The Monte Carlo Method Applied to Study of One-Dimensional Electronic Device (Diode) Based on Hg$_{0.8}$Cd$_{0.2}$Te

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Abstract: We propose in the present work a numerical solution of the Boltzmann Transport Equation using Monte Carlo method. Within a device, both the transport kernel and the field solver are coupled to each other. The field associated with the potential coming from Poisson's equation is the driving force accelerating particles in the Monte Carlo phase, below we give an extensive description of the Monte Carlo particle-based device simulators with emphasis is on the Poisson equation coupling. Numerical results are presented for one-dimensional Hg$_{0.8}$Cd$_{0.2}$Te n+nn+ structure, the presence of velocity overshoot has been observed and it is recognized that the fluctuation of velocity and energy term plays an important role in the simulation of semiconductor devices. Copyright © 2013 IFSA.

Keyword: Transport of carrier, Monte Carlo method, Poisson equation, Semiconductor n+nn+ structure.

1. Introduction

The study of charge transport in semiconductors is of fundamental importance both from the point of view of basic physics and for its application to electronic devices [1]. The performance of semiconductor electronic devices depends on low- and high-field electron transport properties of the materials in which they are fabricated [2]. There are several methods used in the calculation of the transport properties, namely: drift-diffusion models (DD), hydrodynamic models (HD) and Monte Carlo (MC) method. These numerical techniques rely on the discretisation of the semiconductor equations, which were originally derived from approximations based on the Boltzmann transport equation, to obtain solutions. The Monte Carlo method is used to resolve these issues. Emits, instead of solving directly the macroscopic equations that describe the operation of components, as is the case with drift-diffusion model or hydrodynamic, Monte Carlo method simulates statistically the behavior of circulating particles in these components. This does not have only a microscopic view of the function of the components, but also a better understanding of the phenomena that control it. However, due to the statistical nature of this model, it is necessary to monitor a large number of particles for a period time; this method takes extra calculations time. The paper is organized simply in three main parts. Section 1 presents the Monte carol
method as applied to transport calculations in semiconductors and poisons equation. After a brief port in sec. 2 the essential steps of the general algorithm for the application of Monte Carlo simulation. Section 3 present, as examples of application applied to for one-dimensional Hg0.8Cd0.2Te n+nn+ structure, collection of results in covalent semiconductors, and is followed by a brief conclusion.

2. Monte Carlo Simulation

The algorithm for the simulation can be divided essentially into two parts:

- The first part, which manages the movement of particles subject to the electric field.
- The second, which is to update, taking in mind the movement of particles, electric fields in the nodes, and involves solving a Poisson equation.

2.1. Part Monte Carlo

The Monte Carlo method as applied to semiconductor transport is a simulation of the trajectories of individual carriers as they move through a device under the influence of external forces and subject to random scattering events [3]. The duration of the carrier free flights between successive collisions and the scattering events involved are selected stochastically in accordance with the given transition probabilities describing the microscopic processes. In our model, the conduction band is approximated by nonparabolic dispersion relation.

\[ \varepsilon(1 + \alpha\varepsilon) = \frac{\hbar^2 K^2}{2m}, \]  

(1)

Where \( \alpha \), \( m^* \), and \( k \) are the nonparabolicity parameter, effective mass, and wave vector, respectively. Between collisions, the crystal momentum changes according to the local field, while the velocity of the particle is given by.

\[ v(k) = \frac{1}{\hbar} \frac{\partial \varepsilon(k)}{\partial k} \]  

(2)

The duration of the free flight is given by

\[ t_r = -\frac{1}{\Gamma} \ln(r), \]  

(3)

where \( r \) is a random number uniformly distributed between 0 and 1 obtained from the computer random number generator. The total scattering rate, \( \Gamma \), is given by

\[ \Gamma = \Gamma_{pop} + \Gamma_{as} + \Gamma_{imp} + \Gamma_{self}, \]  

(4)

where \( \Gamma_{pop} \), \( \Gamma_{as} \), \( \Gamma_{iv} \), and \( \Gamma_{imp} \) are the various scattering rates considered in the present model due to polar optical phonons, acoustic phonons, and impurities (both ionized and neutral), respectively. The self scattering rate, \( \Gamma_{self} \), corresponds to a fictitious scattering mechanism that changes with time so that the total rate, \( \Gamma \), is constant. Self-scattering does not change the carrier momentum and energy and, thus, does not affect the carrier’s trajectory. Its inclusion is necessary to simplify the random free flight time selection, which is central to the Monte Carlo technique [2].

The type of scattering terminating a free flight is chosen at random according to the relative scattering rates at the end of the flight. The final angle is then chosen randomly according to the differential scattering cross section. Several thousand particles are simulated simultaneously and ensemble averages are performed to obtain the quantities of interest such as the energy and velocity etc.

The material parameters used in the present Monte Carlo simulation and type of scattering are collected in Table 1.

