivity k is given by the Wiedemann-Franz law (which holds for electrons near thermal equilibrium)

$$k = (\frac{5}{2} + c)k_B^2 \frac{nT\tau_p}{m^*}, \tag{6}$$

with τ_p the momentum relaxation time (to be specified later) and c an *adjustable constant*. The default value of c = –2.1 is chosen because it gives the best agreement with the corresponding MC simulations for a particular $n^+ - n - n^+$ diode [6].

ii) Modeling the production terms

Both $\underline{Q}$ and Q_w are assumed to be of the relaxation type

$$\underline{Q} = -\frac{n\underline{u}}{\tau_p}, \tag{7}$$

$$Q_W = -\frac{W - W_0}{\tau_W}, \tag{8}$$

where $W = \frac{1}{2}m^*\underline{u}^2 + \frac{3}{2}nk_BT$ is the total energy density, $W_0 = \frac{3}{2}nk_BT_L$ (T_L being the lattice temperature). τ_W is the energy relaxation time.

Both τ_p and τ_W are assumed to be functions of the electron temperature (and of the doping density). In the original Baccarani-Wordemann formulation they are given by phenomenological expression [4]

$$\tau_p = \frac{m^*\mu_{n0}T_L}{T}, \tag{9}$$

$$\tau_W = \mu_{n0}T_L\left(\frac{m^*}{2qT} + \frac{3T}{2qv_s^2(T+T_L)}\right), \tag{10}$$

where μ_{n0} is the low field mobility and $\upsilon_s = 1 \cdot 10^7 \frac{\text{cm}}{\text{s}}$ is the saturation velocity. However it seems that in the model implemented in ST-HFIELDS, τ_p and τ_W are taken to be constant.

2.2 the APM model

i) The closure problem

This problem is solved by using the methods of extended Thermodynamics [10], [11], i.e. by requiring that the balance equations be compatible with a supplementary conservation law to be interpreted as entropy production law (*entropy principle*). By linearizing around the state of local thermal equilibrium one obtains for $\underline{h}$

$$\underline{h} = -\frac{5}{2}\frac{nk_B^2T\tau_q}{m^*}\nabla T + \frac{5nk_BT\underline{u}}{2}\left(\frac{1}{\tau_p} - \frac{1}{\tau_q}\right)\tau_q, \tag{11}$$

where τ_q is the relaxation time for the energy flux. Notice the convective term

$$\underline{h}_c = \frac{5}{2}nk_BT\underline{u}\left(\frac{\tau_q}{\tau_p} - 1\right), \tag{12}$$

which is absent in the BBW model. According to MC simulations [12], [13] the convective term is the dominant contribution to the heat flux. Furthermore the presence of this term renders the extended model compatible with the *Onsager reciprocity relations* [9] near thermal equilibrium (at variance with the BBW model which has not the correct limit near thermal equilibrium).

ii) Modeling the production terms

For 1-D flow one can assume the same relaxation type expression eqs.(7),(8) as in the BBW model. In 2 or 3 dimensions however a more general expression is required for $\underline{Q}$ [10].

The relaxation times τ_p, τ_q, τ_ω are obtained with the *DAMOCLES*^{TM} code [13] (with parabolic bands for consistency with the derivation of the hydro models) for the structure which will be considered in the next section.

We remark that in the APM model there are **no free parameters** and adjustable constants.

3 THE STRUCTURE

We consider a $n^+ - n - n^+$ diode consisting of a 0.1μ n^+ region followed by a 0.4μ *n*region, and ending with a 0.1μ n^+. In the n^+region the doping density is $N^+ = 10^{18}cm^{-3}$ while in the n region it is $N = 10^{16}cm^{-3}$; the lattice temperature is $T_L = 300°K$. The simplest boundary conditions are:

