

Invited**New Approaches to Device Simulation for Submicron Structures**

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"Classical" concepts of mobility and diffusion constant, are averages over time scales long compared with transit times in submicron-scale devices, and are therefore not applicable to the simulation of devices of this scale. Monte Carlo and Energy Transport methods are feasible for this problem, however. The derivation of the energy transport method from the Boltzmann equation is described, and typical results of energy transport simulations of GaAs MESFETs and Si MOSFETs are reviewed.

I. INTRODUCTION

As semiconductor devices are reduced in size, the time scales in which they operate approach that of the internal dynamical processes that determine their behavior. However, the concepts of "mobility" or "saturation velocity" which have classically been used to describe electron transport behavior are in fact averages over relatively long times. Since these necessary averaging times may exceed the transport time in a submicron-scale device, these concepts are invalid for analysis of such devices, and alternative approaches to their simulation must be developed.

One such simulation approach is probabilistically based, and is appropriately called the Monte Carlo (MC) method. In this method the electron scattering processes in devices are directly simulated, with weighted probability functions based on the real material physics used to determine the type of scattering process, time between scattering events, and state after scattering. The Monte Carlo method has been successful in simulating the properties of bulk--essentially one-dimensional--materials[1], and has also been applied to the simulation of two-dimensional devices[2]. The Monte Carlo method is relatively inexpensive for materials calculations, but may become prohibitively expensive for the simulation of two-dimensional

devices.

An alternative approach, which has been called the "energy transport" (ET) method is now growing in popularity for device simulation due to the relative ease and efficiency with which it can be used. The ET method does require more approximations to the real physics of devices than does the MC method, but is a practical tool for the simulation of submicron-scale devices of virtually any material whose properties can be calculated using a relatively inexpensive one-dimensional MC calculation. The ET method was originally used by Stratton in an analysis of transport in Schottky barriers[3], and has subsequently been applied to the analysis of Gunn diodes[4], GaAs MESFETs[5], and Si MOSFETs[6] and bipolar transistors[7].

II. FUNDAMENTALS OF THE ENERGY TRANSPORT METHOD

The ET method is based on the Boltzmann equation, which is in turn a phenomenological equation which incorporates conservation of mass, energy, and momentum implicitly to describe the rate of change of the distribution of particles in real and momentum space. The distribution function is a function of position, momentum, and time. Upon solution of the Boltzmann equation, this distribution function must be integrated in order to obtain such physically observable properties as energy,

velocity, or density, Therefore, the Boltzmann equation in its classical form yields the most general possible descriptor of the system.

In the ET method, the Boltzmann equation is integrated before solution, and the quantities solved for are the physical observables themselves. Given at least some a priori information about the nature of the distribution function, solution of the integrated Boltzmann-derived equations--called "moments" of the Boltzmann equation--is relatively simple. Different integral operators are used to extract conservation equations for electron density, momentum and energy.

The basic Boltzmann equation

$$\frac{\partial}{\partial t} f(r, k, t) + v(k) \cdot \nabla_r f(r, k, t) - \frac{1}{\hbar} \nabla_r V(r, t) \cdot \nabla_k f(r, k, t) = \left(\frac{\partial f}{\partial t} \right)_{coll} \quad (1)$$

where f is the distribution function in momentum-energy space and E is the electric field, is multiplied by the following operators and integrated over k -space in turn:

$$n = \langle 1 \rangle \quad (2)$$

$$nv = \langle v(k) \rangle \quad (3)$$

$$nw = \frac{m^*}{2} \langle |v(k)|^2 \rangle \quad (4)$$

The following equations for particle, momentum, and energy continuity, result:

$$\frac{\partial n}{\partial t} + \nabla \cdot (nv) = \left(\frac{\partial n}{\partial t} \right)_{coll} \quad (5)$$

$$\frac{\partial v}{\partial t} + (v \cdot \nabla)v = -\frac{1}{m^*} \nabla V - \frac{1}{m^* n} \nabla \cdot (nk_B T) + \left(\frac{\partial v}{\partial t} \right)_{coll} \quad (6)$$

$$\frac{\partial w}{\partial t} + (v \cdot \nabla)w = -(v \cdot \nabla)V - \frac{1}{n} \nabla \cdot (nk_B T \cdot v) - \nabla \cdot Q + \left(\frac{\partial w}{\partial t} \right)_{coll} \quad (7)$$

These equations incorporate the temperature tensor T , the heat-flow vector Q , and the energy w , defined as

$$\frac{1}{2} nk_B T = \frac{m^*}{2} \langle (v(k) - v)(v(k) - v) \rangle \quad (8)$$

$$Q = \frac{m^*}{2} \langle (v(k) - v) |v(k) - v|^2 \rangle \quad (9)$$

$$w = \frac{1}{2} m^* v^2 + \frac{1}{2} Tr(k_B T) \quad (10)$$

The approximation of constant effective mass has been made in writing the equations as above. The set of three equations (5)(7) contains five variables. To allow solution of the set of these

equations then, at least one thing must be known about the distribution function. The usual statement made is that the distribution function is symmetrical, which leads to $Q = 0$, and produces a diagonal temperature tensor T . In addition, if the distribution function is taken to be isotropic, the temperature tensor reduces to a scalar. Under these conditions, equations (5)-(7) reduce to functions of the three variables density (n), velocity (v), and energy (w).

