A Generalized Drift-Diffusion Model for Rectifying Schottky Contact Simulation

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***Abstract*—We present a discussion on the modeling of Schottky barrier rectifying contacts (diodes) within the framework of partial-differential-equation-based physical simulations. We propose a physically consistent generalization of the drift-diffusion model to describe the boundary layer close to the Schottky barrier where thermionic emission leads to a non-Maxwellian carrier distribution, including a novel boundary condition at the contact. The modified drift-diffusion model is validated against Monte Carlo simulations of a GaAs device. The proposed model is in agreement with the Monte Carlo simulations not only in the current value but also in the spatial distributions of microscopic quantities like the electron velocity and concentration.**

***Index Terms*—Schottky barriers, semiconductor device modeling.**

I. Introduction

THE PHYSICAL simulation of Schottky barrier contacts (SBCs) within the framework of partial differential equation (PDE)-based transport models (and neglecting tunneling effects) traditionally exploits boundary conditions (b.c.'s) derived from the thermionic emission and diffusion theory originally developed by Crowell and Sze [1], [2]. In addition to the jump in the surface potential accounting for the potential barrier at the Schottky contact [3] (which, if needed, may be modified to include image-force-lowering effects [4]), current conduction across the barrier on an n-type semiconductor is described by a b.c. on the (majority) carrier continuity equation, i.e.,

$$J = qv_{r0}(n - n_0) \tag{1}$$

where J is the total current density crossing the SBC, n is the electron concentration at the barrier, n_0 is the equilibrium electron concentration at the barrier, v_{r0} is the surface recombination velocity, and q is the absolute value of the electron charge. Within this treatment, only majority carriers (here, electrons) contribute to the current across the SBC, while the minority carrier current is neglected.

The surface recombination velocity v_{r0} is evaluated in [1] assuming a Maxwellian velocity distribution $f_M(v)$ at the contact and shown to be $v_{r0} = v_{\rm th}/4$, where $v_{\rm th} = \sqrt{8k_BT/(\pi m^*)}$ is related the mean thermal velocity (m^* is the electron effective mass, k_B is the Boltzmann constant, and T is the lattice temperature). The Maxwellian assumption becomes less accurate under far-from-equilibrium conditions, particularly in forward bias. Baccarani and Mazzone [5] calculated the distribution function with a Monte Carlo (MC) simulation in strong forward bias (near-flatband conditions), finding a semi-Maxwellian shape, which leads to a surface recombination velocity equal to $2v_{r0} = v_{\rm th}/2$ but, at the same time, to a carrier concentration at the barrier half of the value predicted by the thermionic-diffusion theory; for this reason, (1) for the current across the barrier still holds.

In forward bias, where the Maxwellian assumption breaks down, a modified approach to the definition of the b.c. exploits a bias-dependent surface recombination velocity. Several models have been proposed in the literature along this line [6]–[9]. All of them take the form

$$J = qv'_r(n - n_0) \tag{2}$$

where v'_r now depends on the SBC bias. All these models are characterized by a null v'_r in reverse bias, thus leading to an unrealistically null SBC reverse current.

In this paper, we propose a fully consistent treatment of an SBC and implement it within the framework of a drift-diffusion (DD) transport model. For the sake of simplicity, we neglect in the derivation the tunneling effect across the barrier: notice, however, that, according to the discussion in [2] and [10], thermoionic and tunneling b.c.'s can independently be treated; therefore, the latter effect can readily be included into our model if necessary. Consistency is obtained in two steps: first, we derive a general expression of the contact current density (including the reverse component) based on a piecewise approximation of the distribution function consistent with the physics of carriers moving in opposite directions at the SBC, which, in turn, exhibit a different dependence on the applied

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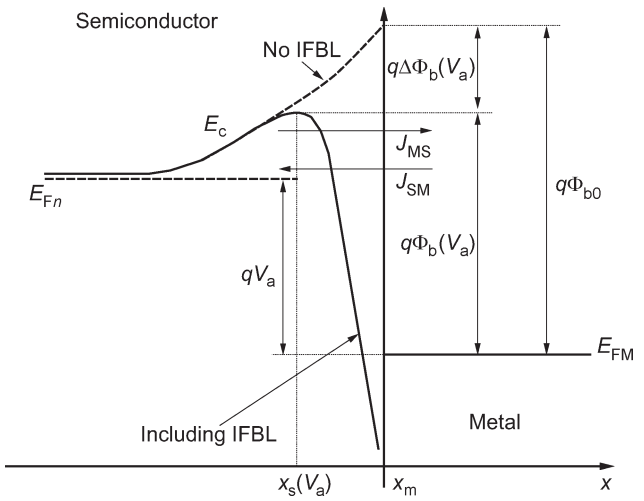

Fig. 1. Band diagram for an SBC on an n-type semiconductor in forward bias (metal is on the right, for $x > x_m$). $E_{\rm Fn}$ and $E_{\rm FM}$ are the electron quasi-Fermi levels in the semiconductor and the metal, respectively. V_a is the bias applied to the metal with respect to the semiconductor, x_m is the position of the SBC (metallurgical junction), and x_s is the position of the peak value of the potential in the semiconductor: neglecting IFBL, $x_s = x_m$. Finally, $q\Phi_{b0}$ is the zero-bias barrier height of the SBC, modified into $q\Phi_b(V_a)$ if IFBL is considered.

bias; as a second step, we define a modified version of the DD equations in the neighborhood of the SBC to correctly implement the current derived in the first step, yielding a model that is valid in both reverse and forward bias. Such a feature is particularly important whenever the SBC works at zero dc bias and is therefore alternatively driven in forward and reverse conditions. Relevant applications are Schottky diodes for fast-switching power supplies and also RF and microwave applications such as resistive mixers and frequency multipliers. The modified DD transport model can easily be implemented into available simulators, since, with a proper formulation, it does not impact on the current density expression and therefore does not require modifications to the Scharfetter and Gummel [3] discretization scheme commonly employed in device modeling tools. This paper is structured as follows. The model is derived in Sections II and III and is validated against MC simulations carried out on a GaAs SBC [12] in Section IV. Finally, conclusions are drawn is Section V.

