



# PHYSICAL MODELS OF OHMIC CONTACT FOR MONTE CARLO DEVICE SIMULATION

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**Abstract**—This paper investigates the problem of modelling ohmic contacts for Monte Carlo simulation of semiconductor devices. Several models are proposed with different velocity distributions for the injected carriers. The influence of each model on the device physics near the contact is discussed. As a prototype for this analysis we investigate the role of the ohmic contact on the electrical characteristics of a GaAs Schottky-barrier diode under forward-bias condition. To get accurate results from the simulations of this device, correct modelling of the ohmic contact is crucial. We have found that the best simulation of the carrier dynamics near the contact is achieved by using a velocity-weighted Maxwellian distribution for injecting the carriers, which provides flat profiles of the different magnitudes near the boundary and a zero voltage drop at the contact. In addition, an appropriate time and space algorithm for carrier injection must be applied.

## 1. INTRODUCTION

The Monte Carlo (MC) method has emerged as a very important tool for the simulation of semiconductor devices. Starting from the bulk properties of materials[1], it has been extensively applied to analyse the behaviour of electronic devices[2]. More and more complex models have been developed to this end[3]. When going from bulk material to devices, an adequate treatment of the boundaries is necessary, which must reflect the physical processes taking place. These boundary conditions (BC) are specially important when the dimensions of the device are very small, and may affect their behaviour[4]. The BC enter the simulation at two levels: in the solution of Poisson's equation and in the carrier dynamics. We shall deal with the second. While there exist well-established and detailed models for the carrier dynamics at boundaries that do not allow particle transmission (usually treated as elastic reflecting boundaries)[5], there is no standard model for the simulation of boundaries that allow particle transmission.

We are specially interested in the modelling of ohmic contacts (OC), which constitute the source and sink of carriers in devices. Usually, an ideal ohmic contact is considered as a region of the device which is in thermal equilibrium even when a current is flowing through it, so that the voltage drop at the contact is negligible and no power is dissipated. To reproduce this behaviour, the condition is generally imposed that the free-carrier concentration of a small region close to each contact should remain constant and equal to the doping density. To do so in an MC simulation, the number of (commonly

thermal) carriers necessary for neutrality to be maintained in these regions are injected at each time step[5]. In addition, the contact absorbs all incident carriers. In the case of charge accumulation, since the charge is expected to diffuse, no carrier is injected or *deleted*. This procedure is common to the different models developed for the OC[2,5-11]. However, there are two aspects in which these models differ, and often very few details on the latter are given. Firstly, the velocity distribution function from which the injected particle is randomly selected (Maxwellian, velocity-weighted Maxwellian, displaced Maxwellian, etc.), and secondly the algorithm used to determine the moment at which the carrier flows into the device and its spatial coordinates. Only recently some attempts have been made to establish an efficient and physically plausible model for the OC[10,11].

The different carrier-injection schemes are not always able to fully accomplish the requirements of an ideal OC (charge neutrality, negligible voltage drop). Frequently, strange spikes in the profile of some magnitudes are observed and unknown contact potentials are introduced. In order to determine the model providing a better behaviour in MC simulation, the aim of the present paper is to investigate the influence of different OC models on the device physics. As a workbench for this analysis, we have made use of a GaAs Schottky-barrier diode (SBD) where the contact directly affects the device performance. In this device the correct simulation of the OC is crucial to get good results, since the barrier height to be surpassed by the carriers for reaching the metal may be strongly modified by the voltage drop at the opposite ohmic boundary. The static characteristics

and noise behaviour of the SBD will be analysed for the different models. The simulation of the SBD is one-dimensional. Although some modifications have to be introduced, the conclusions reached for the contacts may be basically extrapolated to the case of two-dimensional simulations.

The paper is organized as follows. Section 2 describes the various aspects involved in the modelling of an OC and the models to be analysed. Section 3 presents the details of the MC simulation of the SBD. Section 4 reports the results of the implementation of the OC models in the SBD and their influence on the static and noise behaviour. Finally, the main conclusions are given in Section 5.