<table>
<thead>
<tr>
<th>Type of scattering</th>
<th>Expressions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polar Optical Phonon Scattering</td>
<td>( \frac{2\pi^2 K_e \Theta_{\alpha}}{V_k q^2} \left( \frac{1}{E_k} - \frac{1}{E_{k'}} \right) )</td>
</tr>
<tr>
<td>Ionized Impurity Scattering</td>
<td>( \frac{n S \varepsilon^2}{V_k (kE)^2 (q^2 + q^2)} )</td>
</tr>
<tr>
<td>Alloy Disorder Scattering</td>
<td>( \frac{x(1-x)(\Delta e_c)^2}{V_{cd} N_{cd}} )</td>
</tr>
</tbody>
</table>

2.1.2. Poisson Equation

For simple illustration, here we only consider steady-state problem, which means time partial difference item is zero (Fig. 1). At mesh point \( i \), let Poisson’s equation discretized with three-point-center-difference, continuous equation can be discretized by using current value at half point \( i - 1/2 \) and \( i + 1/2 \), yet we get:
\[
\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{(\Delta x)^2} = \frac{q}{\varepsilon (n - N_D)}
\]

(5)

Knowing the position of each particle we determine the charge density in the entire structure then we solve the Poisson equation (6).

\[
\nabla^2 \phi = -\frac{\rho}{\varepsilon \varepsilon_r}
\]

(6)

This is discredited by the finite difference method as follows (7).

\[
\frac{\partial^2 \phi}{\partial x^2} = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{(\Delta x)^2}
\]

(7)

Then we calculates the resulting potentials using a resolution methods associated with partial differential equations using a direct method known as FACR (Fourier Analysis and Cyclic Reduction), or relaxation method such as SOR (Successive Over Relaxation) [7]. Once the potential is known, the electric field is derived by the finite difference method (8):

\[
E = -\Delta \phi
\]

(8)

The field at a point depends on the fields of neighboring points.

The simulation algorithm is a sequence of iterations of these two parts, one after the other. The time loop is executed for a number of time steps until steady state is reached.

3. General Algorithm

Monte Carlo simulation thus begins with initial values (electrostatic potential, energies and speed of the carriers) close to their final values. Then the different sequences carried over to the flowchart in Fig. 2 to loop are performed by the Monte Carlo simulation. After a number of iterations, the system reaches equilibrium where all equations Boltzmann, 1D Poisson are self-consistent. The flow of carriers is then conservative.

4. Study of a Structure n⁺ n n⁺ Weak Voltage (DIODE)

As part of the application of Monte Carlo transport model to real devices, we simulated the case of a device one-dimensional diode n⁺n n⁺ in Hg₀.₈Cd₀.₂Te. This diode made from Hg₀.₈Cd₀.₂Te n of 0.6 µm with a symmetrical doping profile. Its interior region is 0.2 µm wide with a concentration of 10¹³cm⁻³ The emitter and collector are symmetrical with a width of 0.2 µm each, and a concentration of n⁻ 5.410¹³cm⁻³. All this is illustrated in Fig. 3. Note that all the simulation is made at a constant temperature of 77°K.

In our simulation of this system, we use the following boundary conditions n⁺ junction on the left side (cathode) is grounded (polarized with a voltage V_L = 0V), and applying a positive voltage to the anode (n⁺ junction on the right side) of 0.01 V (VR =0.01 V), so that electrons are injected from the left end of the terminal (cathode) move to the far right (anode). We assume that the ohmic contact and ideal, in such a way as to preserve charge neutrality and thermal equilibrium at the contacts.

<table>
<thead>
<tr>
<th>n⁺</th>
<th>n</th>
<th>n⁺</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.410¹³</td>
<td>10¹³</td>
<td>5.410¹³</td>
</tr>
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</table>

0.2 µm 0.2 µm 0.2 µm

Fig. 3. Diagram of the structure of the n⁺nn⁺ diode to study.
5. Results and Discuss

Fig. 4 represents the electron density in the structure. We note that it is almost constant in the area n⁺ (ND=5.4*10¹³ cm⁻³) with a slight excess in contact with a defect in the injector and collector contact. These variations result from the boundary conditions, and indicate the existence of a current diffusive nature. At the border of the n⁺n Junction of the cathode on the left, we see the establishment of a zone of space charge due to a depletion of electrons from the n⁺ side and an electron injection from n⁺ to n zone n creating a zone of accumulation. The same phenomenon exists in the n⁺n junction of the anode and n as the region is very thin, it is entirely accumulation. The electron density is an order of superior greater than the initial density, which means, the density of impurity atoms. The field distribution depends very little of the region of doping n. 

Fig. 5 represents the electric field and the potential change in the structure respectively. In the limits of the n⁺ layer, we have a repulsive field that opposes the diffusion of electrons from the contact, the field distribution in the vicinity of the two n⁺n junction’s correspond well in areas of space charge and the field varies almost linearly in the n⁺ zone.

Knowing the kinetic energy, speed and position of each electron at each moment, we can plot the average kinetic energy and the drift velocity of electrons throughout the structure. The kinetic energy of electrons Fig. (6) is constant in the n⁺ region.

![Fig. 4. Profile of the electron density in the diode.](image1)

![Fig. 5. Profile of the electric field and Profile of the electrostatic potential in the diode.](image2)
Also the velocity in Fig. 6, is low in the n+ region and increases greatly at the beginning of the n region then becomes constant (velocity of saturation or steady state). In the n+ anode side the speed decreases rapidly.

At the front of the n region, the interactions are due to experienced by the electrons acoustic phonons scattering and the interaction probability is very low.

From a certain position, the most energetic electrons have reached energy of about 35meV and begin to emit polar optical phonons. Once the electron energy is becoming increasingly important, the issue of polar phonons then leads to a velocity distribution increasingly anisotropic, this explains the decrease in average velocity.

6. Conclusion

In this paper, we presented: The design of an algorithm for the simulation of one-dimensional systems and the calculation of stationary profiles of a diode n+n based on Hg0.8Cd0.2Te.

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