II. Treatment of the SBC Current

Let us consider a Schottky contact on an n-doped semiconductor, whose band diagram is shown in Fig. 1, where we have chosen to put the metal on the right side of the structure (i.e., for $x > x_m$, where x_m is the position of the metallurgical junction). For the sake of generality, we have also accounted for image force barrier lowering (IFBL): the position where the b.c. is to be derived is the abscissa $x_s(V_a)$ of the peak of the potential distribution inside the semiconductor, where the energy barrier seen from the metal amounts to $q\Phi_b(V_a)$. Expressions for the applied bias dependence of x_s and $q\Phi_b$ can be found, e.g., in [1] and [4]. Neglecting IFBL amounts to setting $x_s = x_m$ and $\Phi_b = \Phi_{b0}$ (the zero-bias value of the SBC barrier).

In the absence of tunneling currents, when the only possible mechanism of current flow through the contact is thermionic

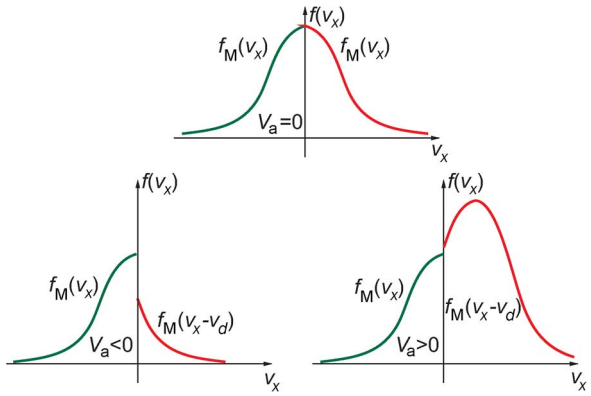

Fig. 2. Assumed piecewise shape of the distribution function at the contact.

emission over the barrier, the development of a physically correct b.c. at $x = x_s$ requires the separate consideration of carriers moving in opposite directions. Indeed, the flow of electrons from the metal to the semiconductor at $x = x_s$ $(v_x < 0)$ is nearly independent of the applied bias V_a, except for IFBL effects, since it is controlled by the Schottky barrier height Φ_b. In contrast, the semiconductor-to-metal flow (electrons with $v_x > 0$ at $x = x_s$) is strongly modulated by V_a. As a consequence, both the density and velocity distribution of electrons moving in opposite directions exhibit a different dependence on the applied bias that must be accounted for to develop a proper b.c.

In order to introduce our approach, we first consider the thermionic-diffusion theory [4] (see also Fig. 1) and, in particular, the following carrier concentration, to which the metal-to-semiconductor current is proportional:

$$n_0'(x_s) = N_c \exp\left(-\frac{\Phi_b(V_a)}{V_T}\right) \tag{3}$$

where V_a is the applied bias (measured on the metal with respect to the semiconductor, and thus, $V_a > 0$ in forward bias), N_c is the conduction band effective density of states, $V_T = k_B T/q$ is the voltage equivalent of temperature. For further details, see [1] and [4].

Our treatment of the SBC is based on the following assumptions.

1) The electron distribution function at the contact (i.e., for $x = x_s$) is represented by the piecewise approximation depicted in Fig. 2. We split the distribution function into two parts, corresponding to the two possible electron fluxes at the contact.
   - For electrons flowing from the metal to the semiconductor (i.e., for negative carrier velocities $v_x < 0$), the distribution function is the left part of a centered Maxwellian $f_M(v_x)$, normalized to yield an electron density equal to $n_0'(x_s)/2$. If IFBL is neglected, this function is also independent of the applied bias V_a.
   - For electrons flowing from the semiconductor to the metal (i.e., for positive carrier velocities $v_x > 0$), the distribution function is the right part of a drifted Maxwellian $f_{\rm DM}(v_x) = f_M(v_x - v_d)$, normalized to yield an electron density equal to $n(x_s) - n_0'(x_s)/2$. As indicated in Fig. 2, the fraction of

$n(x_s)$ corresponding to carriers with $v_x > 0$ is equal to/lower than/higher than that of carriers with $v_x < 0$ for equilibrium/reverse/forward bias, respectively. The peak velocity $v_d(V_a)$ (negative in reverse bias and positive for $V_a > 0$) would correspond to the average velocity of the $n(x_s)$ electrons if all of them were characterized by a drifted Maxwellian distribution function. Since the approximated distribution function for this part of the electron concentration is a drifted Maxwellian (although truncated to positive velocities) as in [6], the Adams and Tang [6] average velocity holds (see (8) below).

2) The electron distribution function in any point in the semiconductor sufficiently far away from the contact (i.e., for $x < x_s - \delta x$, where $\delta x \approx 40 \sim 50$ nm, as discussed further on) is a drifted Maxwellian $f_{\rm DM}(v_x) = f_M(v_x - v_d)$ [9].
3) The metal–semiconductor current density component $J_{\rm MS}$ is associated to free electrons moving from the metal into the semiconductor due to thermionic emission. According to [1] and [4], $J_{\rm MS}$ depends on the height of the barrier only.