## 2. OHMIC CONTACT MODELS

As already explained, an OC is considered as a region of the device which is characterized by local charge neutrality and thermal equilibrium. Trying to reproduce this behaviour, several injection schemes can be applied. In the case of one-dimensional simulations, when the active region of the device is far from the contacts and charge neutrality of the whole structure is expected, periodic BC may be applied: the carriers reaching a contact are reinjected into the opposite end with the same energy and wave vector (or with a state randomly selected from a thermal distribution)[12,13]. This model is specially appropriate for devices like  $n^+nn^+$  structures, where the carriers reach the terminals of the device in a situation close to thermal equilibrium, and the highly doped  $n^+$  regions considerably reduce the effect of carrier injection on the device performance[10,12]. This technique, although providing good results, has a limited applicability. It cannot be used in the simulation of two-dimensional devices with more than two terminals or in the case of devices which are not expected to be charge neutral. This applies for SBDs, which are never charge neutral except under flat-band conditions, and their behaviour is determined by the correct number of carriers inside the device[2,14]. Some modified periodic BC may be used for SBD simulation[15], but always with very restricted application.

Therefore, alternative schemes must be developed, allowing the number of carriers inside the device to fluctuate during the simulation. With this aim, the model was established in which charge neutrality is maintained in a region close to the contact by injecting periodically (usually each time step in which the field is updated) the number of thermal electrons necessary to equal the free-carrier concentration to the impurity density[5]. In addition, any carrier reaching the contact leaves the device. This is the usual description of what is called an OC in MC simulation. However, to know how the carrier injection takes place, further details must be specified: (a) the way to determine the number of carriers which must be injected at each time step, (b) the moment at

which the injected electrons enter the device, (c) their coordinates, and (d) the velocity distribution function from which the state of the new particles is randomly selected. We shall analyse several models, which differ only in the last point (the distribution function). The other details are common to all of them and are explained below for a one-dimensional simulation.

We keep charge neutrality only in the cell adjacent to the ohmic boundary. During each time step of duration  $\Delta t$ , the free-carrier concentration in this cell,  $n_c$ , is calculated according to the expression:

$$n_c = \frac{1}{A \Delta x} \sum_{i=1}^{M_c} \frac{\delta t_i}{\Delta t}, \quad (1)$$

where  $A$  is the cross-sectional area of the device,  $\Delta x$  is the cell length,  $M_c$  is the number of carriers which are present in the cell during the time step, and  $\delta t_i$  is the time each of them spends inside it. Note that  $\delta t_i$  may coincide with  $\Delta t$  (the carrier remains the whole time step inside the cell) or be only a fraction of  $\Delta t$  (the carrier leaves or enters the cell during the time step).

At the end of the time step,  $n_c$  is compared with the value of the doping density in the cell,  $N_c$ . If  $n_c > N_c$ , no carrier is injected: the charge accumulation is expected to disappear by diffusion. If  $n_c < N_c$ , carrier injection takes place. A first carrier is injected with an initial position  $x = 0$  (which corresponds to the cell edge adjacent to the OC) and its dynamics inside the device are simulated during a time  $r\Delta t$ , where  $r$  is a random number uniformly distributed between 0 and 1. The free-carrier concentration in the cell adjacent to the contact  $n_c$  is updated by taking into account the presence of this new particle. The condition  $n_c < N_c$  is checked again. If  $n_c$  remains lower than  $N_c$ , a new carrier is injected in the same way. This procedure continues until the requirement  $n_c = N_c$  is reached to a difference of 0.01%. Before injecting each carrier, the following condition is checked:

$$r\Delta t < t_{\text{rest}} = (N_c - n_c)A\Delta x\Delta t, \quad (2)$$

where  $t_{\text{rest}}$  is the time resting to reach charge neutrality in the cell (by introducing single carriers). If  $r\Delta t > t_{\text{rest}}$ , the time which is simulated for the injected carrier is  $t_{\text{rest}}$ , since in principle, if the carrier remains inside the cell, charge neutrality is exactly achieved with a simulated time  $t_{\text{rest}}$ .

With this carrier injection scheme we are sure to reproduce two important physical aspects at the contact: the electrons are crossing the boundary between the OC and the device (the position  $x = 0$ ) at random times during the time step (and not necessarily at the beginning or at the end), and the proper dynamics of the injected carriers in the cell adjacent to the contact determines the number of particles which must be introduced (depending on the carriers leaving the cell or remaining inside it). The usual number of particles injected by other techniques is the closest integer to  $(N_c - n_c)A\Delta x\Delta t$ , implicitly assuming that electrons enter the device at the beginning of the time step and remain inside the first cell. In our

case, by injecting carriers at random times during the time step and simulating their dynamics, we normally introduce a higher (and more realistic) number of particles.

Within this scheme we are going to analyse several models, which differ in the velocity distribution function from which the state of the new particles is randomly selected. Since the carriers are initially placed at the position  $x = 0$ , the particle velocity must be directed into the device. Thus the velocity (the component perpendicular to the contact surface) is sampled only from the positive part of the distributions. We shall always deal with non-degenerate material.