$$n = N, \quad T = T_L, \tag{13}$$

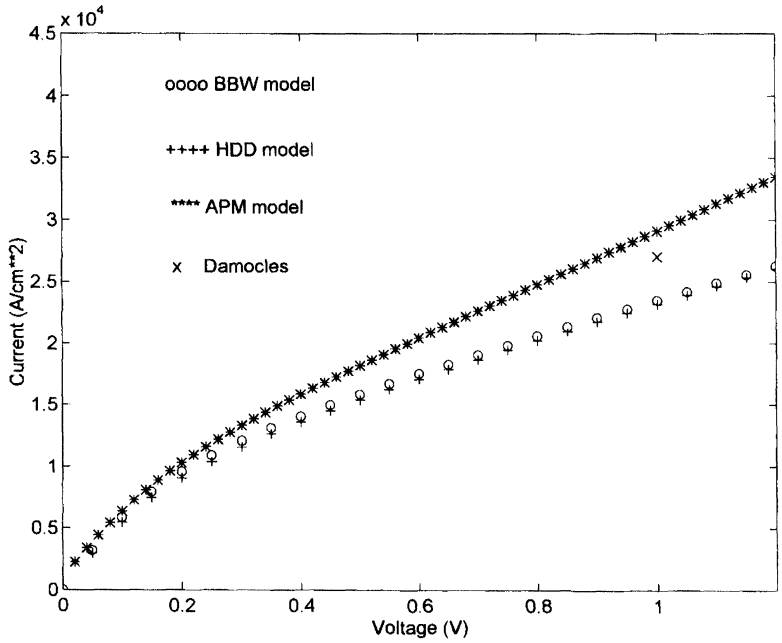

FIGURE 1 Current vs. Voltage computed by using the HFIELDS drift-diffusion model (HDD), the HFIELDS hydrodynamical model (BBW), the APM model and the Monte Carlo code *DAMOCLES*

at x_{min} and x_{max}. Also

$$q\phi(x_{min}) = T\ log(\frac{n}{n_i}), \quad q\phi(x_{max}) = T\ log(\frac{n}{n_i}) + qV_b, \tag{14}$$

where V_b is the applied bias and $n_i$the intrinsic concentration $n_i = 1.4 \times 10^{10} cm^{-3}$. For the numerical solution we employ the methods developed by Gardner, Jerome and Rose [14] and Gardner [15], adapted to this model by Anile, Maccora and Pidatella [16] and Anile, Maccora, Muscato and Pidatella [17]

4 RESULTS AND CONCLUSIONS

In fig.1we plot the characteristics I-V for the structure previously described. We tested this structure with: a) the HDD model (where the mobility model used is the CVT [18]-[19]),b) the BBW model as implemented in HFIELDS (with the default values for the parameters τ_p, τ_W, determined from comparison with homogeneous MC simulations and c = –2.1 obtained by tuning with MC data for a $V_{bias} = 1.5$ V [6]), c) the APM model with the relaxation times obtained from inhomogeneous MC simulations.

We remark that all four curves start from the same initial point, corresponding to a zero bias thermal equilibrium state. This is consistent with the physical requirement that all models must yield indistinguishable results near thermal equilibrium. The curves corresponding to the HDD and BBW models are almost indistinguishable. We notice that at high voltages the difference in current density between the HDD and APM models can be as large as 20%: we ascribe this difference to the fact that the APM model is consistently obtained from the Boltzmann equation. In particular this entails the presence of the convective term in the heat flux constitutive equation at variance with the BBW model where the Fourier equation with the Wiedemann-Franz law is simply postulated.

Furthermore the relaxation times (henceforth the mobility) are consistently obtained from inhomogeneous MC simulations. We notice that the only MC datum we have (through *DAMOCLES*) is much closer to the APM curve as shown in fig. 1. Therefore such a