In the case of a strong-enough forward bias, the previously described model reproduces the so-called *absorbing b.c.* typically considered in MC simulations [12]. Under these conditions, when $n(x_s) \gg n_0'(x_s)$, the extremely low number of electrons injected by the metal into the semiconductor can be neglected as compared to those flowing through the SBC in the opposite direction, and the distribution function at $x = x_s$ can be assumed to be a drifted Maxwellian truncated to positive velocities (i.e., taking a zero value for $v_x < 0$). Thus, the contact acts just as an *absorber* of carriers.

In the general case, the total current density J entering the contact is expressed as the net sum of the currents due to electrons flowing from semiconductor to metal and vice versa, i.e.,

$$J = J_{\rm SM} - J_{\rm MS}. \tag{4}$$

A physically consistent definition of the current density corresponding to the electrons moving from the semiconductor to the metal $J_{\rm SM}$ (i.e., with $v_x > 0$) can be obtained by means of the following considerations. The probability that an electron has, in $x = x_s$, a velocity component along the x-axis between v_x and $v_x + dv_x$ is given by, according to assumption 1, the following:

$$\frac{f_M(v_x - v_d)dv_x}{\int_0^{+\infty} f_M(v_x - v_d)dv_x}. \tag{5}$$

This corresponds to a contribution to the current density

$$dJ_{\rm SM} = q\left[n(x_s) - \frac{n_0'(x_s)}{2}\right] v_x \frac{f_M(v_x - v_d)dv_x}{\int_0^{+\infty} f_M(v_x - v_d)dv_x} \tag{6}$$

therefore

$$J_{\rm SM} = q\left[n(x_s) - \frac{n_0'(x_s)}{2}\right] \frac{\int_0^{+\infty} v_x f_M(v_x - v_d)dv_x}{\int_0^{+\infty} f_M(v_x - v_d)dv_x}. \tag{7}$$

Notice that the integral ratio is the definition of surface recombination velocity exploited in [6]; thus

$$J_{\rm SM} = q\left[n(x_s) - \frac{n_0'(x_s)}{2}\right] v_{r,A} \tag{8}$$

where $v_{r,A}$ is the Adams and Tang [6] average velocity, i.e.,

$$v_{r,A} = \frac{\int_0^{+\infty} v_x f_M(v_x - v_d)dv_x}{\int_0^{+\infty} f_M(v_x - v_d)dv_x}. \tag{9}$$

Since, in equilibrium, $J = 0$ and $v_d = 0$, from (8), we find (notice that, in equilibrium, $v_{r,A} = 2v_{r0}$; see [6])

$$J_{\rm MS}|_{\rm equilibrium} = J_{\rm SM}|_{\rm equilibrium} = q\frac{n_0(x_s)}{2} 2v_{r0} \tag{10}$$

in agreement with [5]. In (10), $n_0(x_s)$ is the $n_0'(x_s)$ calculated for $V_a = 0$ [see (3)]. This allows estimating $J_{\rm MS}$ since, according to assumption 3, when out of equilibrium, we still use (10), apart from the effect of IFBL on the contact electron concentration [4] (and, therefore, on the reverse saturation current), i.e.,

$$J_{\rm MS} = qn_0'(x_s)v_{r0}. \tag{11}$$

If IFBL is neglected, $x_s = x_m$ and $\Phi_b = \Phi_{b0}$ irrespective of bias (and, therefore, a bias-independent reverse saturation current is also obtained).

Using (8) and (11), we finally express the contact current as

$$J = q\left\{\left[n(x_s) - \frac{n_0'(x_s)}{2}\right] v_{r,A} - n_0'(x_s)v_{r0}\right\}. \tag{12}$$

III. Generalized DD Model

At first sight, the current density expression (12) appears to be directly implementable as a b.c. in moment-based models for carrier transport. In practice, this would amount to adding to the equations of the spatially discretized model a discretized version of (12), where the left-hand side (the total current density) is expressed as a function of the model unknowns (including, of course, $n(x_s)$) according, e.g., to the DD transport model. Unfortunately, this approach would lead to inconsistent results, because of a subtle assumption on the carrier distribution function that is implicitly made in the DD model. As discussed, e.g., in [13], the DD model is actually compatible with a carrier distribution function that is a displaced Maxwellian in the entire device volume; this is, of course, in contrast with the piecewise shape of the distribution function we propose close to the Schottky contact. In fact, if the standard DD current expression was used in the left-hand side of (12), it would implicitly also include carriers with a negative velocity (i.e., moving from the metal to the semiconductor), thus resulting, for the same current level, into an electron density and velocity different from those actually present as a consequence of the b.c. derived from the piecewise distribution.

Following the previous remarks and expanding the analysis in [4], we propose a method to reformulate the DD transport model (by introducing in the DD equations an artificial electron

density) in such a way to make it compatible, in the neighborhood of the Schottky contact (i.e., for $x_s - \delta x < x < x_s$), with a piecewise (non-Maxwellian) distribution that is continuously evolving into a shifted Maxwellian distribution ($x \to x_s - \delta x$); this will allow (12) to be implemented as a b.c. in a consistent way.

