Semicond. Sci. Technol. 6 (1991) 602–606. Printed in the UK

9K91

An efficient Monte Carlo particle technique for two-dimensional transistor modelling

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Received 2 August 1990, in final form 14 January 1991, accepted for publication 31 January 1991

Abstract. A novel very efficient technique for charge current calculations in two-dimensional Monte Carlo particle simulation is proposed. The technique obtains accurate results by using a significantly smaller number of particles than the commonly accepted technique. The proposed technique permits the two-dimensional Monte Carlo particle simulation to run on personal computers instead of on supercomputers. The results of field-effect transistor simulation are presented.

1. Introduction

The two-dimensional Monte Carlo particle simulation combines a two-dimensional spatial representation of the potential distribution with a three-dimensional Monte Carlo simulation of the electron motion in momentum space. This technique was first used for field-effect transistor simulation [1]. In principle the Monte Carlo particle technique obtains the numerical solution of the coupled time-dependent Boltzmann equation and Poisson equation. This technique is applied to the detailed study of electron transport in submicrometre MESFETs [2–5] and in MOSFETs [6–8] with submicrometre gate length. The two-dimensional Monte Carlo particle method was used for high-mobility field-effect transistor simulation including 2D electron gas effects [9–11] and for permeable base transistor simulation [12, 13]. The velocity-modulation transistors [14] and real space transfer transistor [15] are studied by the two-dimensional Monte Carlo particle technique.

The two-dimensional Monte Carlo particle simulation consumes much computer time. The computation time for one point of the steady-state current–voltage characteristics obtained by modelling 30 000 to 50 000 particles is 10 to 40 minutes on a CRAY X-MP/28 [16]. A particularly large computation time is necessary for the simulation of a transient response of two-dimensional transistor structures. Even 300 000 particles [17] were simulated for the calculations of transient response of a field-effect transistor.

In this paper an efficient method is proposed for the current evaluation in Monte Carlo particle technique.

2. One-dimensional simulation

The reason for the low efficiency of the conventional two-dimensional Monte Carlo particle technique can be easily understood by comparing this technique with the one-dimensional Monte Carlo particle technique.

In the one-dimensional case the diode current density j can be directly evaluated by counting the number of particles entering and leaving the diode through the cathode and anode per time step Δt. However, there is an essentially more efficient way of calculating the current [18, 19]. In general the total current density can be expressed as

$$j = e\int v_x f(v, x, t)\,\mathrm{d}v + \varepsilon\varepsilon_0 \frac{\partial E(x, t)}{\partial t} \qquad (1)$$

where v is the electron velocity, $f(v,x,t)$ is the distribution function normalized to the electron concentration and E is the electric field strength. In the one-dimensional case the total current density including the displacement current is position independent. Therefore, integrating both sides of (1) over the diode length L we obtain

$$j(t) = \frac{e}{L}\int_0^L \mathrm{d}x \int \mathrm{d}v\, v_x f(v, x, t) + \frac{\varepsilon\varepsilon_0}{L}\frac{\partial U}{\partial t} \qquad (2)$$

where U is the voltage applied to a diode. The last term of the right-hand side of (2) represents the displacement current caused by a time dependence on the applied voltage. For simplicity let us assume that the applied

oltage is time independent. Then (2) can be rewritten as

$$j(t) = e\int v_x F(v,t)\,dv \tag{3}$$

where

$$F(v,t) = \int_0^L f(v,x,t)\,dx. \tag{4}$$

Physically $F(v,t)$ represents the electron velocity distribution averaged over the sample. From (2) we obtain the expression for the current density evaluation by the one-dimensional Monte Carlo particle technique

$$j(t) = \frac{\sigma}{L}\sum_{i=1}^{N} v_i(t) \tag{5}$$

where σ is the surface charge density of the particle, v_i is the instant velocity of the ith particle and N is the number of particles under simulation inside the sample.