### 2.1. Model 1 (M1): Maxwellian distribution

The carriers are injected according to a Maxwellian distribution at the lattice temperature  $T$ :

$$f(v) \propto e^{-\frac{m^* v^2}{2K_B T}}, \quad (3)$$

where  $m^*$  is the effective mass of electrons in the semiconductor,  $K_B$  is Boltzmann's constant and  $v$  is the carrier velocity. In principle, this model would predict zero current at the boundary.

### 2.2. Model 2 (M2): displaced Maxwellian distribution

In this case the carriers are injected according to a displaced Maxwellian distribution at the lattice temperature:

$$f(v) \propto e^{-\frac{m^*(v-v_d)^2}{2K_B T}}, \quad (4)$$

where  $v_d$  is the mean velocity which the carriers in the cell adjacent to the contact should have according to the current density flowing through the device,  $J$ :

$$v_d = \frac{J}{qN_c}. \quad (5)$$

The value of  $v_d$  is determined in each time step from the current density calculated in the previous step. This distribution only applies for the velocity component perpendicular to the contact surface; the parallel components are determined according to a Maxwellian distribution. In principle, this model would preserve current conservation at the boundary [10,11].

### 2.3. Model 3 (M3): velocity-weighted Maxwellian distribution

Since in our injection scheme we are simulating carriers crossing the boundary between the OC and the adjacent cell inside the device, to account for the higher probability of particles with a large velocity to enter the device, the Maxwellian distribution should be weighted by the perpendicular velocity [9]. This model considers the OC as a thermal gas touching the boundary of the device, with its electrons escaping into the cell adjacent to the contact. In this case:

$$f(v) \propto v e^{-\frac{m^* v^2}{2K_B T}}. \quad (6)$$

This is the distribution of the carriers crossing a given position in a semiconductor at thermal equilibrium. Note that carriers with null/low velocity have null/very small probability of crossing the boundary. Again, this distribution only applies for the velocity component perpendicular to the contact surface, and the parallel components are determined according to a Maxwellian distribution.

The weighted Maxwellian could also be displaced according to the mean velocity the carriers should have to conserve the current:

$$f(v) \propto v e^{-\frac{m^*(v-v_d)^2}{2K_B T}}. \quad (7)$$

Since the results show that the displacement in velocity changes very slightly the behaviour of the contact, we shall not consider this case. The distribution of eqn (6) already provides very satisfactory results.

### 2.4. Model 4 (M4): reservoir method

This model is rather different from the previous ones. Here we try to get an appropriate distribution of carriers in a reservoir region adjacent to the semiconductor, so that the carrier dynamics in this reservoir determines the injection into the device [16]. The reservoir acts as a source of carriers.

This model is sketched in Fig. 1. A small region (commonly a few cells) adjacent to the device in the position of the contact is considered (reservoir), with the same doping as the adjacent semiconductor. The bias potential is applied to the node between the reservoir and the device. The injection of carriers into the reservoir occurs at the first cell of the opposite side, and following M1. Poisson's equation is only solved inside the device, but not in the reservoir, and the field in all cells of the reservoir takes the same value as that of the first cell inside the device. This ensures that in the boundary reservoir-device current is conserved. Any strange unwanted effect associated to the injection of carriers in the reservoir is far from the edge of the device, and the particles have enough time (and space) to stabilize their state according to the electric field before entering the device, so that in

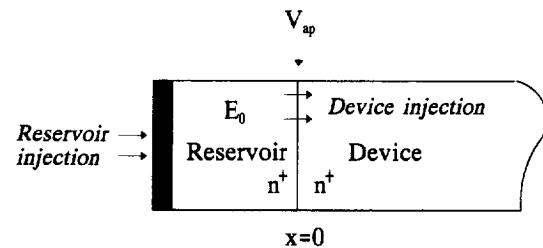


Fig. 1. Schematic presentation of the reservoir model for an ohmic contact.

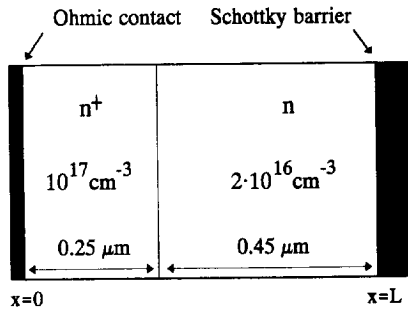


Fig. 2. Schematic drawing of the Schottky-barrier diode under study.

the boundary we get an adequate distribution. The real injection of carriers into the device occurs when the particles naturally cross the boundary reservoir-device.

