Device simulation by means of a direct solution of the coupled Poisson/Boltzmann Transport equations

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Abstract

A method for directly solving the coupled Poisson/Boltzmann Transport equation including a new model for the collision term is presented. This method yields the complete momentum distribution function from which all quantities of interest to the device modeller can easily be calculated. Current continuity is implicit in the model. The method is demonstrated by simulating an n^+-n-n^+ silicon structure.

I Introduction

With decreasing device dimensions there is a need to accurately model the effects of hot carriers. Solutions of the drift-diffusion and hydrodynamic models have been widely used to model the behaviour of many submicron devices [1]. However, in the analysis of the programming of EPROMs [2] and many other phenomena found in modern small geometry devices, the complete carrier distribution function in both ordinary space and momentum space is required for accurate simulation. Recently there has been increased interest in solving the Boltzmann Transport Equation (BTE) to obtain the distribution function [3, 4]. Knowing the distribution function and electric potential, all other quantities of interest can be calculated. In this paper a method for solving the coupled Poisson/Boltzmann Transport equations is presented.

II Mathematical model

The BTE for steady state conditions for a semiconductor device is

$$\vec{v}.\,\vec{\nabla}_r f - \frac{q}{\hbar}\vec{E}.\,\vec{\nabla}_k f = -\left(\frac{\partial f}{\partial t}\right)_{COLL} \tag{1}$$

where $\vec{v}$ is the carrier velocity, $\vec{E}$ is the electric field and f is the distribution function. The right hand side of equation 1 is the collision term and is often approximated using the relaxation time approximation [5] as

$$\left(\frac{\partial f}{\partial t}\right)_{COLL} \simeq \frac{f - f_0}{\tau} \tag{2}$$

where f_0 is the distribution function at equilibrium and τ is the relaxation time. Integrating equation 1 over momentum gives the current continuity equation in the abscence of generation-recombination. However, if the relaxation time approximation is used the integral of the collision term over momentum is, in general, not equal to zero because the electron concentration differs

from equilibrium to non-equilibrium conditions. Thus the relaxation time approximation does not satisfy the condition of current continuity, and is therefore invalid for non-equilibrium conditions.

A new approximation is made to the collision term of the BTE

$$\left(\frac{\partial f}{\partial t}\right)_{COLL} \simeq \frac{f - g(\vec{k})n}{\tau} \tag{3}$$

$$\int g(\vec{k})d\vec{k} = 4\pi^3 \tag{4}$$

where $g(\vec{k})$ is a Gaussian function in $\vec{k}$ and n is the carrier concentration. The carrier concentration is given by

$$n = \frac{1}{4\pi^3}\int f d\vec{k} \tag{5}$$

If τ is a function of ordinary space only, then the integral of equation 3 over momentum space is always equal to zero. Therefore this approximation always satisfies the condition of current continuity. Close to equilibrium the new approximation approaches the relaxation time approximation because

$$g(\vec{k})n = f_0(\vec{k}) \tag{6}$$

at equilibrium.

III Discretization in one spatial and one momentum dimension

The discretization of the governing equations in all three spatial and three momentum dimensions would lead to a very large system of equations to be solved simultaneously. Therefore only one spatial and one momentum dimension are included. Poisson's equation is discretized in one spatial dimension using finite differences. The BTE is discretized in one spatial and one momentum dimension using finite differences, the gradients being approximated using central differences. With just one spatial and one momentum dimension it is assumed that the distribution of carriers in the other two momentum dimensions is the same as at equilibrium and that collisions only scatter carriers forwards or backwards in that one momentum dimension. The velocity is modelled on a parabolic band structure. For simplicity the BTE and Poisson's equation are solved using Gummel's method [5] subject to appropriate boundary conditions.

IV Boundary conditions

The contacts are taken to be Ohmic. The potential at the contacts is set equal to the sum of the applied voltage and the built in potential. For the BTE a Dirichlet boundary condition is imposed at the extremities of momentum and a natural boundary condition is applied at the contacts. At the maximum and minimum values of momentum, the distribution function is set equal to the equilibrium distribution function. At the contacts the gradient of the distribution function is set equal to zero assuming there is a neutral space charge region close to the contacts.