Let us estimate the accuracy of the current density calculated from (5). For this let us assume that the electric field in the diode is evaluated precisely so that particles in the diode move in a self-consistent electric field. Then, according to (5), the statistical fluctuations of the calculated current density are caused by the fluctuations of particle velocities. It is evident from (4) that the distribution function $F(v,t)$ represents the probability density for an electron having the velocity v at any point in the diode at the time t. The statistical fluctuations of the calculated current density can be estimated by employing $F(v,t)$. This may be done in the same manner as in [20], where the statistical fluctuations of the results obtained by the ensemble Monte Carlo technique in a uniform electric field are evaluated. By using equation (15) of [20] we obtain

$$\frac{\langle\Delta j^2\rangle}{j_0^2} = \frac{1}{N}\left\{\left[\int v_x^2 F(v,t)\,dv \Big/ \left(\int v_x F(v,t)\,dv\right)^2\right] - 1\right\} \tag{6}$$

where $\langle\Delta j^2\rangle$ is the mean square deviation of current density at the time t evaluated according to (5), N is the number of simulated particles and j_0 is the exact value of the current density. A convenient expression for the direct estimation of $\langle\Delta j^2\rangle$ during the calculations can be obtained from (6). The result is

$$\frac{\langle\Delta j^2\rangle}{j} = \frac{1}{N}\left\{\left[N\sum_{i=1}^{N} v_{xi}^2(t) \Big/ \left(\sum_{i=1}^{N} v_{xi}(t)\right)^2\right] - 1\right\}. \tag{7}$$

The current density estimated according to (5) is considerably higher in accuracy than the results obtained by counting the number of particles entering and leaving the contacts of the diode. This is because (5) takes into account all the simulated particles, while only a small number of them is considered when the current density is evaluated from the particles crossing the contacts. In the last case the current density is estimated from the particles that are placed near contacts.

In the two-dimensional Monte Carlo particle technique the current through terminals is calculated from the number of particles crossing the contacts per time step. Therefore, only a small number of the total simulated particles contribute to the current. Consequently, the accuracy of the current evaluation is low even though the electric field and the carrier velocity distribution function inside the device would be defined precisely. In this paper we present a novel efficient method for current calculation. This method takes into account the contribution to the current by essentially all the simulated particles.

3. A method for two-dimensional simulation

First we consider the general well known relations. From the continuity equation

$$\oint_S \boldsymbol{j}_c\,d\boldsymbol{S} + \frac{\partial}{\partial t}\int_V \rho\,dV = 0 \tag{8}$$

and from the Gaussian theorem

$$\int_V \rho\,dV = \varepsilon\varepsilon_0\oint_S \boldsymbol{E}\,d\boldsymbol{S} \tag{9}$$

we obtain

$$\oint \boldsymbol{j}\,d\boldsymbol{S} = 0 \tag{10}$$

where the total current $\boldsymbol{j}$, including the displacement current, is given by

$$\boldsymbol{j} = \boldsymbol{j}_c + \varepsilon\varepsilon_0\frac{\partial \boldsymbol{E}}{\partial t}. \tag{11}$$

In equations (8)–(11) $\boldsymbol{j}_c$ is the conduction current and ρ is the space charge density. The integration is performed over the volume V and surface S.

For the sake of completeness we consider the geometry of the field-effect transistor presented in figure 1. The standard boundary conditions are usually applied for the device, i.e. Dirichlet boundary conditions to all metal–semiconductor interfaces and Neumann boundary conditions (the zero normal derivative of the potential) to other surfaces. The total current density normal to these surfaces equals zero. The normal conduction current equals zero because the carriers cannot pass through surfaces, and the normal displacement current equals

