

**NUMERICAL SIMULATION OF SUBMICRON DEVICES  
USING ENERGY BALANCE AND HYDRODYNAMIC MODELS  
IN THE GENERAL-PURPOSE DEVICE SIMULATOR SPISCES-2B.**

**Y. Apanovich, E. Lyumkis, B. Polsky, A. Shur and P. Blakey**  
*SILVACO International*  
*4701 Patrick Henry Drive, Bldg.3, Santa Clara, CA 95054*

**Abstract**

Energy balance and hydrodynamic models have been added to the general purpose device simulator SPISCES-2B. Attention was paid to developing a stable spatial discretization, achieving reliable convergence in steady-state, and implementing stable time-stepping for transient problems. The new capabilities are demonstrated for a range of silicon devices that include ballistic diode, MOS, and bipolar structures. Differences between results obtained using the energy balance and hydrodynamic models are discussed.

**I. INTRODUCTION**

Carrier transport in advanced submicron silicon devices is not always described with sufficient accuracy by the conventional drift-diffusion model (DDM). The DDM does not describe velocity overshoot, diffusion associated with carrier temperature gradients, or the dependence of impact ionization rates on the carrier energy distributions. The limitations of the DDM indicate the need for more general transport models. Solutions of the full Boltzmann transport equation (BTE) are desirable, but the associated computational requirements are presently too high for general use. Approximations applied to the full BTE lead to more tractable transport models. Two of the more significant classes of such transport models are energy balance models (EBM's) [1] and hydrodynamic models (HDM's) [2].

The full HDM [2] is a set of equations that describes conservation of carrier density, momentum and energy. The equations are tightly coupled and highly nonlinear. Reliable algorithms for 1D solutions have been developed only recently [3]. A simplified HDM is widely used and gives results that are generally similar to the full HDM [4,5,6]. The simplified HDM is obtained by neglecting a time dependent term and a convective term in the carrier momentum equation, and neglecting the drift-related part of the electron energy in the energy balance equation. The EBM starts from the perspective of energy balance [1]. The simplified HDM and the EBM lead to similar equations, but there are differences in the expressions for current and energy flux densities.

Industry has an immediate need to simulate advanced submicron transistors accurately, but the relative merits of EBM and HDM variants is still an academic research topic. The EBM and the simplified HDM have therefore *both* been incorporated into the general purpose device simulator SPISCES-2B. The implementation, and results obtained using the models, are described in this paper.

## II. MATHEMATICAL MODEL AND NUMERICAL TECHNIQUES

The focus here is on the differences that arise in the current density and energy flux equations for the EBM and the HDM. The electron current density equations of the EBM and simplified HDM models are:

$$\mathbf{J}_n = q \mu_n \left[ \frac{k_B T_n}{q} \nabla n - n \nabla \psi + \frac{k_B}{q} (1 + \xi_n) n \nabla T_n \right] \quad (EBM)$$

$$\mathbf{J}_n = q \mu_n \left[ \frac{k_B T_n}{q} \nabla n - n \nabla \psi + \frac{k_B}{q} n \nabla T_n \right] \quad (HDM)$$

The electron energy flux equations of the models are:

$$\mathbf{S}_n = - K_n (T_n) \nabla T_n - \frac{k_B \delta_n}{q} \mathbf{J}_n T_n \quad (EBM)$$

$$\mathbf{S}_n = - K_n (T_n) \nabla T_n - \frac{5}{2} \frac{k_B}{q} \mathbf{J}_n T_n \quad (HDM)$$

$$K_n (T_n) = q n \mu_n \left( \frac{k_B}{q} \right)^2 \delta_n T_n \quad \delta_n = \frac{5}{2} + \xi_n, \quad \xi_n = \frac{d \ln \mu_n}{d \ln T_n}$$

The EBM and simplified HDM would correspond if  $\xi_n$  was identically equal to zero. (i.e. if mobility was independent of carrier temperature). This condition is never met in practice. A popular model for the temperature dependence of the electron mobility in silicon is:

$$\mu_n (T) = \frac{\mu_0}{\left[ 1 + \left( \frac{3}{2} \frac{k_B \mu_0}{q v_s^2 \tau_e} \right)^2 (T_n - T_0)^2 \right]^{1/2}}$$

