SIMULATION OF SEMICONDUCTOR DEVICES AND PROCESSES Vol. 4
Edited by W. Fichtner, D. Aemmer - Zurich (Switzerland) September 12-14, 1991 - Hartung-Gorre

An Impact Ionization Model for Two-Carrier Energy-Momentum Simulation

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Abstract

Conventional numerical drift-diffusion simulation assumes that the carriers are in equilibrium with the local electric field at all times. It is well-known however that at high fields, significant carrier heating can occur and these high temperatures may affect the device response. Thus, a wide variety of hydrodynamic or energy/momentum numerical models have been developed to allow the simulation of non-equilibrium effects such as velocity overshoot and carrier diffusion due to temperature gradients.

Although mobility models for such simulations have been extensively investigated, far less work has been done in modelling carrier generation and recombination, especially impact ionization. Thus, it is still unclear how the effects of carrier heating will modify the response of devices in which impact ionization is significant.

In this paper, we investigate this area by comparing a conventional two-carrier drift-diffusion model incorporating a field-dependent impact ionization coefficient with a hydrodynamic formulation in which the carrier generation is a function of local carrier temperature. These models are applied to the simulation of a $p^+n^-n^+$ IMPATT device. We show that in forward bias where little carrier heating occurs, the two models are equivalent. At high reverse bias however, the results are quite different. The drift-diffusion model overestimates the reverse leakage current compared to the energy/momentum formulation. We show that this is due not only to a larger ionization coefficient for the field-based model, but also a different spatial distribution of carrier generation. This is a non-local effect that cannot be predicted using the conventional approach.

1 The Model Equations

Two-dimensional simulation models using the drift-diffusion formulation have been used successfully in many devices [1, 2, 3]. Our model is based on a two-carrier formulation including conservation of momentum and energy (hydrodynamics) [4] implemented in the CHORD simulator [5]. For electrons we have

$$\frac{\partial n}{\partial t} = \nabla \cdot (n\mathbf{v_n}) = n_{scat} \quad (1)$$

$$\frac{\partial \mathbf{p_n}}{\partial t} = \nabla \cdot (\mathbf{v_n}\mathbf{p_n}) - qn\nabla\psi + \nabla(nkT_n) = \mathbf{p}_{nscat} \quad (2)$$

$$\frac{\partial w_n}{\partial t} + \nabla \cdot (\mathbf{v_n} w_n) - qn\mathbf{v_n}\nabla\psi + \nabla \cdot (\mathbf{v_n} nkT_n) - \nabla \cdot (\kappa_n \nabla T_n) = w_{nscat} \quad (3)$$

and for holes

$$\frac{\partial p}{\partial t} = \nabla \cdot (p\mathbf{v_p}) = p_{scat} \quad (4)$$

$$\frac{\partial \mathbf{p_p}}{\partial t} = \nabla \cdot (\mathbf{v_p p_p}) + qp\nabla\psi + \nabla(pkT_p) = \mathbf{p_{pscat}} \quad (5)$$

$$\frac{\partial w_p}{\partial t} + \nabla \cdot (\mathbf{v_p} w_p) + qp\mathbf{v_p}\nabla\psi + \nabla \cdot (\mathbf{v_p} pkT_p) - \nabla \cdot (\kappa_p \nabla T_p) = w_{pscat} \quad (6)$$

We also require Poisson's equation and the heat conduction equation:

$$\nabla^2\psi + \frac{q}{\epsilon}(p - n + N_D - N_A) = 0 \quad (7)$$

$$\rho c_l \frac{\partial T_l}{\partial t} - \nabla \cdot \kappa_l \nabla T_l = T_{lscat} \quad (8)$$

The energy, momentum and lattice heat intra-band scattering terms are modelled using the relaxation time approximation[6] Inter-band scattering includes emission and capture via traps, Auger recombination and impact ionization. We now focus on the impact ionization term in the carrier scattering terms n_{scat} and p_{scat}.