It must be stressed that the four contact models provide reasonable (and similar) results in the case of long devices, where the possible effects associated to the contacts are not crucial for their behaviour. However, in the case of short devices these effects may be very important on their performance, and here lies the interest in finding an OC model with an ideal behaviour. The description of the four models given previously is for the case of one-dimensional MC simulations. Though it may require some slight modifications, their extension to two- or three-dimensional simulations is relatively simple.

### 3. MONTE CARLO SIMULATION

To check the behaviour of the four contact models, we have implemented them in the simulation of a GaAs SBD under forward-bias conditions. We have chosen this device because its performance is greatly affected by the number of carriers inside it and by the possible voltage drop at the ohmic contact, which may change the potential barrier the electrons have to surpass in order to reach the metal. A similar analysis in other one-dimensional devices, like  $n^+nn^+$  structures, would also show the effects appearing at the OCs, but their overall influence on the device performance would be practically negligible due to the presence of the highly doped  $n^+$  regions[10,12].

The simulated SBD is shown schematically in Fig. 2. It is modelled as a one-dimensional GaAs  $n^+-n$ -metal structure[17]. The  $n^+$  region is  $0.25\ \mu\text{m}$  long with a doping of  $10^{17}\ \text{cm}^{-3}$ . The OC is at its left side. The  $n$  region is  $0.45\ \mu\text{m}$  long with a doping of  $2 \times 10^{16}\ \text{cm}^{-3}$ . The Schottky barrier is at its end, with the metal contact acting as a perfect absorbing boundary: any carrier reaching the metal leaves the device and no carrier is injected from the metal. The barrier height used in the simulation is  $0.738\ \text{eV}$  (barrier seen by the electrons at the Fermi level in the metal), which leads to an effective built-in voltage (at equilibrium)  $V_{bi}$  of  $0.658\ \text{V}$  between the  $n$  region of

the semiconductor and the metal. No image-force lowering is included.

The GaAs model takes into account the first conduction band within a three-valley model ( $\Gamma$ ,  $L$  and  $X$ ), all isotropic and non-parabolic. Material parameters and scattering mechanisms can be found in Ref.[18]. The MC simulation follows the standard scheme[2]. The device is divided into equal cells of  $100\ \text{\AA}$  each, and the electric field is updated each  $10\ \text{fs}$  by employing a self-consistent one-dimensional Poisson solver. Carrier injection takes place before the field update. The cross-sectional area adopted for the device in the simulation is  $2 \times 10^{-13}\ \text{m}^2$ , which means an average number of simulated carriers ranging from 6300 to 6750 (depending on the bias and the model). In the case of M4, the reservoir is formed by 10 extra cells, leading to an additional number of carriers around 2000 and to a substantial increase in the computation time. The simulations are performed at a temperature of  $300\ \text{K}$ .

### 4. RESULTS

First we analyse the static characteristics of the SBD obtained with the different OC models. Figure 3 shows the profiles of several quantities along the device for an applied voltage of  $0.55\ \text{V}$ . These profiles were calculated by averaging over  $100\ \text{ps}$  of simulation once the device has reached the steady state. We shall focus on the effects taking place near the OC. In the case of the free-carrier concentration [Fig. 3(a)], the only model providing a uniform characteristic is M3. M1 and M2 show similar effects: although in the mesh close to the OC they reproduce the doping density (as is imposed by the model), in the following cells a dip in the concentration occurs, then approaching again the expected value. We attribute this effect to the fact that the above models inject carriers at the boundary with a too low velocity, which move slowly into the device. Thus, although charge neutrality is imposed by the models in the first cell, they are not able to provide adequate carriers to maintain it in the following cells, since the injected electrons need too long a time to reach them. In fact, the electrons must be accelerated by the electric field appearing because of the charge depletion, and after some distance ( $500\text{--}600\ \text{\AA}$ ) charge neutrality is achieved again. Note that even the displaced Maxwellian of M2 is not able to provide carriers with the appropriate velocity. Regarding M4 it is observed that the reservoir approaches much more the ideal concentration, but still presents some problems near the boundary introducing a slightly lower number of carriers. We conclude from these results that a right velocity distribution of the injected electrons is essential to get a uniform concentration near the contact and that the velocity-weighted Maxwellian is the most appropriate one.

