Time-Dependent Solution of a Full Hydrodynamic Model Including Convective Terms and Viscous Effect

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Sub-picosecond turn-on transient behavior of ballistic diodes ($N^+ - N - N^+$ structures) is studied by solving a system of time-dependent hydrodynamic (HD) equations. Convective terms as well as viscous effect are included in the study. The simulation result indicates that the diode undergoes approximately one quarter of a plasma oscillation before it relaxes to the steady-state value through collisions.

Keywords: transient simulation, full hydrodynamic model, convective terms, viscous effect, ballistic diode.

INTRODUCTION

Recently the hydrodynamic model has been widely used in submicrometer semiconductor device simulations in order to more accurately describe the non-equilibrium and non-local phenomena occurring in these devices. However, most of these simulations are limited to the steady-state operation. Although some work has been performed for transient simulation [1],[2], the transport models used are often simplified. In this study, we used a unique set of HD model which has been calibrated by Monte Carlo (MC) data [3].

HYDRODYNAMIC TRANSPORT MODEL

The new system of HD transport equations consists of [3]:

$$\frac{\partial^2 \psi}{\partial z^2} = -\frac{q}{\epsilon}(-n + N_D). \quad (1)$$

$$\frac{\partial n}{\partial t} + \frac{\partial(nV)}{\partial z} = 0, \quad (2)$$

$$\frac{\partial(nV)}{\partial t} + \frac{\partial(nA)}{\partial z} - nFM^{-1} = -\frac{nV}{\tau_v} + \lambda_v n \frac{\partial A}{\partial z}, \quad (3)$$

$$\frac{\partial(nW)}{\partial t} + \frac{\partial(nS)}{\partial z} - nFV = -n \frac{W - W_0}{\tau_e}. \quad (4)$$

where $V = \langle v_z \rangle$, $A = \langle v_z v_z \rangle$, $W = \langle \epsilon \rangle$, $M^{-1} = \frac{1}{n} \langle \frac{\partial v_z}{\partial k_z} \rangle$, $S = \langle v_z \epsilon \rangle$, $F = -qE$, τ_v and τ_e represent the velocity and the energy relaxation time respectively, and λ_v is a dimensionless parameter (0.1 for $\frac{dA}{dz} > 0$, 0.35 for $\frac{dA}{dz} < 0$) determined from the MC simulation data.

Convective and Viscous Terms

The macroscopic quantity A and the inverse effective mass M^{-1} appearing in Eq.(3) are modeled as [3]:

$$A = VV + 2.85(2\alpha W)VV + a(W) - \eta\tau_v VV \left(\frac{dV}{dz}\right), \quad (5)$$

$$M^{-1} = \frac{1}{m_c} [1 - 1.3(2\alpha)m_c VV - 1.85(2\alpha)^2 m_c WVV] + b(W), \quad (6)$$

where $\alpha = 0.5eV^{-1}$ denotes the non-parabolicity factor and $a(W)$ and $b(W)$ represent the empirical formulas fitted from the MC simulation data [3]. The first two terms on the r.h.s. of (5) and the second and third terms on the r.h.s. of (6) represent the convective terms. These terms cannot be easily handled by the conventional Scharfetter-Gummel (S-G) [4] type discretization scheme and therefore are often neglected in the device simulation. The last term on the r.h.s. of (5) represents the viscous term. The viscous effect is a second-order effect which becomes important when the velocity-gradient is large. The dimensionless parameter η is determined from the MC simulation and is approximately $2 \sim 3$ [5].

NUMERICAL SCHEMES

Spatial Discretization Scheme

The well known S-G scheme [4] for spatial discretization is very effective in dealing with the drift-diffusion (DD) equations as well as the simplified energy-balance equation. However, all exponentially weighted schemes have one common disadvantage: the velocity V is not treated as one of the state variables. Thus neither the convective terms nor the viscous effect can be included in the HD model in a natural way.

In this work we use the second upwind as the spatial discretization scheme which has been successfully used by Gardner [6] to solve the simplified HD system under the steady-state condition.

We impose the following boundary conditions to our discretized system :

$$\begin{aligned} \psi(0) &= \psi_{eq}, \quad \psi(L) = \psi_{eq} + \psi_a \\ n(0) &= n_{eq}(0) \\ \frac{dV}{dz} \Big|_{z=0} &= \frac{dV}{dz} \Big|_{z=L} = 0 \\ W(0) &= W(L) = W_{eq} \end{aligned}$$

where ψ_{eq} , n_{eq} and W_{eq} are the equilibrium values of the electrostatic potential, the electron concentration and the average energy, respectively.

Time Advancing Scheme

In this study we use Bank's trapezoidal rule/backward-differentiation-formula (TR-BDF2) composite method as the time-stepping scheme. The detailed discussion of this method can be found in [2]. An automatic time-step adjustment mechanism is built in with this scheme through monitoring the local truncation error at each time step. The relative error during the course of time advancement is chosen to be 10^{-3} .

SIMULATION RESULTS

We use an $N^+ - N - N^+$ structure (not shown) as our testing device. A step bias of 2 Volts is applied at $t = 0+$. Figs. 1, 2, and 3 show the time evolution of the electron velocity, the average energy and the electron current density, respectively. The average energy

FIGURE 1 Time evolution of the electron velocity

FIGURE 2 Time evolution of the electron energy

FIGURE 3 Transient response of the electron current density

increases smoothly from W_{eq} to its final distribution (Fig.2). However, the velocity has a rapid overshoot (Fig.1) at around $0.1ps$ and then gradually relaxes to a much lower steady-state value. During approximately the same time period ($t \sim 0.1ps$), the electron current density also shows a similar peak (Fig.3). The time duration from $t = 0$ to $t = 0.1ps$ represents approximately one quarter of the plasma oscillation period. After $t \approx 0.1ps$, the free plasma oscillation is quickly taken over by the collision processes and the velocity, as well as the current density, relax towards their steady-state values.

As we mentioned before, the viscous term, which has a dissipating effect, is included in our HD system.

FIGURE 4 A comparison between the velocity profiles obtained with and without the viscous effect. The MC data is also included for comparison

The effect of including the viscous term on the final steady-state result is shown in Fig.4. It is clear that the velocity overshoot obtained with the viscous term near the $N^+ - N$ junction region is substantially lower than that without the viscous term, and is in a better agreement with the MC data. This difference is expected to be more significant in the simulation of the narrow-base BJT's.

CONCLUSIONS

We have tested our new HD transport model and the existing numerical schemes with the transient simulation of an $N^+ - N - N^+$ diode. The HD model is considered as "full" in the sense that the conservation of "momentum" is solved explicitly with time. Although the problem considered is somewhat artificial (a step voltage is directly applied to the diode), it serves to demonstrate the utility of the HD model and the numerical solution schemes being used. We have also shown that the inclusion of the convective and viscous terms in the HD model yields a result in better agreement with the MC simulation data. We are now extending this work to the simulation of narrow-base BJT's in which the viscous effect is expected to play a more significant role.

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Biographies

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