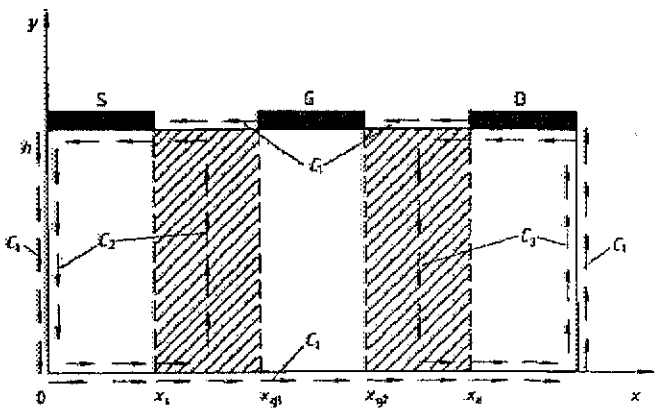

Figure 1. The field-effect transistor geometry.

zero due to Dirichlet boundary conditions. With regard to this, integrating (10) over contour C_1 (figure 1) yields

$$I_s = I_g + I_d \tag{12}$$

where I_s, I_g and I_d are the source, gate and drain currents respectively. By integrating (10) over contour C_2 we obtain

$$I_s(t) = \int_0^h j_x(x, y, t)\,dy \qquad x \in (x_s, x_{g1}) \tag{13}$$

where j_x is the component of the total current density along x axes. The integration of both sides of (13) over x from $x = x_s$ to $x = x_{g1}$ gives

$$I_s(t) = \frac{1}{x_{g1} - x_s} \int_0^h \int_{x_s}^{x_{g1}} j_x(x, y, t)\,dx\,dy. \tag{14}$$

In a similar manner integrating (10) over contour C_3 and over x yields

$$I_d(t) = \frac{1}{x_d - x_{g2}} \int_0^h \int_{x_{g2}}^{x_d} j_x(x, y, t)\,dx\,dy. \tag{15}$$

By substituting (11) into (14) and (15) we finally obtain

$$I_s(t) = \frac{1}{x_{g1} - x_s}\left(\int_0^h \int_{x_s}^{x_{g1}} j_{cx}(x, y, t)\,dx\,dy + \varepsilon\varepsilon_0 \frac{\partial}{\partial t}\int_0^h [\varphi(x_s, y, t) - \varphi(x_{g1}, y, t)]\,dy\right) \tag{16}$$

and

$$I_d(t) = \frac{1}{x_d - x_{g2}}\left(\int_0^h \int_{x_{g2}}^{x_d} j_{cx}(x, y, t)\,dx\,dy + \varepsilon\varepsilon_0 \frac{\partial}{\partial t}\int_0^h [\varphi(x_{g2}, y, t) - \varphi(x_d, y, t)]\,dy\right) \tag{17}$$

where φ is a potential. The gate current is defined according to (12). In a similar way for the device geometry presented in figure 2 we obtain

$$I_s(t) = \frac{1}{x_{g1}}\left(\int_0^h \int_0^{x_{g1}} j_{cx}(x, y, t)\,dx\,dy - \varepsilon\varepsilon_0 \frac{\partial}{\partial t}\int_0^h \varphi(x_{g1}, y, t)\,dy\right) \tag{18}$$

and

$$I_d(t) = \frac{1}{x_d - x_{g2}}\left[\int_0^h \int_{x_{g2}}^{x_d} j_{cx}(x, y, t)\,dx\,dy + \varepsilon\varepsilon_0 \frac{\partial}{\partial t}\left(\int_0^h \varphi(x_{g2}, y, t)\,dy - U_d h\right)\right] \tag{19}$$

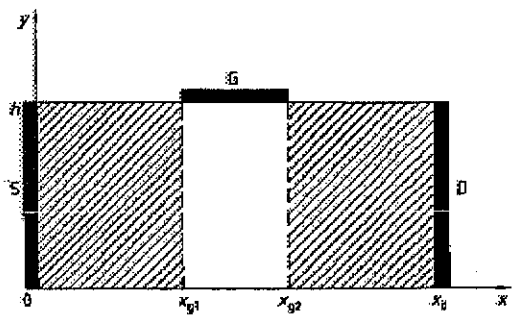

Figure 2. The simulated field-effect transistor geometry.