We start by evaluating, at the SBC, the current density due to electrons flowing toward the metal according to a shifted Maxwellian approximation; this "modified-DD" semiconductor–metal current is expressed as

$$J_{\mathrm{SM,DD}}(x_s) = qn_{\mathrm{DD}}(x_s)\frac{\int_0^{+\infty} v_x f_M(v_x - v_d)dv_x}{\int_{-\infty}^{+\infty} f_M(v_x - v_d)dv_x} = qn_{\mathrm{DD}}(x_s)v_{r,S} \tag{13}$$

where $n_{\mathrm{DD}}(x_s)$ is a "modified-DD" SBC electron density, and $v_{r,S}$ is the surface recombination velocity proposed by Shibkov *et al.* [9], i.e.,

$$v_{r,S} = \frac{\int_0^{+\infty} v_x f_M(v_x - v_d)dv_x}{\int_{-\infty}^{+\infty} f_M(v_x - v_d)dv_x}. \tag{14}$$

Concerning the MS current, we assume that this is always given at the SBC by (11); from (4), we obtain the following "modified-DD" total SBC current expression:

$$J_{\mathrm{DD}}(x_s) = qn_{\mathrm{DD}}(x_s)v_{r,S} - qn_0'(x_s)v_{r0}. \tag{15}$$

Equating (12) and (15), we can readily relate the "modified-DD" SBC electron density $n_{\mathrm{DD}}(x_s)$ to the physical SBC electron density $n(x_s)$ as follows. Let us define the coefficients

$$r_n = \frac{n(x_s)}{n_{\mathrm{DD}}(x_s)} \quad r_{v_r} = \frac{v_{r,A}}{v_{r,S}}. \tag{16}$$

We have

$$r_n = \frac{1}{r_{v_r}} + \frac{1}{2}\frac{n_0'(x_s)}{n_{\mathrm{DD}}(x_s)} \tag{17}$$

therefore

$$n_{\mathrm{DD}}(x_s) = \frac{n(x_s)}{r_n} = \left[\frac{1}{r_{v_r}} + \frac{1}{2}\frac{n_0'(x_s)}{n_{\mathrm{DD}}(x_s)}\right]^{-1} n(x_s) = \hat{r}_{v_r}(x_s)n(x_s) \tag{18}$$

where $\hat{r}_{v_r} \to r_{v_r}$ for $n_{\mathrm{DD}}(x_s) \gg n_0'(x_s)$, and $\hat{r}_{v_r} \to 1$ for $n_{\mathrm{DD}}(x_s) \to n_0'(x_s)$.

If we assume that, beyond a boundary layer of thickness δx, the carrier distribution thermalizes into a shifted Maxwellian, we can extend (18) to the whole thickness of the boundary layer as

$$n_{\mathrm{DD}}(x) = \hat{r}_{v_r}(x)n(x) \tag{19}$$

where the coefficient $\hat{r}_{v_r}(x)$ satisfies (18) for $x = x_s$ and tends to 1 for $x \to x_s - \delta x$ (see assumption 2). In other words, the "modified-DD" current (which continuously evolves into the standard DD current from the SBC to the boundary-layer limit) can be expressed by inserting the modified charge density $n_{\mathrm{DD}}(x)$ into the standard DD equations as follows (μ_n and D_n are the electron mobility and diffusivity, respectively):

$$J_{\mathrm{DD}}(x) = q\left[\mu_n \hat{r}_{v_r} n\mathcal{E} + D_n\frac{\partial(\hat{r}_{v_r}n)}{\partial x}\right]. \tag{20}$$

In (20), $\mathcal{E}$ denotes the electric field that depends, through Poisson's equation, on n. Notice, however, that $\hat{r}_{v_r}(x_s)$ is actually a model unknown, since it depends on the solution $n_{\mathrm{DD}}(x_s)$, and thus, it has to be determined through the self-consistent numerical solution of the entire model.

The last step is the introduction of a suitable parameterization and approximation of the unknown function $\hat{r}_{v_r}(x)$. We exploit a third-order power series expansion, i.e.,

$$\hat{r}_{v_r}(x) = \begin{cases} 1, & \text{if } x < x_s - \delta x \\ 1 + \frac{\hat{r}_{v_r}(x_s)-1}{\delta x^3}(x - x_s - \delta x)^3, & \text{if } x_s - \delta x \le x \le x_s \end{cases} \tag{21}$$

where the coefficients are derived by imposing the value of $\hat{r}_{v_r}(x)$ in x_s and $x_s - \delta x$ and the continuity of the electric field and of the first and second derivatives of n in $x_s - \delta x$.

In summary, to describe, within the DD model, the SBC so that a current consistent with the b.c. derived from the piecewise distribution is obtained in both forward and reverse bias, the following modified DD model (from now on referred to as the "generalized DD model") should be employed[1]:

$$\frac{\partial \mathcal{E}}{\partial x} = \frac{q}{\epsilon_S}\left[N_D^+(x) - n(x)\right] \tag{22a}$$

$$\frac{\partial}{\partial t}n(x) = \frac{1}{q}\frac{\partial J_{\mathrm{DD}}}{\partial x} - U_n \tag{22b}$$

where the symbols have the usual meaning, the current density is given by the constitutive relation (20), the SBC b.c. for the current is (12), and the $\hat{r}_{v_r}(x)$ parameter is given by (21).

