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MONTE CARLO SIMULATION FOR ELECTRON DYNAMICS IN SEMICONDUCTOR DEVICES

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Abstract- The single-particle Monte Carlo simulation for the electron transport in semiconductor devices is presented. The Monte Carlo method is briefly compared with alternative theoretical techniques. Flowchart of the simulation program is given and selections of free flight time, scattering mechanism and electron wave vector are explained. Determination of mean electron velocity and energy is presented.

Keywords- Monte Carlo Method, Semiconductor Devices, Electron Transport

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: variational principle (VP), iterative method (IM), relaxation time approximation (RTA), Matthiessen rule (MR) formalism, and Monte Carlo (MC) method [3]. 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 has a quite different methodology, although the solution is still based on the Boltzmann equation. Monte Carlo techniques are statistical numerical methods, which are applied to the simulation of random processes. Monte Carlo methods have been used in a wide variety of fields to solve problems spanning from the analysis of sub-atomic quantum physics to the development of galaxies. An important feature of the Monte Carlo models is that they can be applied to both material and device simulations. A particularly attractive feature of this method is that it allows the simulation of physical processes, which cannot always be observed or reduced directly from laboratory experiments. Many transport characteristics used in simulations, such as velocity field characteristics, are obtained using Monte Carlo simulation [4]. The majority of mobility, diffusion, energy, relaxation time and effective mass characteristics, which are usually taken as a function of electric field, are obtained using Monte Carlo model [5].

2. MONTE CARLO SIMULATION OF ELECTRON TRANSPORT IN SEMICONDUCTORS

The single Monte Carlo Method, as applied to charge transport in semiconductors, consist of a simulation of the motion of one electron inside the crystal subject to applied

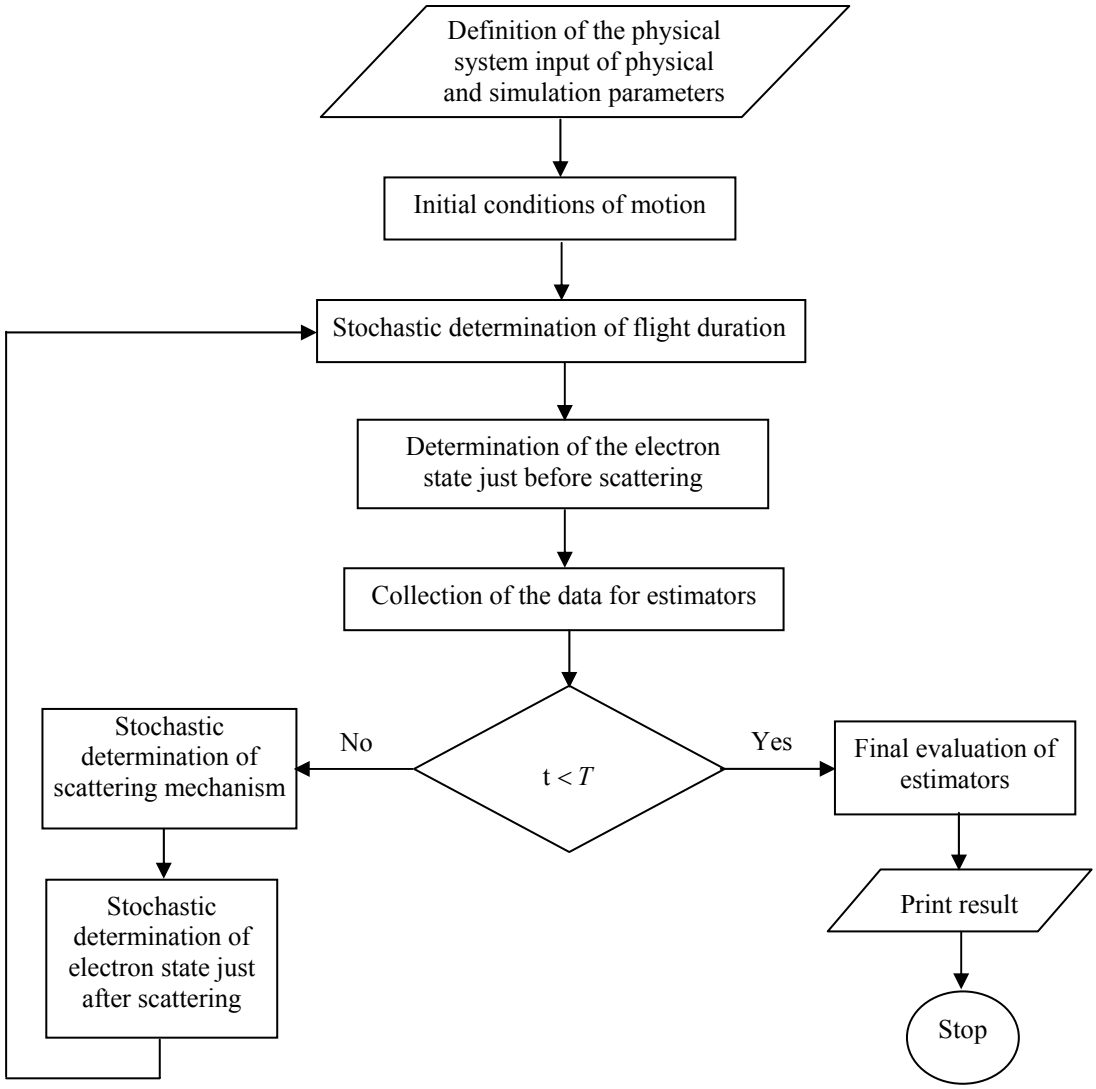

Figure 1. Flowchart of a typical Monte Carlo program [6].