The potential along the structure is shown in Fig. 3(b). Here, the influence of the contact models

can be clearly detected. The charge depletion observed near the OC with M1 and M2 leads to a voltage drop which is very important for the device behaviour, since it modifies the potential distribution along the structure. Thus the barrier which the carriers in the  $n$  region of the semiconductor must surpass to reach the metal is increased by this voltage drop. The charge depletion near the Schottky contact noticed in Fig. 3(a) is consistent with this potential barrier, being slightly more pronounced for the case of M1 and M2. M3 and M4 provide a very similar shape of the potential, with a very small voltage drop appearing near the boundary in the case of M4. The only model providing a completely flat characteristic at the OC is M3. The electric field in the SBD according to this potential profile is shown in Fig. 3(c). Near the OC, the field associated with the charge depletion of M1 and M2 is observed, reaching a value of  $2.5 \text{ kV cm}^{-1}$  at  $x = 0$ . In order to achieve charge neutrality in the adjacent cells, this field tends to accelerate into the device the too-slow carriers injected by the boundary. It is clear that both models lead to an OC which is not at thermal equilibrium. M4 shows an intermediate behaviour, and again the velocity-weighted Maxwellian (M3) provides the best

shape of the electric field. The field related to the built-in potential between the  $n^+$  and  $n$  regions is the same for all contacts. Near the Schottky barrier M1 and M2 yield higher values of the electric field as corresponds to the higher barrier.

Of course, when trying to get zero field at the contact we refer to the mean value along the whole simulation. At a given moment the field may be positive or negative at the boundary because of the presence of space charge. What the contact should do in such a case is to recover charge neutrality, so that on average the mean value of the field along the simulation is null.

Figure 3(d) gives the mean energy of the carriers along the diode. Again, the influence of the contact model is evident. While M3 and M4 inject carriers providing an energy near the OC which corresponds to the expected thermal energy  $\frac{3}{2}k_B T$ , M1 and M2 show significantly lower values. This fact supports our hypothesis that the Maxwellian and the displaced Maxwellian distributions inject carriers with a physically inconsistent velocity component perpendicular to the contact. The value of this component in the carriers introduced at the boundary should be higher, as occurs when these distributions are weighted by