From an implementation standpoint, the generalized DD model (22) can conveniently be rephrased in terms of the unknown $n^*(x) = \hat{r}_{v_r}(x)n(x)$, since, in this case, we have

$$\frac{\partial \varepsilon}{\partial x} = \frac{q}{\epsilon_s}\left[N_D^+(x) - \frac{n^*(x)}{\hat{r}_{v_r}(x)}\right] \tag{23a}$$

$$\frac{\partial}{\partial t}\left[\frac{n^*(x)}{\hat{r}_{v_r}(x)}\right] = \frac{1}{q}\frac{\partial J_{\mathrm{DD}}}{\partial x} - U_n \tag{23b}$$

where

$$J_{\mathrm{DD}}(x) = q\left[\mu_n n^*\mathcal{E} + D_n\frac{\partial n^*}{\partial x}\right]. \tag{23c}$$

The b.c. becomes

$$J = q\left[n^*(x_s)v_{r,S} - n_0'(x_s)v_{r0}\right]. \tag{23d}$$

A. Evaluating v_d

The surface recombination velocity $v_{r,S}$ used in (23) was originally proposed by Shibkov *et al.* [9], i.e.,

$$v_{r,S} = \frac{1}{2}v_d\left[1 + \mathrm{erf}\left(\frac{v_d}{2\sqrt{\pi}v_{r0}}\right)\right] + v_{r0}\exp\left(-\frac{v_d^2}{4\pi v_{r0}^2}\right). \tag{24}$$

[1]We consider here the 1-D monopolar case. The extension to a bipolar transport model is straightforward.

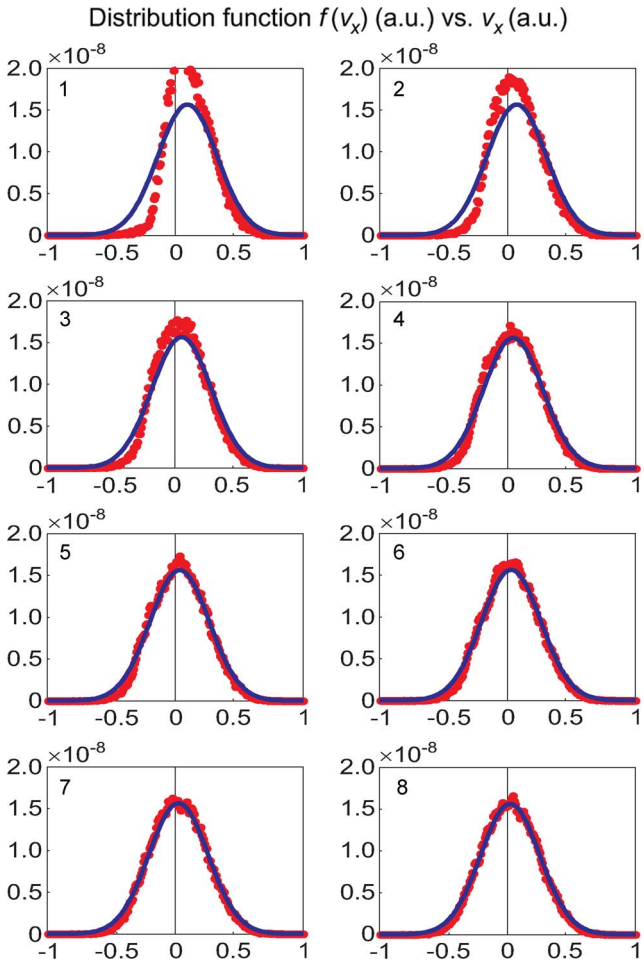

Fig. 3. Comparison between the distribution function calculated with Monte Carlo (symbols) and its approximation with a drifted Maxwellian (full line) in several positions near the SBC for a forward bias $V_a = 0.6$ V. The distances of the distribution functions from the contact are given as follows: 1: 4.125, 2: 12.375, 3: 20.625, 4: 28.875, 5: 37.125, 6: 45.375, 7: 53.625, and 8: 61.875 nm.

Notice that, in equilibrium conditions, $v_d = 0$, and (24) reduces to $v_r = v_{r0}$. The main difficulty in applying (24) in the presence of bias is the determination of the average drift velocity v_d, which is quite generically defined as given by $J(x)/(qn(x))$ for some x "near" the contact [9]. According to the previous discussion, in principle, v_d should correspond to the peak of the drifted Maxwellian representing the distribution function in $x_s - \delta x$. Examining the MC distribution function (see Fig. 3), we conclude that the distribution function is reasonably approximated by a drifted Maxwellian for $\delta x \approx 40 \sim 50$ nm. Therefore, we estimate v_d by calculating

$$v_d(x_i) = \frac{J(x_i)}{qn(x_i)}, \qquad i = 1, 2 \tag{25}$$

where x_i are the two mesh points nearest to $x_s - \delta x$, and we use these values to calculate $v_d(x_s - \delta x)$ through linear extrapolation.