For high temperatures such that  $T_n \gg T_0$ ,  $\xi_n = -1$ ,  $\delta_n = 3/2$ , and  $1 + \xi_n = 0$ . The  $\nabla T_n$  term of the current density equation is effectively eliminated for the EBM, but not for the HDM. The above equations have been incorporated in SPISCES-2B. Great care was taken with the spatial discretization of the energy balance equations. Expressions for the energy flux densities were reformulated in a form similar to the current densities, and associated Scharfetter-Gummel type approximations were derived. Spatial oscillations encountered with previous approaches were thereby virtually eliminated. Somewhat related ideas are discussed elsewhere [5, 7]. For steady-state calculations two iterative procedures are used. The first uses Gummel iteration for all equations. The second uses a Newton method for updating  $\psi$ ,  $n$ , and  $p$ , followed by decoupled solution of the energy balance equations. The second procedure is invoked automatically if the first procedure has not converged after a certain number of Gummel iterations. For each bias point the initial guess for the potential is determined using the solution of the total current equation. An extension of the absolutely stable half-implicit scheme [8] is used for time-stepping.

### III. RESULTS

The first example is a 1D  $n^+nn^+$  ballistic diode with an  $n^+$  doping of  $5 \cdot 10^{17}$ , an  $n$  doping of  $2 \cdot 10^{15}$ , and an  $n$  region length of 0.4 microns. An energy relaxation time of 0.4 ps was assumed. Fig.1 shows electron velocity profiles for an applied bias of 1.5V for the EBM and HDM models. The HDM predicts a spurious velocity spike in the vicinity of the collecting  $nn^+$  junction. This confirms earlier indications that the EBM gives results in better agreement with Monte-Carlo simulation [5]. HDM results are believed to be due to overestimation of the thermal diffusion

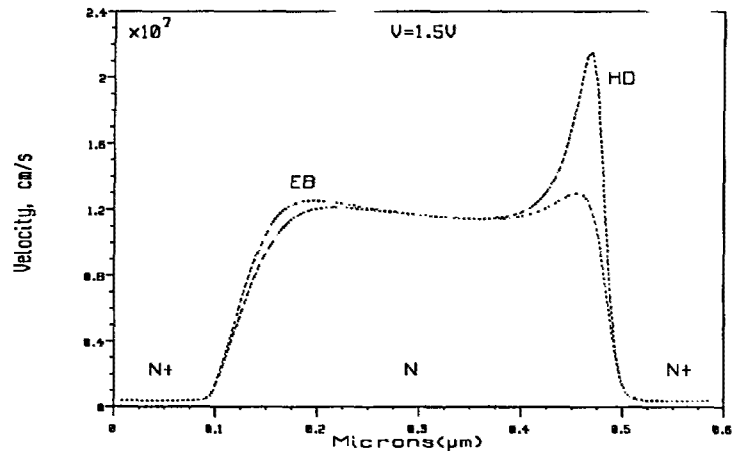


Figure 1. Electron Velocity Distribution in the  $n^+nn^+$  Diode

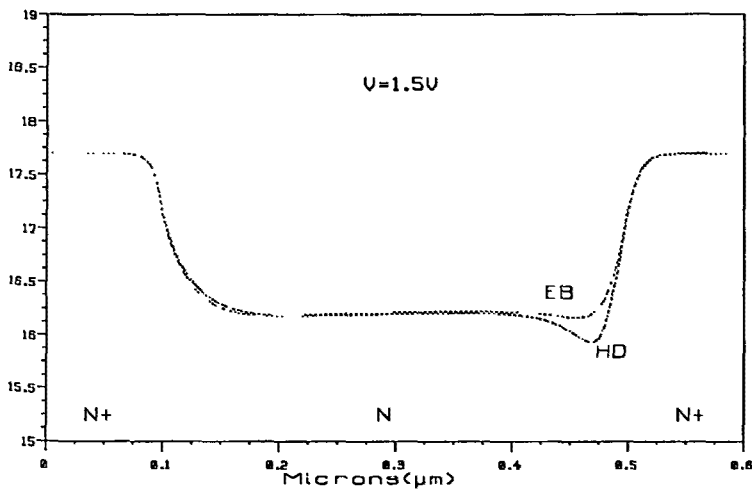


Figure 2. Log Electron Concentration in the  $n^+nn^+$  Diode

qualitative form as the EBM and HDM results. The failure of the DDM to predict *qualitatively* correct substrate currents is because it neglects the nonlocal nature of impact ionization and consequently overestimates the amount of impact ionization. The EBM and HDM results are qualitatively similar, but the substrate current predicted by the HDM is only about half that predicted by the EBM, because the HDM has fewer carriers in the region of peak carrier temperature.

current in the current density expression. Thermal diffusion makes carriers leave the point where the carrier temperature is at a maximum. The electron concentration is thus lower in this region (see figure 2), and to maintain current continuity the mean velocity must be higher.