2 Energy Based Impact Ionization

The inter-band scattering term due to impact ionization is usually expressed as the product of the local particle current and an ionization rate

$$n^{ii}_{scat} = n|v_n|\alpha_n \qquad p^{ii}_{scat} = p|v_p|\alpha_p \quad (9)$$

In traditional drift-diffusion based simulation, the ionization rates are based on the local electric field, usually in an exponential relationship such as the Chynowth model[7]

$$\alpha_n = a_n e^{-b_n/E} \qquad \alpha_p = a_p e^{-b_p/E} \quad (10)$$

This formulation will over-estimate the ionization rates in very small devices since cool carriers entering a high field region must travel several tenths of a micron before they gain sufficient energy to ionize i.e. the dark space effect[8]. One way to overcome this effect is to write the ionization rates as functions of the carrier energy or velocity. This is problematic in a drift-diffusion model, but simple using a hydrodynamic formulation.

Wang[9] proposed a model in which the ionization rates were expressed as functions of the average carrier velocity. Scholl et. al.[10] and Quade et. al.[11] base their model on carrier energy. In our approach, we derive an expression relating electric field and carrier energy[4]

$$E(W_n) = \frac{W_n - W_l}{2v_{sat}q\tau_{wn}} + \left\{ \left[\frac{W_n - W_l}{2v_{sat}q\tau_{wn}}\right]^2 + \frac{W_n - W_l}{q\mu_0\tau_{wn}} \right\}^{\frac{1}{2}} \quad (11)$$

Here $E(W_n)$ is a scalar function of energy and can be used as an equivalent field parameter. Since we are interested only in energies $W >> W_l$, this becomes

$$E(W_n) = \frac{W_n}{qv_{sat}\tau_{wn}} \quad (12)$$

The energy dependent ionization rates are now given by

$$\alpha_n = a_n \exp\{-b_n q v_{sat} \tau_{wn}/w_n\} \qquad \alpha_p = a_p \exp\{-b_p q v_{sat} \tau_{wp}/w_p\} \tag{13}$$

This result may also be used to generate consistent expressions for energy, momentum and lattice temperature scattering.

3 Simulation Results

The forward bias simulation for both drift-diffusion and energy-momentum formulations is shown in Figure 1. Since the electric field is low in this case, hot carrier effects are minimal and the two models show excellent agreement. The same results for reverse bias are shown in Figure 2. Here we see a dramatic difference between field-based impact ionization and energy-based. The field-based model produces currents many orders of magnitude greater the the energy model. The reason for this is shown in Figure 3. Here we plot the ionization rates across the device at a bias of -20 V . We can see that the region in which ionization is possible is about 30% smaller in the energy model than in the field-based model. This is due to the finite distance carriers must travel to reach high energy, an effect impossible to model in a drift-diffusion simulation. Note also that the energy model has a high ionization rate only in regions where the carrier concentration is low. The field-based model allows high ionization rates in the transition regions near the junctions where carrier densities rise rapidly to their equilibrium values. Since the generation rate is proportional to the product of the carrier concentrations and α, a much higher current is produced in this case.

Since our impact ionization model is based on Equation 11, we show in Figure 4 how well this ties in with the simulated energy. Here we plot the peak carrier temperature along with the values predicted by Equation 11. The energy is converted to temperature using $W_n = 3kT_n/2$. We see that there is good agreement except at very high reverse bias where the large numbers of cool carriers generated by impact ionization lower the temperature.

