DEVICE MODELING USING HYDRODYNAMIC BALANCE EQUATIONS

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ABSTRACT

We describe a semiconductor device modeling program based on hydrodynamic balance equations. This program is is capable of treating multiple carriers in compositionally nonuniform (such as heterostructures) and spatially inhomogeneous device structures, as well as high electric field and associated nonlinear effects. Unlike other balance equation based approaches to device modeling, where the various relaxation rates are treated phenomenologically, or imported from Monte Carlo calculations, our approach is self-contained in that these rates are calculated within the simulation program. The momentum and energy relaxation rates are cast in the form of electric field dependent frictional force and energy transfer functions, with full account of carrier-carrier interaction effects, such as dynamical screening/descreening. These effects are embodied in the dielectric function of the system, which is treated within the random-phase approximation here but can also include exchange-correlation effects. Another advantage of our balance equation approach is that arbitrary energy band structures can be treated, making it suitable for high-field and microwave applications. The simplicity of our technique permit fast and efficient modeling of device performance characteristics, requiring only a fraction of the CPU time needed for Monte Carlo simulations. We have tested the modeling program on simple devices such as an n^+-n-n^+ diode and have obtained good agreement with Monte Carlo simulations.

I. INTRODUCTION

An increasingly popular approach in device modeling is the hydrodynamic balance equation technique, which solves the first few moments of the Boltzmann equation. But the moments equations by themselves do not form a closed set of equations, requiring input of momentum and energy relaxation rates from outside the system. These relaxation rates are supplied from experimental measurements, or from Monte Carlo calculations, and sometimes they are simply taken to be constants. A third way of circumventing this difficulty is to postulate the distribution function with unknown parameters, and use balance equations to solve for these parameters.

Recently, a new balance-equation method for high-field transport in uniform system has been developed[1]. This has subsequently been generalized to weakly nonuniform systems[2]. In addition to the simplicity and transparency of its mathematical structure, the advantages of this method also include its generality of description of nonlinear transport in the presence of an electric field of arbitrary strength, and its ease of treating dynamic, nonlocal carrier-carrier scattering. All the important transport properties are expressed in terms of the carrier density-density correlation function which includes full carrier-carrier interaction within the random-phase approximation (RPA) or beyond.

In this presentation we will describe our balance equation based device modeling, giving particular attention to points of departure from other, more conventional balance equation based device modeling programs.

II. BALANCE EQUATIONS

Within the balance equation approach the following balance equations are used to describe the carrier transport. These are, the equation of continuity,

$$\frac{\partial n}{\partial t} + \vec{\nabla} \cdot (n\vec{v}) = 0, \tag{1}$$

the force/momentum balance equation,

$$\frac{\partial \vec{v}}{\partial t} + \vec{v}(\vec{\nabla} \cdot \vec{v}) = -\frac{2}{3}\frac{\vec{\nabla} u}{mn} + \frac{e}{m}\vec{E} + \frac{1}{mn}\vec{f}, \tag{2}$$

and the energy balance equation

$$\frac{\partial u}{\partial t} = \vec{v} \cdot \vec{\nabla} u = -\frac{5}{3}u(\vec{\nabla} \cdot \vec{v}) - w - \vec{v} \cdot \vec{f}, \tag{3}$$

along with the Poisson equation

$$\nabla^2 \phi = -\frac{e}{\epsilon_0}[n(\vec{R}) - N_D]. \tag{4}$$

These are supplemented by the expression of the average local kinetic energy density of the carrier

$$u(\vec{R}) = 2\sum_{\vec{k}} \epsilon_{\vec{k}} f_0[(\epsilon_{\vec{k}} - \mu(\vec{R}))/k_B T_e(\vec{R})], \tag{5}$$

and that of the local chemical potential $\mu(\vec{R})$ which is related to the local electron density $n(\vec{R})$ via the relation

$$n(\vec{R}) = 2\sum_{\vec{k}} f_0[(\epsilon_{\vec{k}} - \mu(\vec{R}))/k_B T_e(\vec{R})], \tag{6}$$

where $\epsilon_{\vec{k}} = \hbar^2 k^2/2m$ and f_0 is the Fermi-Direc function.