B. Including Velocity Saturation Effects

The generalized DD model calls for a consistent modification of the mobility model exploited to account for velocity saturation. This is due to the fact that, at the contact, the average carrier velocity derived from the approximated distribution function should be equal to the value dictated by the inclusion of the saturation velocity effect. Having in mind the simulation of Schottky contacts on III–V compound semiconductors, we use the standard GaAs mobility model [3], i.e.,

$$\mu_n(x) = \frac{\mu_{n0} + v'_{\rm sat}(x)\left[\mathcal{E}(x)^3/\mathcal{E}_0^4\right]}{1 + \left[\mathcal{E}(x)/\mathcal{E}_0\right]^4} \tag{26}$$

where the coefficients μ_{n0} and $\mathcal{E}_0$ are determined from MC simulations. The spatial dependence of the modified saturation velocity is derived similar to (21), as given in (27), shown at the bottom of the page. Finally, the contact saturation velocity is approximated as

$$v'_{\rm sat}(x_s) = v_{\rm sat}\left[1 - \frac{|n(x_s) - n'_0(x_s)|}{n(x_s)}\right] + \frac{\max(2v_{r0}, v_{r,A})}{\hat{r}_{v_r}(x_s)}\frac{|n(x_s) - n'_0(x_s)|}{n(x_s)}. \tag{28}$$

For $V_a = 0$, $n(x_s) = n'_0(x_s)$ and $\hat{r}_{v_r}(x_s) = 1$ so that, according to the Maxwellian electron distribution function at the contact, $v'_{\rm sat}(x_s) = v_{\rm sat}$. Furthermore, $2v_{r0} > v_{r,A}$ for $V_a < 0$, and $2v_{r0} < v_{r,A}$ for $V_a > 0$. Therefore, we have the following.

1) If $V_a \ll 0$ and $v_{\rm sat} > v_{\rm th}/2$, $n(x_s) \to n'_0(x_s)/2$, and thus, $v'_{\rm sat}(x_s) \to 2v_{r0}/\hat{r}_{v_r}(x_s)$. Taking into account (26), the current density expression of the generalized DD model yields $J_{\rm DD}(x_s) \to -qv_{r0}n'_0(x_s)$. Notice that if $v_{\rm sat} < v_{\rm th}/2$, the contact electron concentration cannot reach the limit $n'_0(x_s)/2$ value.
2) For $V_a \gg 0$, $n(x_s) \gg n'_0(x_s)$, and thus, $v'_{\rm sat}(x_s) \to v_{r,A}/\hat{r}_{v_r}(x_s)$. The current density becomes $J_{\rm DD}(x_s) \to qv_{r,A}n(x_s)$.

Both asymptotic current expressions are consistent with (12).

IV. Comparison With MC Simulations

To validate the generalized DD model discussed in Section III, we have simulated a 1-D GaAs SBC [12] made of a Schottky contact (with barrier height $\Phi_{b0} = 0.737$ V and IFBL not included in all simulations) on an n region (with doping level $N_D = 10^{16}$ cm^{-3} and a length of 350 nm), an n$^+$ region (with doping level $N_D^+ = 10^{17}$ cm^{-3} and a length of 350 nm), and an ohmic contact. The Schottky contact is placed on the right side of the structure, while the x-axis origin used in the following figures is at the left ohmic contact. Since we neglect IFBL here, the SBC position is therefore $x_s = x_m = 700$ nm. According to the model developed, we also neglect, in this case, tunnel effects. In order to substantiate this approximation, we

$$v'_{\rm sat}(x) = \begin{cases} v_{\rm sat}, & \text{if } x < x_s - \delta x \\ v_{\rm sat} + \frac{v'_{\rm sat}(x_s) - v_{\rm sat}}{\delta x^3}(x - x_s - \delta x)^3, & \text{if } x_s - \delta x \le x \le x_s \end{cases} \tag{27}$$

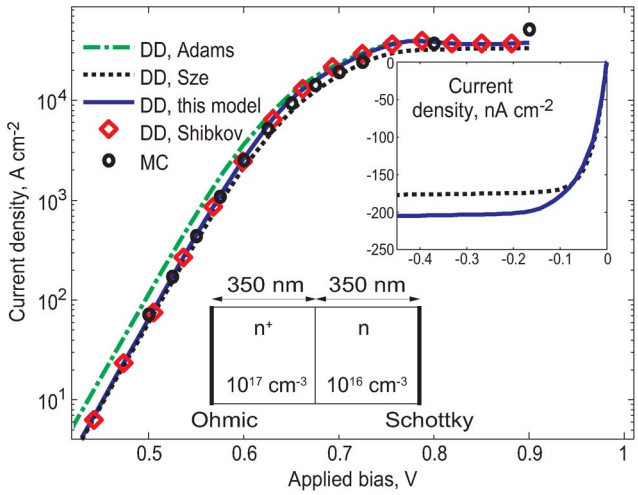

Fig. 4. DC characteristics of the GaAs Schottky barrier diode. Comparison among MC, the DD model for different v_r models, and the generalized DD model. The reverse-bias characteristic is shown in the inset.

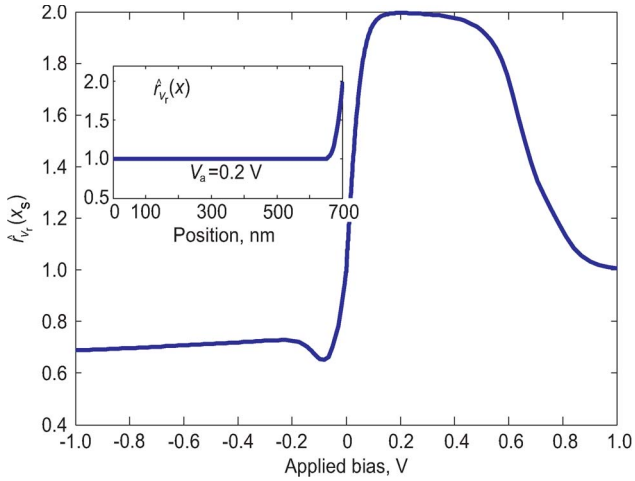

Fig. 5. Bias dependence of $\hat{r}_{v_r}(x_s)$. The inset shows the spatial dependence of $\hat{r}_{v_r}(x)$ near the SBC for $V_a = 0.2$ V.

consider the theory developed in [11] where it is shown that thermionic emission is the dominating transport mechanism for those SBCs where

$$E_{00} = \frac{\hbar}{2}\sqrt{\frac{N_D}{m^* \epsilon_S}} \ll V_T \tag{29}$$

where $\hbar$ is the reduced Planck's constant. Since, in our case, $E_{00} = 1.95$ mV $\ll V_T = 25.85$ mV, we can safely neglect tunneling effects.