V Results

The model is applied to simulating the operation of a lightly doped n^+-n-n^+ diode. The n^+-n-n^+ diode has an overall length of 10 microns with the outer 2.5 microns at each side doped at 10^{14} cm^{-3}. The 5 micron region in the centre is doped at 10^{13} cm^{-3}. The contact at the right is grounded and a bias is applied to the left contact. Figure 1 shows the potential distribution across the device for an applied bias of 400 mV. Figure 2 shows the electron concentration under the same conditions. The distribution function at the right contact is shown in figure 3 along with the distribution function where the carrier concentration is lowest (3.5 μm from the left contact). The greater displacement from equilibrium of the distribution function where the carrier

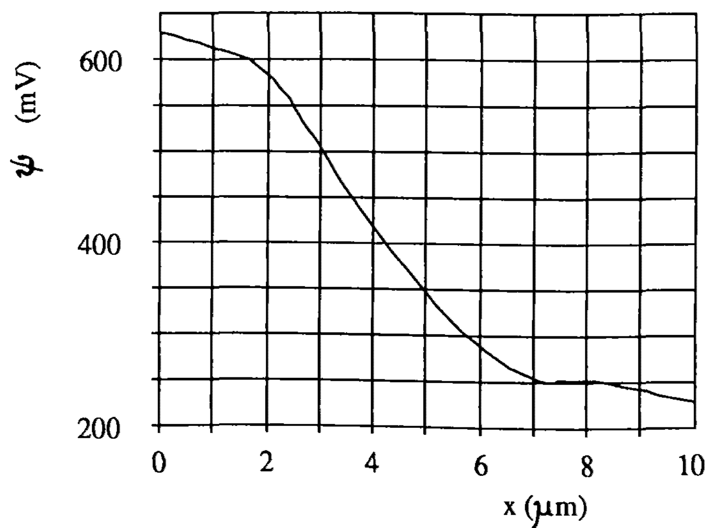

Figure 1: Electric potential (ψ) for a bias of 400 mV applied to the left contact.

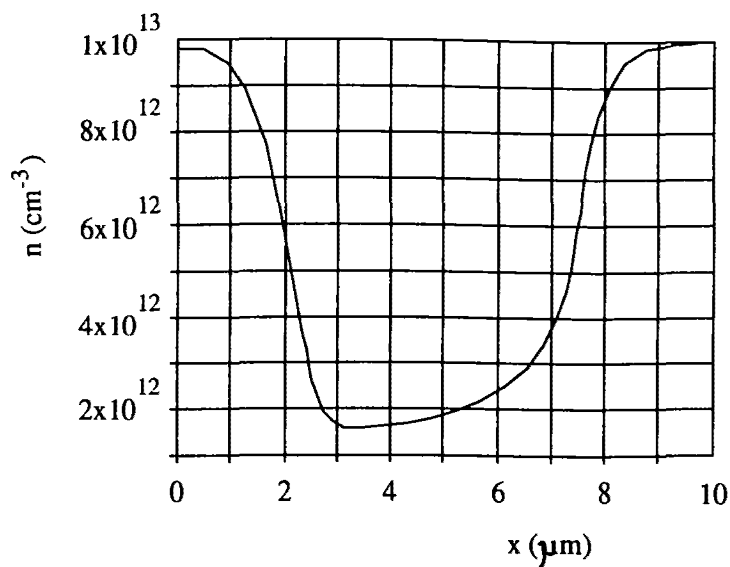

Figure 2: Electron concentration for a bias of 400 mV applied to the left contact.