The resistive force and the energy loss rate are

$$\begin{aligned} \vec{f} &= n_I \sum_{\vec{q}} |u(\vec{q})|^2 \vec{q} \Pi_2(\vec{q}, \omega_0) \\ &\quad + 2\sum_{\vec{q},\lambda} |M(\vec{q},\lambda)|^2 \vec{q} \Pi_2(\vec{q}, \omega_0 + \Omega_{\vec{q}\lambda}) \left[N\left(\frac{\hbar\Omega_{\vec{q}\lambda}}{k_B T}\right) - N\left(\frac{\hbar(\Omega_{\vec{q}\lambda} + \omega_0)}{k_B T_e}\right)\right], \end{aligned} \tag{7}$$

$$w = 2\sum_{\vec{q},\lambda} |M(\vec{q},\lambda)|^2 \Omega_{\vec{q}\lambda} \Pi_2(\vec{q}, \omega_0 + \Omega_{\vec{q}\lambda}) \left[N\left(\frac{\hbar\Omega_{\vec{q}\lambda}}{k_B T}\right) - N\left(\frac{\hbar(\Omega_{\vec{q}\lambda} + \omega_0)}{k_B T_e}\right)\right], \tag{8}$$

where $\omega_0 = \vec{q} \cdot \vec{v}(\vec{R})$, $N(x)$ is the Bose-Einstein factor, n_I is impurity density, $\Omega_{\vec{q}\lambda}$ is the phonon frequency of wave vector $\vec{q}$ and branch index λ, $u(\vec{q})$ is the electron-impurity interaction potential, $M(\vec{q},\lambda)$ is the electron-phonon coupling matrix element, $\Pi_2(\vec{q},\omega)$ is the density-density correlation function of electrons which can be obtained within the RPA or beyond. Note that $\vec{f}$ and w depend on the position vector $\vec{R}$ through the quantities $n(\vec{R})$, $T_e(\vec{R})$, and $\vec{v}(\vec{R})$.

These equations will uniquely determine $\vec{v}(\vec{R})$, $T_e(\vec{R})$, $u(\vec{R})$, $n(\vec{R})$, $\mu(\vec{R})$, and $\phi(\vec{R})$, for given initial and boundary conditions. All these variables may be time dependent for transient or ac transport processes. Following standard procedures[3,4], these differential equations are turned into difference equations on a space-time grid. The resulting simultaneous nonlinear difference equations are solved using the Newton method[4].

III. AN EXAMPLE—MODELING OF AN n^+-n-n^+ DIODE

The process of device simulation developed here is applied to the simulation of a one-dimensional problem, an $n^+ - n - n^+$ Si diode. This is a symmetric, 0.55 μm structure, with the middle 0.25 μm doped to $N_D = 10^{15}\, cm^{-3}$, and the anode and cathode (each is 0.15 μm long) doped to $5 \times 10^{17}\, cm^{-3}$. There is some smooth grading in doping density at the junctions between the electrodes and the middle, low doping region.

We carry out our modeling for a lattice temperature $T = 300\, K$. In addition to ionized impurity scattering, we include nonpolar optical phonon scattering and deformation potential acoustic phonon scattering. All materials parameters are those of single crystal Si.

For a bias voltage of $0.5\, V$ we have calculated the steady-state carrier density, drift velocity, energy, and electrostatic potential, all as functions of position along the device length. These are depicted in Figure 1. In addition, we also present the calculated resistive force and energy-loss rate in Figure 2.

In summary, we have developed a semiconductor device modeling program, based on hydrodynamic balance equation approach to charge transport. Instead of the usual relaxation rates employed in traditional balance equation based modeling, our method relies on a resistive force function and an energy-loss rate function, which are calculated within the program.