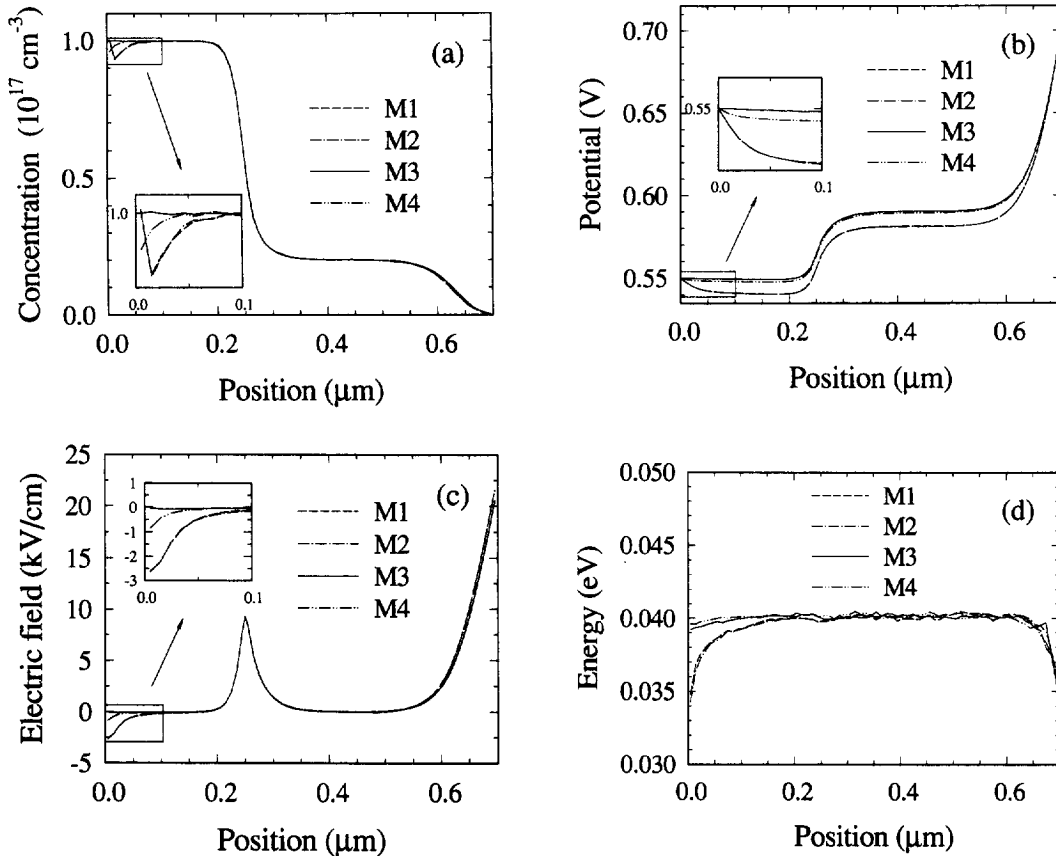


Fig. 3. Stationary profiles obtained with different ohmic contact models: (a) free-carrier concentration, (b) potential, (c) electric field and (d) energy at an applied voltage of 0.55 V in the Schottky-barrier diode under study.

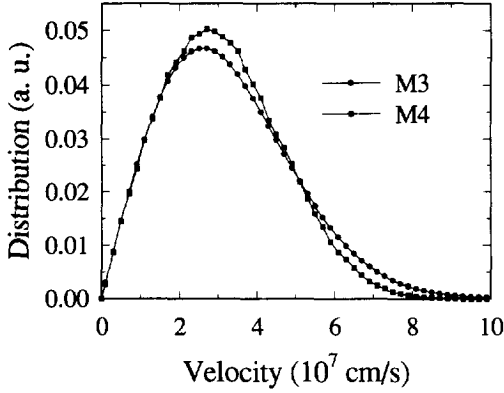


Fig. 4. Comparison between the velocity distribution of the carriers crossing the boundary reservoir-device in M4 at an applied voltage of 0.55 V and the velocity-weighted Maxwellian distribution (M3).

the velocity. At the side of the Schottky contact the cooling effect due to the barrier is clearly detected[19].

In Fig. 4, the velocity-weighted Maxwellian distribution (M3) is compared with the velocity distribution of carriers crossing the boundary reservoir-device in M4 for an applied voltage of 0.55 V. As can be observed, both curves are very similar, which means that M3 reproduces correctly the velocity of the carriers injected at the boundary without any additional simulation of particles.

The current-voltage characteristic of the SBD obtained with the different models of the OC is shown in Fig. 5. We also present the results for the current under forward-bias conditions given by the analytical thermionic emission theory:

$$J = \frac{qm^*(K_B T)^2}{2\pi^2\hbar^3} e^{-\frac{q(\phi_m - \chi_s)}{K_B T}} e^{\frac{qV}{K_B T}}, \quad (8)$$

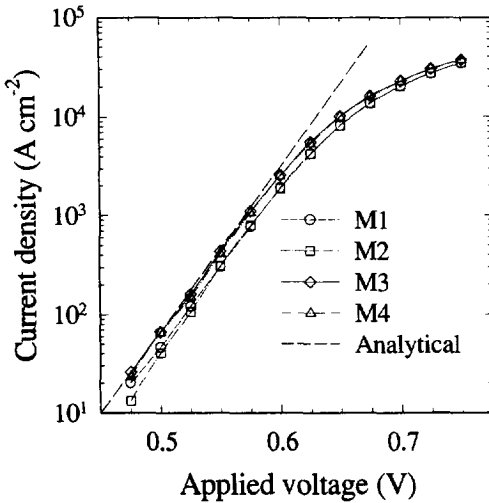


Fig. 5. Current-voltage characteristic of the Schottky-barrier diode under forward-bias conditions obtained with different ohmic contact models, together with the analytical estimation according to thermionic emission theory.

where  $q$  is the absolute value of the electron charge,  $\hbar$  is Planck's constant divided by  $2\pi$ ,  $\phi_m$  is the work function of the metal,  $\chi_s$  is the electron affinity of the semiconductor and  $V$  is the applied voltage.  $\phi_m - \chi_s$  corresponds to the barrier height, 0.738 V in our case. Since our aim is to reproduce the ideal behaviour of a contact (and not the real effects which could take place inside it) we compare our results with the ideal theory of the Schottky diode (and not with experimental data where non-ideal effects at the contact could occur).

Two different regions can be clearly observed in all curves according to the conditions  $V < V_{bi}$  and  $V > V_{bi}$ . In the former the current exhibits an exponential behaviour, which is determined by the thermionic emission of carriers over the barrier. In the latter the current tends to a linear behaviour due to the disappearance of the barrier, and it is the semiconductor series resistance which controls the current in the device. Therefore, the comparison with the analytical theory [eqn (8)] must be carried out in the first region. M3 and M4 achieve an excellent agreement with the analytical result in this range. The values of M4 are marginally lower than those of M3. However, M1 and M2, showing a similar exponential behaviour, provide considerably lower values of the current, as may be expected from the increase in the semiconductor-metal barrier introduced by the voltage drop at the OC. Therefore, we can conclude that in MC simulation of a SBD, the role played by the OC is decisive for obtaining correct results. M3 and M4 are found to be the most suitable and physically plausible models of an OC. M3 results to be the most efficient one, since its implementation is easier and the computation time required for the simulations is appreciably shorter.