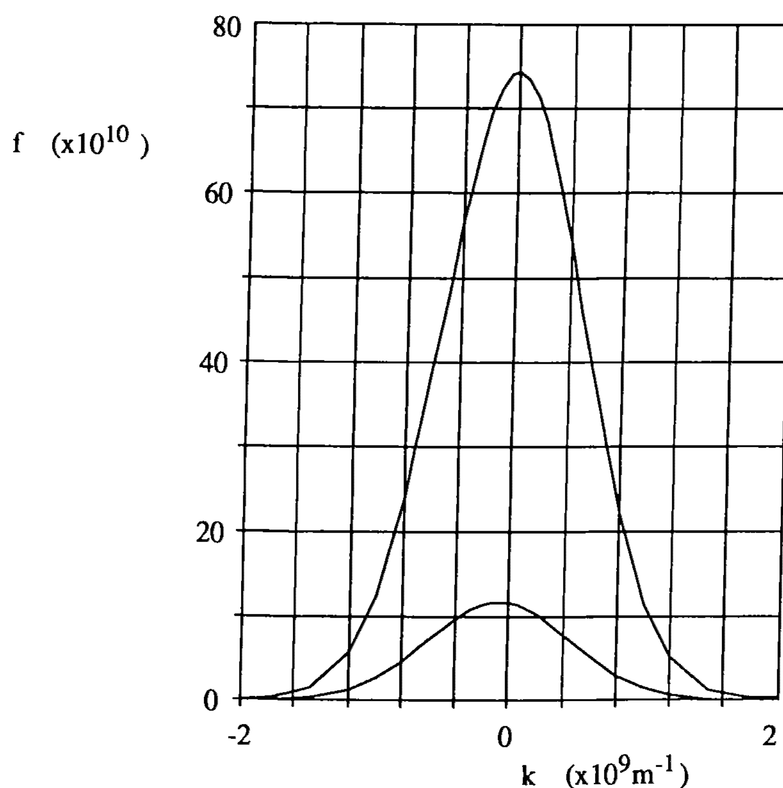

Figure 3: Shape of distribution function

concentration is lower corresponds to a greater average energy of the carriers towards the centre of the device. Figure 4 shows the average energy of electrons at 300K across the device. Note that the carriers a distance 2.5 microns from the right contact (barrier region) have an average energy lower than the lattice thermal energy, a phenomenon which occurs when carrier diffusion is in the same direction as the external force on the carriers [6]. Current continuity is implicit in the model and is observed for all applied biases. Current density in the device is easily calculated from the momentum distribution function. The current density versus applied bias for this structure is shown in figure 5. This result is identical to that predicted by the drift diffusion model.

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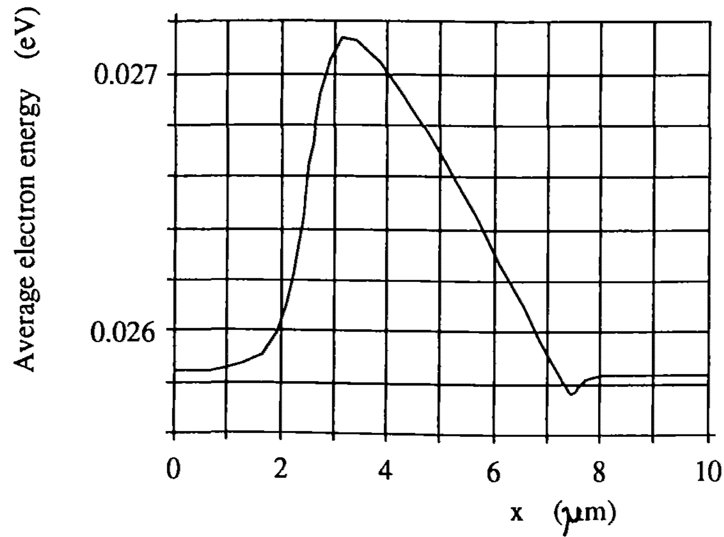

Figure 4: Average electron energy for a bias of 400 mV applied to the left contact.

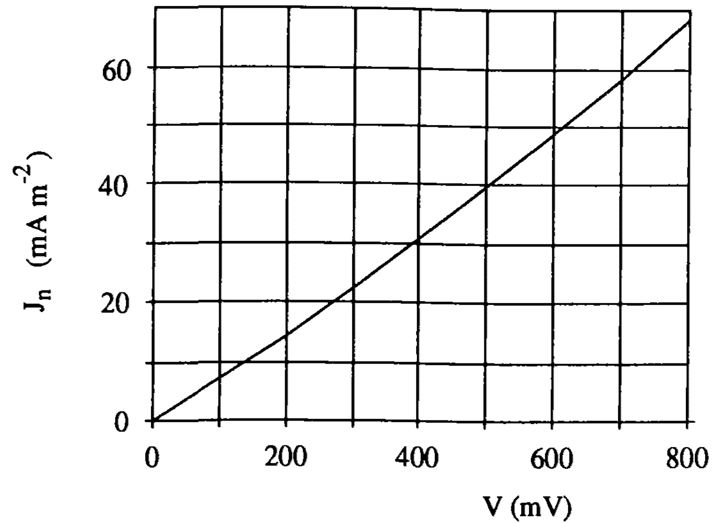

Figure 5: Current density versus applied voltage.