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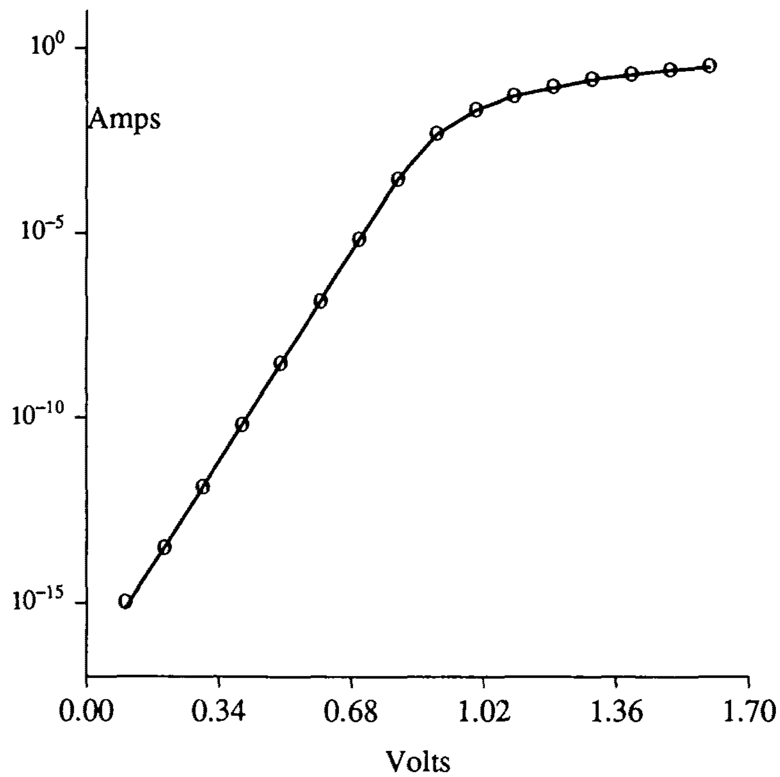

Figure 1: Comparsion of the forward I-V characteristics using drift-diffusion (solid line) and energy-momentun (o) models

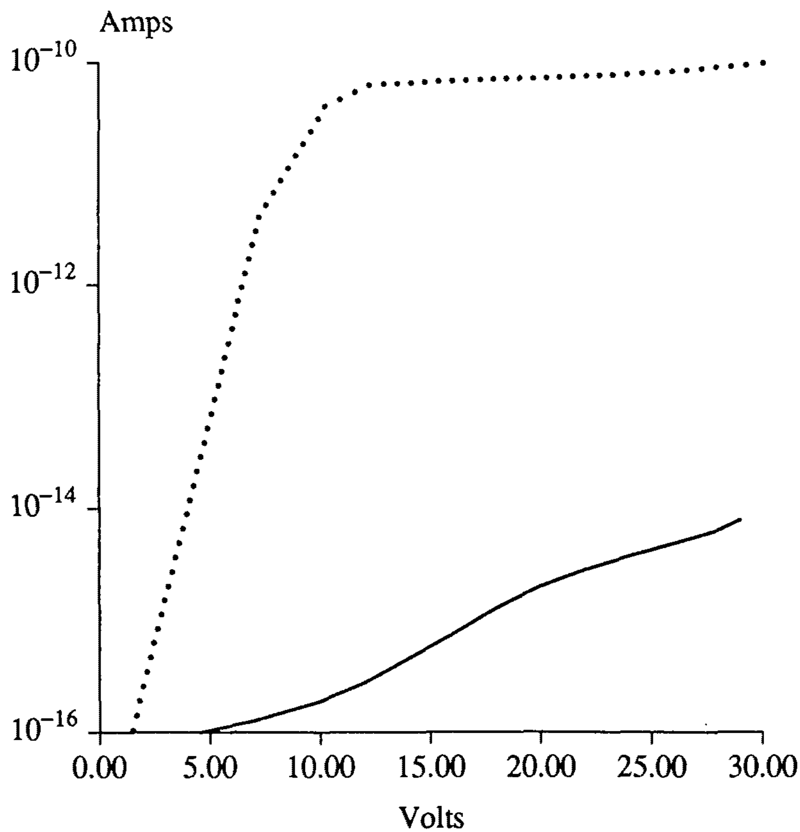

Figure 2: Reverse bias I-V characteristics using energy-momentum results with energy dependent impact ionization rate (solid) and drift-diffusion with field-dependent rate (dotted).