At this point it must be emphasized that in the case of other more "symmetric" devices (like  $n^+nn^+$  structures) it has been checked that the  $I$ - $V$  characteristics are not appreciably modified by the model used for the OC. However, the same anomalous effects are found near the contacts when using M1, M2 and M4.

In order to illustrate the influence of the OC model on second-order terms, we present some results on the noise behaviour of the SBD. Figure 6(a) shows the autocorrelation function of current fluctuations  $C_1(t)$  at an applied voltage of 0.6 V, and Fig. 6(b) shows its Fourier transform, the spectral density  $S_1(f)$ . The details of the calculation of these magnitudes can be found in [17,20]. It is clear that the contact model also affects the noise performance of the device. Although the four models provide analogous shapes of the curves, there are significant differences. The autocorrelation functions exhibit an oscillatory behaviour associated to the coupling between carrier velocity and self-consistent electric field introduced by the  $n^+-n$  homojunction[12,17,20]. As in the results previously shown, the pairs of models M1-M2 and

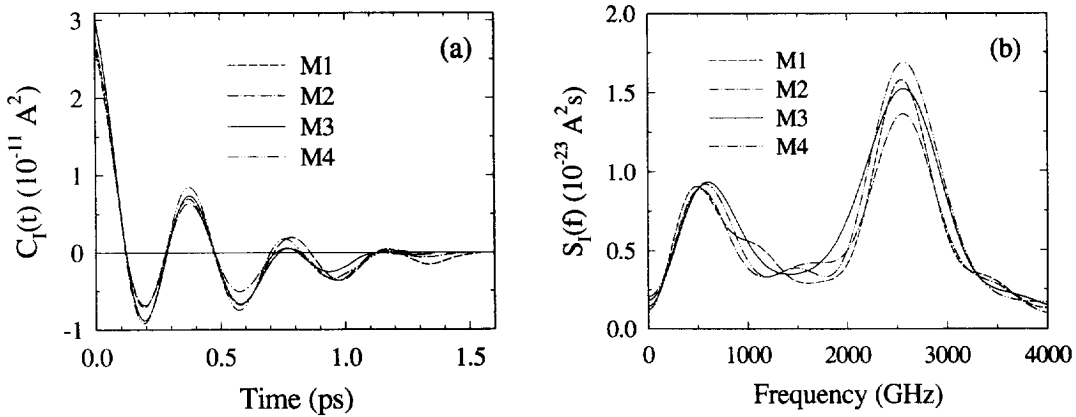


Fig. 6. (a) Autocorrelation function and (b) spectral density of current fluctuations in the Schottky-barrier diode obtained with different ohmic contact models at an applied voltage of 0.6 V.

M3–M4 present similar results. In particular, the correlation extends for longer times with M1 and M2.

The low-frequency value of the spectral density with the four models fits rather well (to an accuracy of about 15%, and within the error of the MC method) the expectation of finding pure shot noise, i.e.  $S_I(0) = 2qI$  [15,17,20,21]. At higher frequencies two peaks are observed. The first one is originated by the carriers that have insufficient kinetic energy to surpass the barrier and return to the neutral semiconductor [21]. The second one is associated with the above-mentioned oscillatory behaviour in the autocorrelation function [17,20]. While the frequency of the second peak is independent of the model (but its amplitude changes), the first one is displaced towards higher frequencies for models M3 and M4 due to the shorter depletion region near the Schottky contact [21].

In the case of the noise, there is no clear criterion to establish which one is the most appropriate model, except the low-frequency value of the spectral density, which is favourable for the four models within the statistical error of the MC technique. Nevertheless, it can be concluded that the OC model also affects the behaviour of the fluctuations.