electric field and given scattering mechanisms. Flowchart of a typical Monte Carlo program is shown in Figure 1. The motion of the electron inside the crystal subject to electric field consists of drift and collision processes. The effect of external forces is deterministic but the collision processes affect the trajectories in a probabilistic manner. The drift process may be calculated by applying the classical laws of motion, but the collision process requires probability theory [7]. This is done in the Monte Carlo method by generating uniformly distributed random numbers [8], and by using them to determine the time between collisions and the nature of the collisions using the following procedure.

2.1 Determination of the free flight time

The motion of electrons is simulated as a series of free flights interrupted by instantaneous scattering events, representing the carrier-phonon, the carrier-impurity, and the carrier-carrier interactions. After a scattering, the carrier will emerge with a crystal momentum $\vec{k}(0)$ at time t=0. The time evolution of the momentum during the flight is

$$\vec{k}(t) = \vec{k}(0) + (\frac{\vec{F}}{\hbar})(t - t_0) \quad , \text{since } \vec{F} = \frac{d}{dt}(\hbar\vec{k}), \tag{1}$$

where $\vec{F}$ is the external force on the electron [9]. However, as the electron moves it may suffer a scattering at any time. The scattering is a random event. At each instant there is a definite total scattering rate $\lambda(k)$, function of the magnitude of the momentum. The total scattering rate $\lambda(k)$ is defined as the sum of the individual scattering rates over all the n scattering mechanisms.

$$\lambda(k) = \sum_{i=1}^{n} \lambda_i(k) \tag{2}$$

The scattering rate indicates the average number of scatterings, which a particle would suffer in the unit time; therefore it has units of inverse seconds. The probability of the particle being scattered between time t and $t + dt$ is determined by

$$P_f(t)dt = \lambda(k)\exp\left(-\int_0^t \lambda(k_{t'})dt'\right)dt \tag{3}$$

where $P_f(t)$ is the probability density of scattering at time t and $\lambda(k)$ is the total scattering rate [5]. The free-flight time $t = t_f$ is obtained by generating random numbers

$$P_f(t)dt = P(r_1)dr_1$$

$$\int_0^t P_f(t')dt' = \int_0^{r_1} P(r_1')dr_1' = r_1 \tag{4}$$

where the random numbers r_1 lies in the range 0 to 1 and it is related to the total scattering rate by

$$r_1 = 1 - \exp\left(-\int_0^{t_f} \lambda(k(t'))dt'\right) \tag{5}$$

If the logarithm of both sides is taken,

$$-\ln(1 - r_1) = \int_0^{t_f} \lambda(k(t'))dt' \tag{6}$$

Since r_1 and $(1 - r_1)$ have identical distributions,

$$-\ln r_1 = \int_0^{t_f} \lambda(k(t'))dt' \tag{7}$$

The free flight time t_f can be obtained using a random number r_1. But the integral equation would need to be solved for each scattering event. Rees introduced self-scattering concept to overcome this difficulty [10]. If the total scattering rate is written as a constant

$$\Gamma = \lambda(k(t)) + \lambda_{ss} \tag{8}$$

where λ_{ss} called self-scattering rate. Equation 7 can be rearranged as

$$t_f = -\frac{\ln r_1}{\Gamma} \tag{9}$$

If the self-scattering is selected as the scattering mechanism, there is no any changing on the electron energy and momentum.

After a free flight of duration t_f the momentum $\vec{k}$ is given by

$$\vec{k} = \vec{k}_0 + \frac{q}{\hbar}\int_0^t dt' \vec{E}(t')$$

$$\vec{k} = \vec{k}_0 + \frac{q\vec{E}t_f}{\hbar} \tag{10}$$

where $\vec{k}_0$ is the wave vector of electron just before scattering event and $\vec{E}$ is the applied electric field.

2.2 Selection of a scattering mechanism

At the end of each free flight a scattering mechanism must be selected. Selection of a scattering mechanism (n) can be made using functions $\Lambda_n(k)$ defined as

$$\Lambda_n(k) = \frac{\sum_{i=1}^{n} \lambda_i(k)}{\Gamma} \tag{11}$$

which are the successive summations of the scattering rates normalized with Γ. A scattering mechanism for an electron is selected by generating a random number r_2 lying between 0 and 1, and comparing it to $\Lambda_n(k)$; thus, the n-th scattering mechanism is chosen if the condition given by

$$\Lambda_{n-1}(k) < r_2 \leq \Lambda_n(k) \tag{12}$$

is satisfied [11]. If the self-scattering mechanism is selected, then the energy and wave vector of the electron are not changed.