where U_d is the drain voltage, which can be time-dependent. From (16) and (17) we obtain the expressions for the two-dimensional Monte Carlo particle simulation of the device presented in figure 1. The result is

$$I_s(t) = \frac{1}{x_{g1} - x_s}\left[Q\sum_i v_{xi}(t) + \frac{\varepsilon\varepsilon_0 \Delta y}{\Delta t}\sum_{j=1}^{m_y} \times \Big(\varphi(x_s, j\Delta y, t) - \varphi(x_s, j\Delta y, t - \Delta t) - \varphi(x_{g1}, j\Delta y, t) + \varphi(x_{g1}, j\Delta y, t - \Delta t)\Big)\right] \tag{20}$$

$$I_d(t) = \frac{1}{x_d - x_{g2}}\left(Q\sum_i v_{xi}(t) + \varepsilon\varepsilon_0 \frac{\Delta y}{\Delta t}\sum_{j=1}^{m_y} \times [\varphi(x_{g2}, j\Delta y, t) - \varphi(x_{g2}, j\Delta y, t - \Delta t) - \varphi(x_d, j\Delta y, t) + \varphi(x_d, j\Delta y, t - \Delta t)]\right) \tag{21}$$

where Q is the linear charge density of a particle and m_y is the mesh number along the y axes. In (20) the summation over i is performed over all the particles that occur at the time t between the source and the gate. Correspondingly, in (21) the summation over i is performed over the particles occurring between the gate and the drain. The regions of the simulation are indicated by shaded areas in figure 1. Analogous expressions can be deduced for (18) and (19) that correspond to the device geometry presented in figure 2. The summation in this case is performed by the particles found in the hatched areas of figure 2.

Under steady state the potential distribution is time independent and the final terms of (16)–(21) containing the potential can be omitted. Moreover under the steady state and under typical transistor bias voltages the gate current I_g equals zero, and thus $I_s = I_d$. In this case (16)–(21) can be simplified. For the device geometry presented in figure 1 we obtain

$$I_s = I_d = \frac{1}{x_d - x_s}\int_0^h \int_{x_s}^{x_d} j_{cx}(x, y)\,dx\,dy. \tag{22}$$

From (22) we can derive an expression for the current calculation in the Monte Carlo particle technique. The result is

$$I_s = I_d = \frac{Q}{x_d - x_s}\sum_i v_{xi}. \tag{23}$$

The summation in (23) is performed over all the particles found between the source and drain contacts. In a similar way for the device geometry shown in figure 2 we obtain

$$I_s = I_d = \frac{1}{x_d}\int_0^h \int_0^{x_d} j_{cx}(x, y)\,dx\,dy \tag{24}$$

and

$$I_s = I_d = \frac{Q}{x_d}\sum_i v_{xi}. \tag{25}$$

The summation in (25) is performed over all the simulated particles independently of their position.

Evidently the proposed method permits a calculation of the current in two-dimensional structures with an essentially higher accuracy than the method of counting the number of particles entering and leaving the contacts. The method can be applied to other transistor structures: HEMTs, permeable-base transistors etc.

The accuracy of the proposed method can be estimated in a similar manner to that above for the one-dimensional Monte Carlo technique. We assume that the potential is precisely defined and hence the statistical fluctuations of the estimated current are caused by the particle velocity fluctuations. We introduce the spatially averaged distribution function. In the steady state we have

$$F(v) = \int_s f(v, x, y)\,dx\,dy. \tag{26}$$

The integration in (26) is performed over the hatched areas in figures 1 and 2. The distribution function $F(v)$ corresponds to the probability density for an electron with velocity v. Following equation (15) of [20] we can write

$$\frac{\langle \Delta I^2 \rangle}{I_0^2} = \frac{1}{N}\left\{\left[\int v_x^2 F(v)\,dv \Big/ \left(\int v_x F(v)\,dv\right)^2\right] - 1\right\} \tag{27}$$

where I_0 is the exact value of the current, $\langle \Delta I^2 \rangle$ is the mean-square deviation and N is the number of particles inside the corresponding shaded region. According to (26) and (27) the mean-square deviation $\langle \Delta I^2 \rangle$ can be estimated directly during the simulation. From (26) and (27) we find

$$\frac{\langle \Delta I^2 \rangle}{I_0^2} = \frac{1}{N}\left\{\left[N \sum_i v_{xi}^2 \Big/ \left(\sum_i v_{xi}\right)^2\right] - 1\right\}. \tag{28}$$

The summation in (28) is performed over the particles found in the corresponding region.