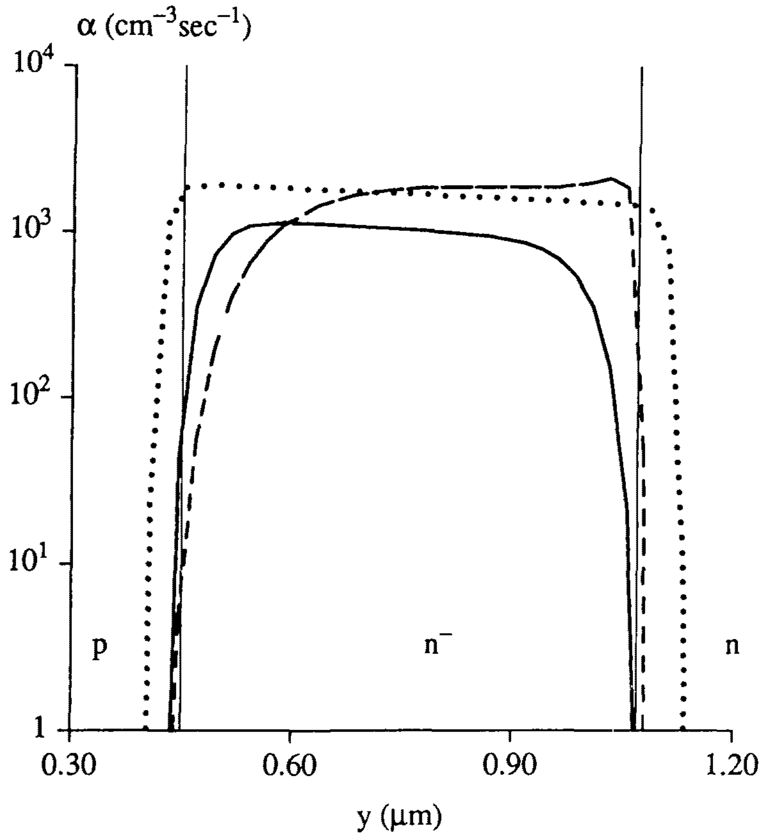

Figure 3: Ionization rates versus distance for the field-based model (dotted) and energy-based electrons (dashed) and holes (solid). The straight lines mark the junctions

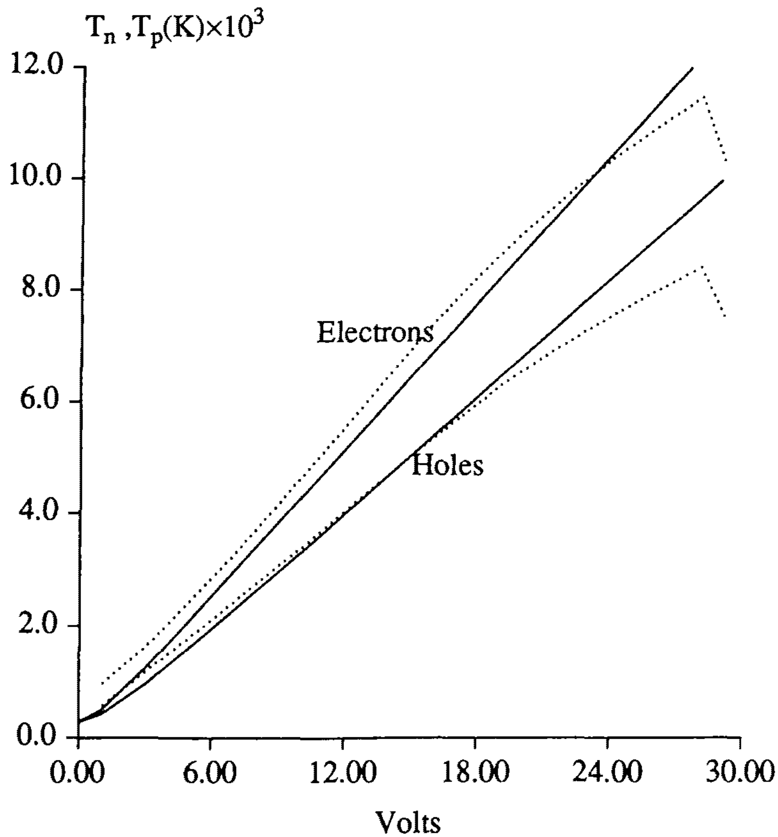

Figure 4: Peak electron and hole temperatures as a function of reverse bias from simulation(dotted) and Equation 11.