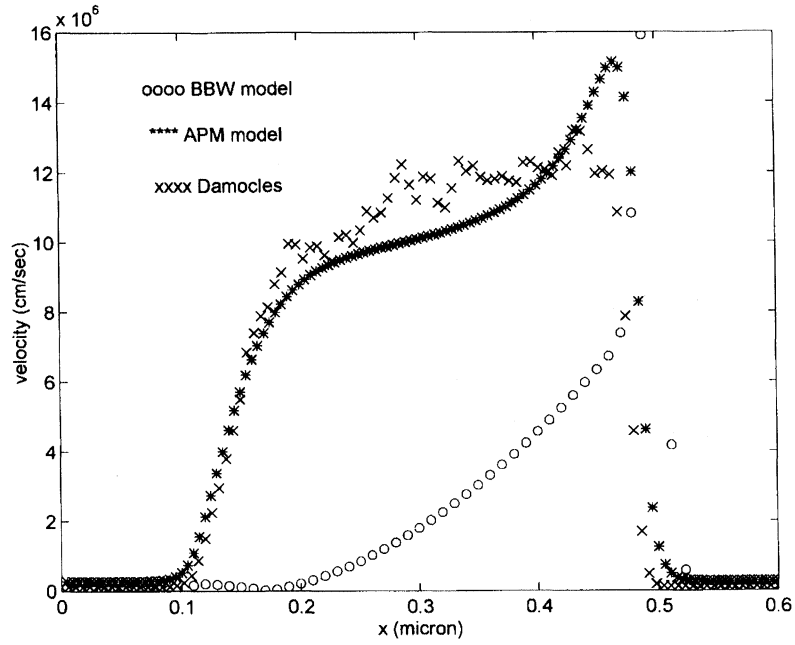

FIGURE 2 Electron temperature vs. distance computed by using the HFIELDS hydrodynamical model (BBW), the APM model and the Monte Carlo code *DAMOCLES* for V_{bias}=1 V

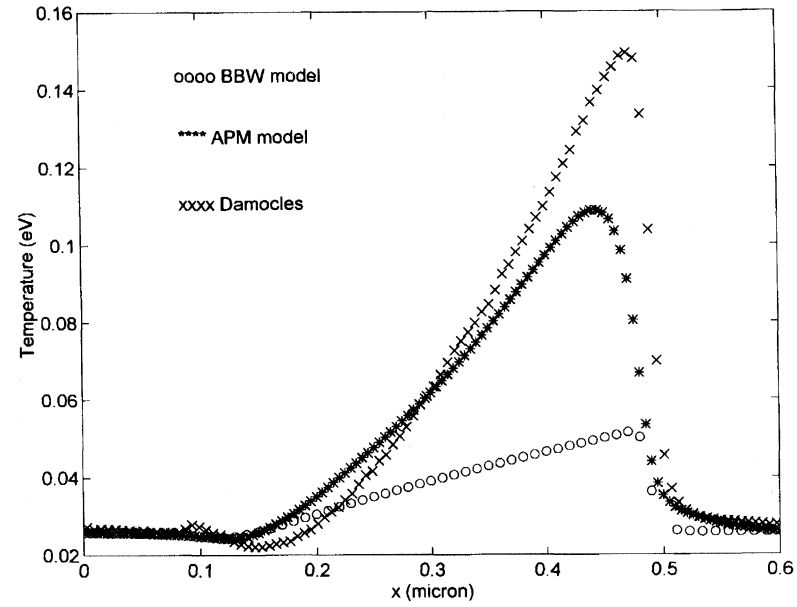

FIGURE 3 Electron velocity vs. distance computed by using the HFIELDS hydrodynamical model (BBW), the APM model and the Monte Carlo code *DAMOCLES* for V_{bias}=1 V

difference should be amenable to experimental discrimination.

In fig.2 we plot the velocity obtained with the APM model, the BBW model and *DAMOCLES* for V_{bias}=1 V. In fig.3 we plot the temperature obtained with the APM model, the BBW model and *DAMOCLES* for V_{bias}=1 V .

We remark that care must be exercised when comparing the theoretical curves with the experimental ones, due to the several approximations employed in deriving the theoretical models (neglect of non-parabolicity, of the hole current, 1-D geometry, etc.). In particular a rigorous assessment of the non parabolicity effects is required, following approaches employed by Tang et al. [20].

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