The reference solution is provided by an ensemble MC simulator self-consistently coupled with a 1-D Poisson solver. The conduction band consists of three nonparabolic spherical valleys Γ, L, and X. The structure is divided into a uniform mesh of step equal to 100 Å, with the electric field updated every 2 fs. More details about the MC model can be found in [12].

The generalized DD model described in Section III has been implemented in an in-house simulator. We solve the unipolar model (i.e., neglecting holes), with material parameters estimated from bulk MC simulations: the electron mobility is $\mu_{n0} = 7480$ cm^{2}V^{-1}s^{-1} for the lightly doped region and $\mu_{n0} = 4960$ cm^{2}V^{-1}s^{-1} in the n$^+$ region. The other parameters of the mobility model are estimated as $\mathcal{E}_0 = 4.37$ kV/cm and $v_{\rm sat} = 1.01 \times 10^7$ cm/s. For the sake of comparison, we have also implemented the surface recombination velocity models proposed in [1], [6], and [9].

The comparison of the dc characteristics in forward bias is shown in Fig. 4. Consistently with the discussion in [9], the DD simulation with the Adams *et al.* model for v_r' [6] does not correctly reproduce the SBC current in low forward bias, although the comparison in stronger forward bias is favorable. The generalized DD model we propose gives results in very good agreement with the reference MC solution, as well as the Shibkov *et al.* model [9], at least if the forward bias is low enough to induce negligible nonstationary transport effects. Notice, however, that, as discussed in the previous section, the model in [9] guarantees the same current value of the novel b.c. but at the price of a different value of the electron concentration and velocity. The inset in Fig. 4 shows the reverse-bias characteristic, calculated with our approach and with the model

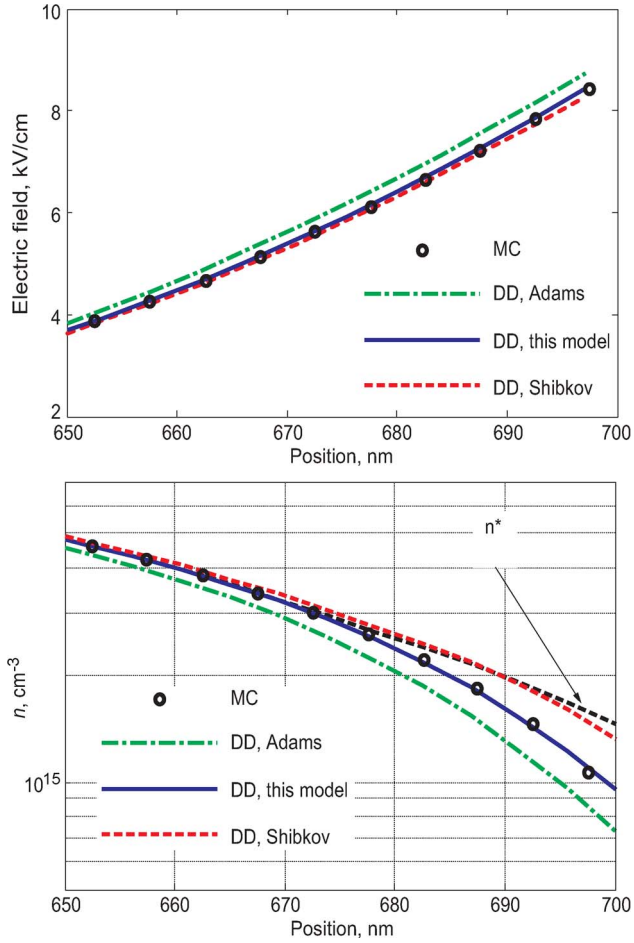

Fig. 6. Position dependence of the electric field and electron concentration near the SBC for $V_a = 0.6$ V.

in [1] since only this can be used in such conditions: only the generalized DD model provides the expected limit value of the reverse saturation current (i.e., $qn_0'(x_s)v_{r0}$).

To gain further insight, we discuss the behavior of the microscopic variables into the simulated device. Fig. 5 shows the bias dependence of the coefficient $\hat{r}_{v_r}(x_s)$. In forward bias, the coefficient reaches a value of 2 in the voltage range in which