$$\frac{\partial n}{\partial t} + \nabla \cdot (nv) = \left(\frac{\partial n}{\partial t} \right)_{coll} \quad (11)$$

$$\frac{\partial v}{\partial t} + (v \cdot \nabla)v + \frac{1}{m^*} \nabla V + \frac{1}{m^* n} \nabla \cdot (nk_B T) = \left(\frac{\partial v}{\partial t} \right)_{coll} \quad (12)$$

$$\frac{\partial w}{\partial t} + (v \cdot \nabla)w + (v \cdot \nabla)V + \frac{1}{n} \nabla \cdot (nk_B T \cdot v) = \left(\frac{\partial w}{\partial t} \right)_{coll} \quad (13)$$

and the total energy is simply

$$w = \frac{1}{2} m^* v^2 + \frac{3}{2} k_B T \quad (14)$$

The system is taken to be in a steady state, i.e., although the distribution function is itself a function of time, that function of time does not change with time.

Solution of equations (11)-(13) is further simplified if the kinetic energy of the drifting electrons is assumed to be negligible compared to their thermal kinetic energy; and the electron scattering processes are described by energy-dependent relaxation times. The relative magnitudes of thermal and kinetic energy may be checked by calculation, but the use of relaxation times may be more troublesome. The scattering processes of importance in silicon, such as impurity and acoustic and optical phonon scattering, may be described by relaxation times, but polar optical phonon scattering, which is of major importance in compound semiconductors at high fields, rigorously may not. However, if the electron energy is much higher than the polar optical phonon energy use of a scattering time for this process is not a bad approximation [8]. One dimensional calculations performed to compare the MC and ET methods [9] do in fact show good agreement in the initial stages of electron acceleration, when electrons have not yet had time to lose energy in intervalley scattering processes; agreement is somewhat less good as time passes. In

the end, As we have noted elsewhere [5], the equations which result "provide a good engineering-level description of the important hot electron effects in the device".

The energy-dependent relaxation times may be obtained from onedimensional MC calculations. for the properties of bulk material under the influence of a uniform electric field. If devices in which multi-valley transport phenomena occurs are to be simulated (e.g., GaAs, or where quantum electron confinement is important) either separate equation sets, in which the appropriate effective mass and relaxation-time values for each valley are inserted, or a model which uses quantities averaged over both upper and lower-valley electrons must be used. In the latter case the fraction of the total electron population in each valley, a function of electron energy, may also be obtained from one-dimensional Monte Carlo calculations, and the resulting energy equation is

$$w = \frac{1}{2} m^* v^2 + \frac{3}{2} k_B T + G_U(w) \Delta_{LU} \quad (15)$$

An energy-dependent effective mass may be used in the calculations at the cost of some additional computing time. The incorporation of such energy dependence may be justified in regions where electrons can reach very high energies and where the band structure is known with sufficient accuracy. It is further not necessary to take the distribution function as symmetrical, in which case an additional moment equation for Q would have to be solved.

The subject of approximations in device simulation calculations should, in any case, always be viewed in the light of how well both the materials and device parameters are known. The materials themselves are often sufficiently variable, and device processing and measurement techniques yield sufficiently ambiguous results, to make "engineering-level" formulations quite adequate.

III. EXAMPLES OF TWO-DIMENSIONAL CALCULATIONS

Calculations of the properties of both Si and GaAs MESFETs may be simplified in certain cases by making use of certain qualitative features of the electron dynamics of these devices as illustrated

by conventional two-dimensional simulations. The features that have been used are (a): electrons cannot be heated by the field in certain regions of the device where the electrostatic potential is depressed below the source potential by the charge density; and (b) in regions where carrier heating is significant both drift velocity and electric field are almost entirely in the longitudinal direction. As a result of these features, the carrier heating can be ignored entirely in certain parts of the device, and the problem can be considered as primarily a one-dimensional one over the remainder. Results using these simplifications have shown good agreement with two-dimensional Monte Carlo models, an electron-temperature hydrodynamic model, and with experiment[10].

The ET method has also been used to study electron heating along the surface of a short-channel Si MOSFET, leading to a measure of the dependence of gate leakage current on drain doping profile[11], and a full two-dimensional ET MOSFET analysis has shown that velocity overshoot should play an important role in determining the behavior of Si devices with channel lengths under about 0.5 micron and drain voltages over about two volts[6].

IV. CONCLUSIONS

The energy transport method can make two-dimensional simulations of complicated submicron-scale structures a reasonable and relatively economical way of learning more about how they work, and how they may be better designed. Solution of the equations involved may be done using standard computer algorithms, and the approximations involved in their solution are consistent with the accuracy with which simulated device parameters are usually known.

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