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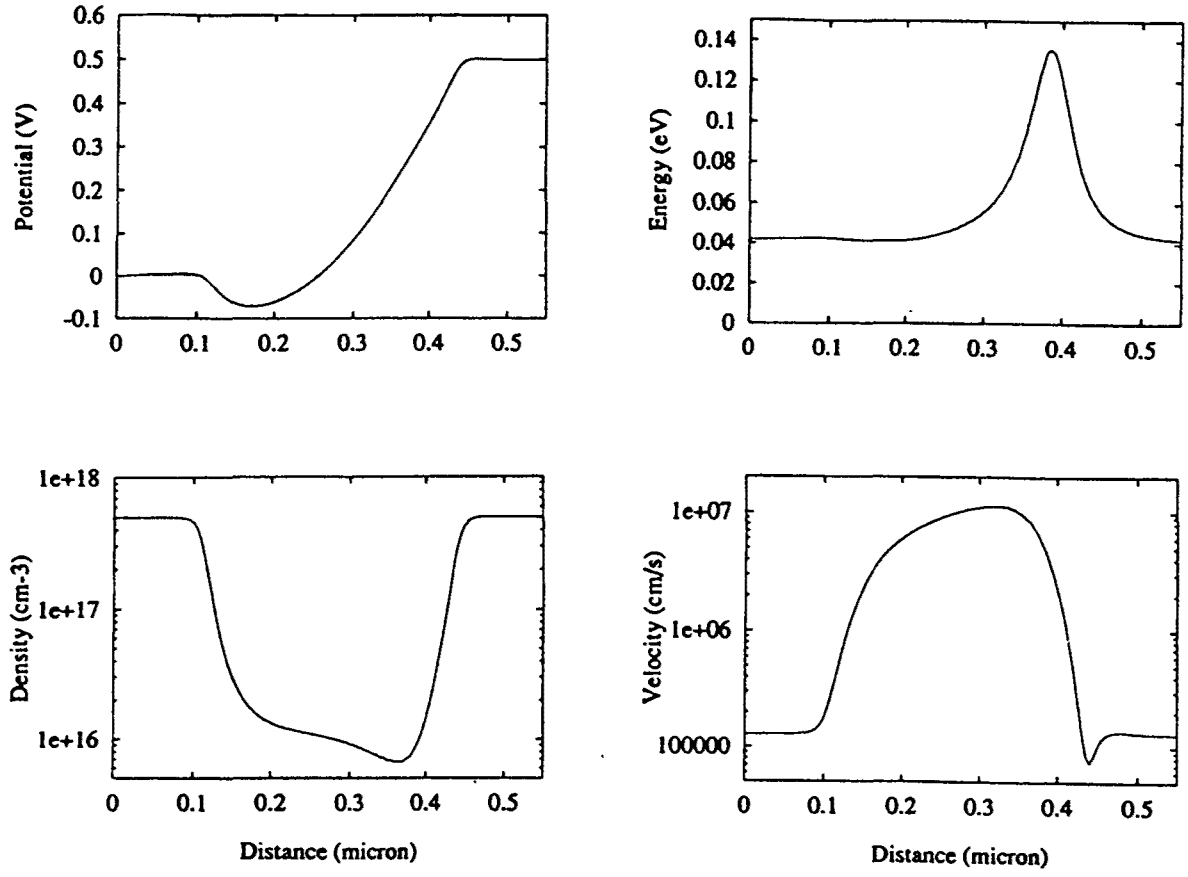

Figure 1: Electron density, drift velocity, energy, and electrostatic potential as functions of position for a bias of 0.5 V.

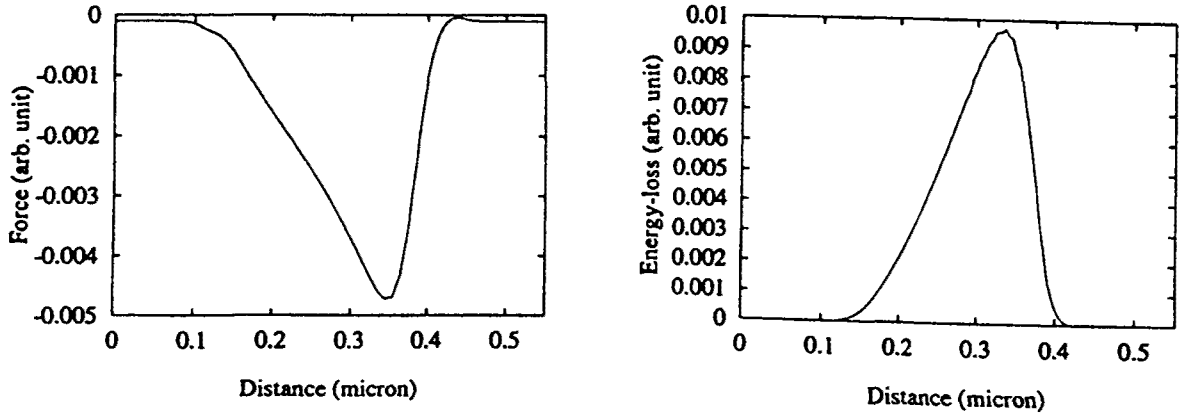

Figure 2: Resistive force and energy-loss rate as functions of position for a bias of 0.5 V.