Figure 3 shows substrate currents calculated using the DDM, EBM, and HDM for a conventional LDD MOSFET with a  $0.7 \mu\text{m}$  channel length. Experimental measurements on such structures have the same

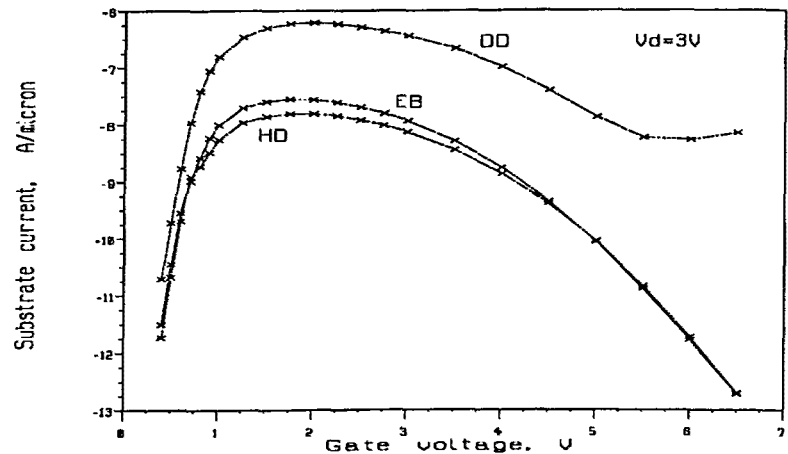


Figure 3. Log Substrate Current Versus Gate Voltage for the DD, EB and HD Models

A similar effect is observed in the results of BJT simulation. A realistic structure with an effective base width of  $0.15 \mu\text{m}$  and a collector region doped at  $7 \cdot 10^{16} \text{cm}^{-3}$  was simulated. Figure 4 shows the base current as a function of the collector-emitter voltage with the base-emitter voltage held at  $0.75\text{V}$ . The DDM overestimates the amount of impact ionization and predicts an earlier drop off in base current. The EBM and HDM both predict higher breakdown voltages. The HDM again predicts less impact ionization than the EBM due to its overestimation of thermal diffusion.

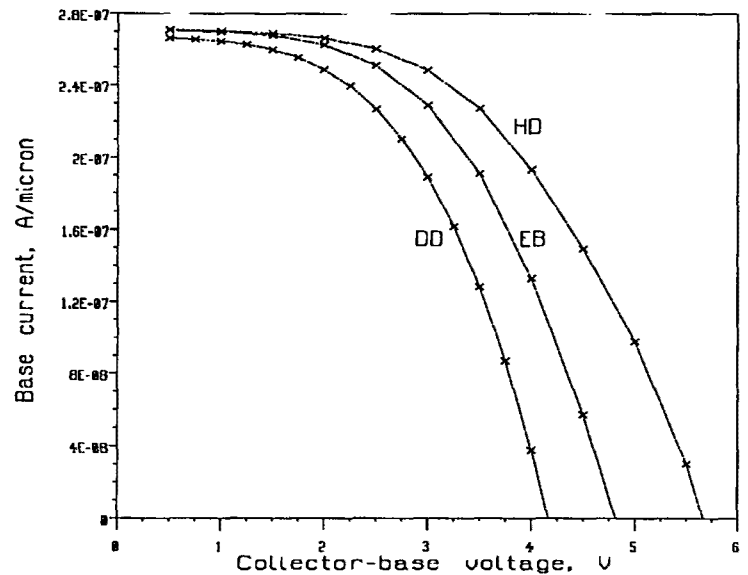


Figure 4. Base Current Versus Collector-Base Voltage for the DD, EB and HD Models

#### IV. CONCLUSIONS

Two nonlocal models of charge transport have been added to the general purpose device simulator SPISCES-2B. The numerical techniques employed provide a robust and reliable implementation. The evidence suggests that the EBM may be more useful than the HDM, but this conclusion must be tentative until confirmed by careful comparisons with experimental data.

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