2.3 Determination of the electron wave vector after the scattering

The scattering processes change the wave vector of the electron and it is necessary to have a method of determining the wave vector $\vec{k}'$ after scattering event. The magnitude of $\vec{k}'$ is known by the energy conversation, and the direction of $\vec{k}'$ needs to be determined in terms of its components in a Cartesian coordinate. The components k_x', $k_y'$and k_z' can be found by considering a sphere with radius 1, centered at the space location where the scattering occurs. In Cartesian coordinates ϕ azimuth and θ polar angels need to be determined, in order to identify every point on the sphere. The probability to select a point P on an element ds of the surface is equal to $ds/4\pi$ since in spherical coordinates;

$$ds = Sin\theta\, d\theta\, d\phi$$

$$\frac{ds}{4\pi} = \frac{Sin\theta}{4\pi} d\theta\, d\phi = P(\theta,\varphi) d\theta\, d\phi \tag{13}$$

where

$$P(\theta,\phi) = \frac{Sin\theta}{4\pi}$$

is the density of probability. The separate densities of probability $P(\theta)$, and $P(\phi)$ for the two angels are independent [12].

$$P(\theta) = \int_0^{2\pi} P(\theta,\phi)\, d\phi = \frac{Sin\theta}{2} \tag{14}$$

$$P(\phi) = \int_0^{\pi} P(\theta,\phi)\, d\theta = \frac{1}{2\pi} \tag{15}$$

$P(\theta,\phi) = P(\theta)P(\phi)$, which proves the independence of θ and ϕ [13]. Values of θ and ϕ in any particular scattering can be determined by using two random numbers (between 0 and 1) r_3 and r_4 as,

$$r_3 = \int_0^{\phi} P(\phi)\, d\phi = \frac{\phi}{2\pi} \qquad \phi = 2\pi r_3 \tag{16}$$

$$r_4 = \int_0^{\theta} P(\theta) d\theta = \frac{1-\cos\theta}{2} \qquad Cos\,\theta = 1 - 2r_4 \tag{17}$$

then components of the $\vec{k}'$ can be calculated using the angels in Cartesian coordinates.

2.4 Mean velocity and energy calculation

The instantaneous carrier velocity in a bulk semiconductor subject to applied electric field is given by

$$\vec{v} = \frac{1}{\hbar}\vec{\nabla}_{\vec{k}} E_{\vec{k}} \tag{18}$$

therefore, the mean carrier velocity during flight time τ can be written as

$$< \vec{v} >_{\tau} = \frac{1}{\hbar}\frac{\Delta E_{\vec{k}}}{\Delta \vec{k}} \tag{19}$$

where $\Delta E_{\vec{k}}$ and $\Delta \vec{k}$ are small increments of the carrier energy and wave vector during τ, respectively. Using the Equation 10 mean velocity is obtained as

$$< \vec{v} >_{\tau} = \frac{\Delta E_{\vec{k}}}{q\vec{E}\tau} \tag{20}$$

The mean carrier velocity during the total simulation time T is obtained as

$$\begin{aligned} < \vec{v} >_{\tau} &= \frac{1}{T}\sum < \vec{v}_{\tau} > \tau \\ &= \frac{1}{q\vec{E}T}\sum \Delta E_{\vec{k}} \\ &= \frac{1}{q\vec{E}T}\sum \left(E_f - E_i\right) \end{aligned} \tag{21}$$

where E_f is the carrier energy at the end of the electron flight and E_i is the energy at the start of the flight [14]. The summation must be made for all free flight.

Mean carrier energy during the total simulation time T can be calculated as

$$< E >_T = \frac{1}{T}\sum < E_{\tau} > \tau \tag{22}$$

where

$$< E_{\tau} >= \frac{E_i + E_f}{2}$$

3. CONCLUSION

The characterisation of semiconductor materials and devices requires their physical and electrical properties. Experiments can provide considerable information on the semiconductors. However; it is important to obtain information on processes which influence the experimental characteristics but which cannot be directly observed. To obtain theoretical description of any semiconductor device Boltzmann's equation must be solved, or the quantum mechanical equivalent of it. Monte Carlo method in which the Boltzmann equation is not directly solved, but the transport properties are evaluated by the simulation of electron trajectories using random numbers.

The simulation starts with one electron with wave vector $\vec{k}_0$; then the duration of the first free flight is chosen with a probability distribution determined by the scattering

probabilities. At the end of the free flight electron velocity, electron energy and momentum are calculated using the motion equations. Then a scattering mechanism is chosen as responsible for the end of the free flight, according to the relative probabilities of all possible scattering mechanisms. A new $\vec{k}$ state after scattering is randomly chosen as initial state of the new free flight, and entire processes is iteratively repeated. Reliable results are usually obtained within 80-100 thousand scattering events. The mean values of velocity and energy can be calculated by taking an average over all free flights.

We have used the single particle Monte Carlo method to examine the electron transport in InSb and $Hg_xCd_{1-x}Te$ semiconductor materials [15,16]. In this paper we have briefly reviewed the method.

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