4. Numerical results

The gallium arsenide field-effect transistor model employed is the same as in [17] and is shown in figure 2. Such a model is chosen to compare the results of the present work with those obtained in [17], because the calculations in [17] were performed with an extremely high number of simulated particles $N = 300\,000$.

The device length parameters are as follows: $x_{g1} = 0.5\ \mu m$, $x_{g2} = 1\ \mu m$, $x_d = 1.5\ \mu m$, $h = 0.1\ \mu m$. The uniform doping density $10^{17}\ cm^{-3}$ and the lattice temperature $T_0 = 300$ K are assumed. The simplified two-valley gallium arsenide model is adopted in accordance with [17].

The two-dimensional Poisson equation was solved using the marching algorithm [21]. The Dirichlet boundary conditions were applied to the contacts, and the Neumann boundary conditions were applied to other surfaces of the device. The uniform mesh spacing was 117 Å × 63 Å. The time step $\Delta t = 5$ fs is accepted. The electron density distribution is assigned to the meshes by the cloud in the cell method [22]. The number of particles employed is about 10 000.

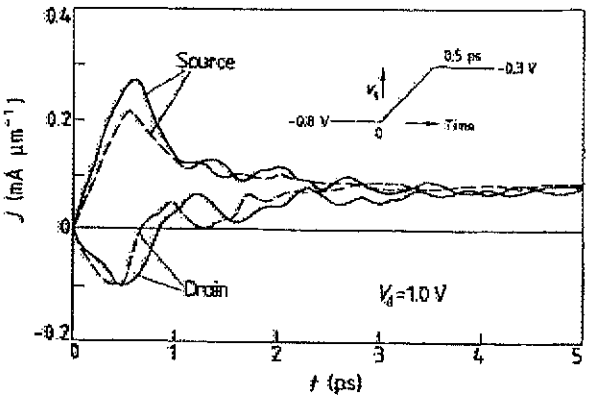

Figure 3. The transient response of source and drain currents. The full curves represent our results; the broken curves represent the results of [17]. The drain voltage $V_d = 1$ V. The time variation of the gate voltage is shown in the inset.

The polar optical, acoustic, intervalley and ionized impurity scattering processes are taken into account. The source and drain are considered as ohmic contacts (absorbing boundaries). Other surfaces including the gate region are treated as reflecting boundaries. The thermal electron injection from the source and drain contacts is simulated by an injection of a corresponding number of particles for each time step from both contacts. The number of particles necessary to be injected is defined by the electron concentration at the contacts, and is taken to be $10^{18}\ cm^{-3}$. Considering the thermal equilibrium at the source and drain contacts the velocity distribution of the injected particles is

$$f(v) \simeq v_x \exp(-mv^2/2kT_0). \tag{29}$$

The calculated transient response of the source and drain current is presented in figure 3. The time variation of the gate voltage is shown in the inset of figure 3. The comparison of the present results with those obtained in [17] shows approximately the same accuracy despite the fact that the number of simulated particles in [17] exceeds the particle number used in the present paper by 30 times.

5. Conclusions

An efficient technique for the current evaluation in two-dimensional Monte Carlo particle simulation is proposed. The efficiency of the technique is examined by the simulation of the field-effect transistor. The proposed technique can be easily generalized to other two-dimensional structures: permeable-base transistors, high electron mobility transistors etc. This technique appears to be particularly promising for the transient response and intrinsic noise calculations.

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