## 5. CONCLUSIONS

We have presented a detailed analysis of the influence of ohmic contact (OC) models on Monte Carlo (MC) simulation of semiconductor devices. An algorithm to determine the number of carriers to be injected at a contact, the moment at which they enter the device and their coordinates has been presented. Four different distributions for the velocity of the injected carriers have been analysed. A GaAs Schottky-barrier diode (SBD) under forward-bias conditions has been used to implement the four models, and their effect on the static characteristics and on the noise performance has been studied. The main conclusions can be summarized as follows:

- (i) The role played by an OC in MC simulation of semiconductor devices may be essential, specially in the case of short structures or when the number of carriers inside the device determines its performance (like in SBDs).
- (ii) In order to introduce the correct number of particles for achieving charge neutrality, not only in the cell adjacent to the boundary but in a longer region of the device close to the contact, an appropriate time and space algorithm to inject the carriers at the OC must be applied.
- (iii) Maxwellian or displaced-Maxwellian velocity distribution functions for the injected carriers lead to physically inconsistent effects in the vicinity of the OC, affecting the free-carrier concentration, the potential, the electric field, the energy, etc., and modifying the ideal  $I$ – $V$  characteristics of the SBD due to a voltage drop at the contact.
- (iv) The reservoir method and the velocity-weighted Maxwellian distribution provide similar and correct results, specially the latter. Flat profiles of the different magnitudes, zero voltage drop at the contact and  $I$ – $V$  characteristics in excellent agreement with the thermionic emission theory are obtained with them for the SBD.
- (v) The noise behaviour of the SBD is also affected by the choice of the OC model.
- (vi) As a final conclusion we consider the velocity-weighted Maxwellian injection as the most appropriate and efficient model among those analysed in this work. It reproduces all physical requirements of an ideal OC, needs lower computation time with respect to the reservoir method and its implementation in a MC simulator is easier.

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# REFERENCES

1. M. V. Fischetti, *IEEE Trans. Electron Devices* **ED-38**, 634 (1991), and Refs cited therein.
2. C. Jacoboni and P. Lugli, *The Monte Carlo Method for Semiconductor Device Simulation*, p. 224. Springer, Berlin (1989).
3. K. Hess (Ed.) *Monte Carlo Device Simulation: Full Band and Beyond*. Kluwer, Boston (1991).
4. J. J. Rosenberg, E. J. Yoffa and M. I. Nathan, *IEEE Trans. Electron Devices* **ED-28**, 941 (1981).
5. R. W. Hockney and J. W. Eastwood, *Computer Simulation Using Particles*, p. 358. IOP, Bristol (1988).
6. M. V. Fischetti and S. E. Laux, *Phys. Rev.* **B38**, 9721 (1988).
7. K. Tomizawa, *Numerical Simulation of Submicron Semiconductor Devices*, p. 125. Artech House, Boston (1993).
8. C. Moglestue, *Monte Carlo Simulation of Semiconductor Devices*, p. 183. Chapman & Hall, Cambridge (1993).
9. S. E. Laux and M. V. Fischetti, in *Monte Carlo Device Simulation: Full Band and Beyond* (Edited by K. Hess), p. 1. Kluwer, Boston (1991).
10. D. L. Woolard, H. Tian, M. A. Littlejohn and K. W. Kim, *IEEE Trans. Electron Devices* **ED-41**, 601 (1994).
11. D. L. Woolard, H. Tian, M. A. Littlejohn and K. W. Kim, *IEEE Trans. Computer-Aided Des. Integr. Circuits Syst.* **13**, 1241 (1994).
12. L. Varani, T. Kuhn, L. Reggiani and Y. Perlès, *Solid-St. Electron.* **36**, 251 (1993).
13. T. González and D. Pardo, *J. appl. Phys.* **73**, 7453 (1993).
14. U. Ravaioli, P. Lugli, M. A. Osman and D. K. Ferry, *IEEE Trans. Electron Devices* **ED-32**, 2097 (1985).
15. J. G. Adams, T.-W. Tang and L. E. Kay, *IEEE Trans. Electron Devices* **ED-41**, 575 (1994).
16. A. di Carlo, *Dissertation*, University of Rome-La Sapienza (1991).
17. T. González, D. Pardo, L. Varani and L. Reggiani, *Appl. Phys. Lett.* **63**, 3040 (1993).
18. T. González, J. E. Velázquez, P. M. Gutiérrez and D. Pardo, *Semicond. Sci. Technol.* **6**, 862 (1991).
19. R. Stratton, *Phys. Rev.* **126**, 2002 (1962).
20. L. Varani, L. Reggiani, T. Kuhn, T. González and D. Pardo, *IEEE Trans. Electron Devices* **ED-41**, 1916 (1994).
21. M. Trippe, G. Bosman and A. van der Ziel, *IEEE Trans. Microw. Theory Tech.* **MTT-34**, 1183 (1986).