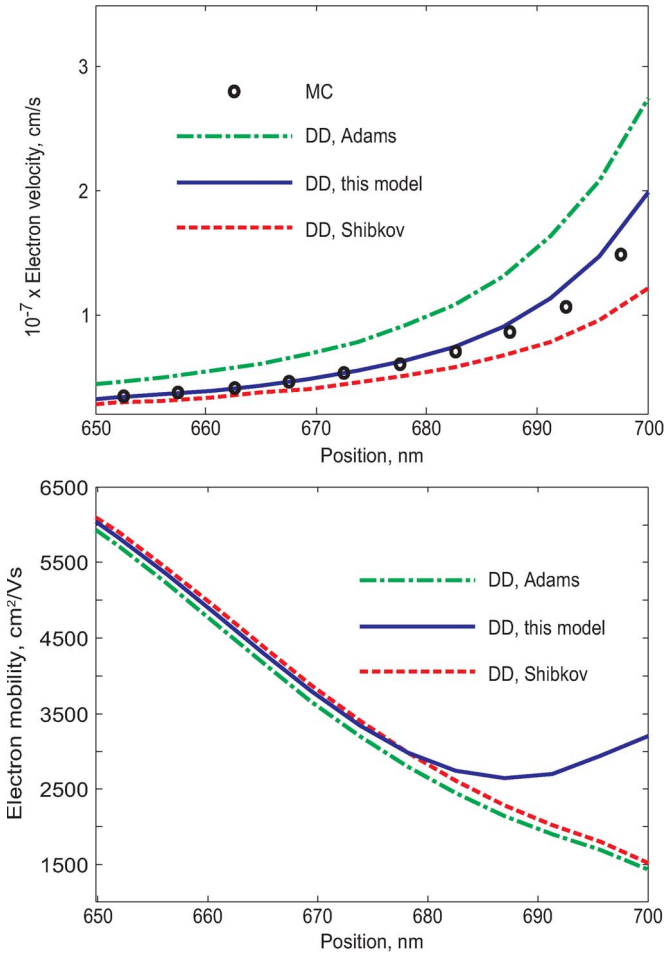

Fig. 7. Position dependence of the electron velocity and mobility near the SBC for $V_a = 0.6$ V.

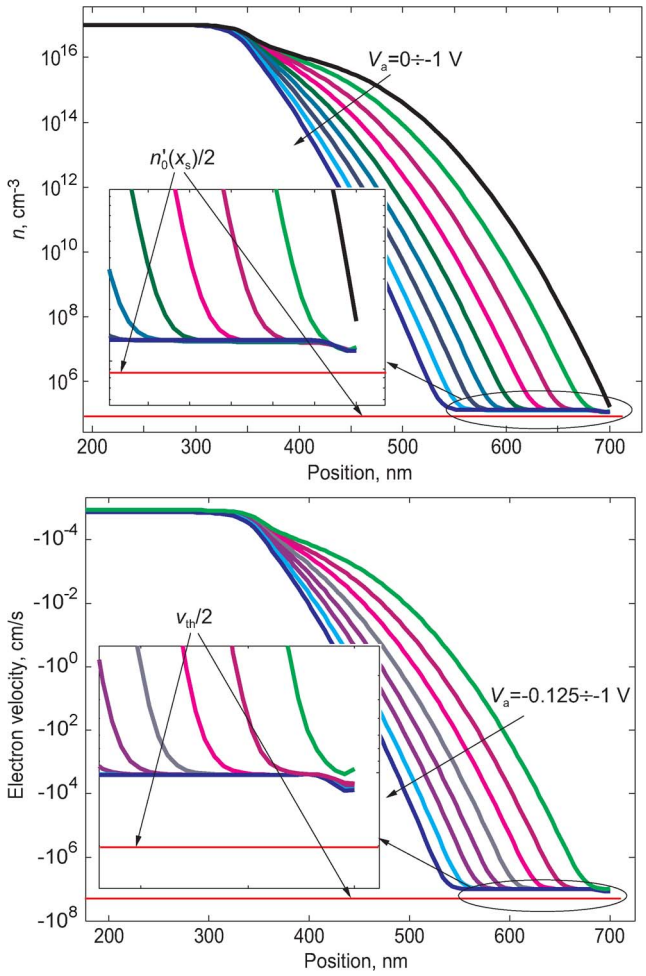

Fig. 8. Spatial and reverse-bias dependence of (from top to bottom) electron concentration and carrier velocity calculated with the generalized DD model.

v_d is so small that carriers with $v_x > 0$ essentially obey a semi-Maxwellian distribution. For higher voltages, when v_d becomes significant, an increasing portion of the drifted Maxwellian describing carriers in the semiconductor corresponds to positive velocities, so that $\hat{r}_{v_r}(x_s)$ decreases and finally approaches 1. A minimum value of 0.58 is attained in reverse bias. The inset in the same figure represents the spatial dependence of $\hat{r}_{v_r}(x)$ in moderate forward bias: as the observation position is moved of around 50 nm away from the SBC, the coefficient becomes equal to 1.

Figs. 6 and 7 report the spatial dependence of the microscopic variables near the SBC for a forward bias $V_a = 0.6$ V, as compared with MC simulations. As previously discussed, the results clearly show that only the generalized DD model allows to reproduce the behavior imposed by the b.c. derived from the piecewise distribution, thus providing profiles in agreement with the MC results. Near the SBC, the Shibkov *et al.* [9] model exhibits a higher carrier concentration and a lower electron velocity than the generalized DD model, but the same current values are obtained in both cases (see Fig. 4). Notice also that the n^* concentration, calculated with the generalized DD model, is practically coincident with the results of the standard DD model with the b.c. in [9]: this is due to the fact that, for this static analysis, the only difference between these two models is in the right-hand side of Poisson's equation. The mobility near the SBC corresponding to the generalized model exhibits the influence of the modified technique used to consistently include velocity saturation effects.

Finally, we discuss the reverse-bias behavior, where MC simulations are extremely difficult because of the very low current level. We compare in Figs. 8 and 9 the spatial and (reverse) bias dependence of two microscopic variables calculated with the generalized and standard (using the b.c. in [1], the only one available in such conditions) DD models, respectively. The standard model shows the foreseen unphysical values of electron concentration and carrier velocity at the contact (notice in particular that $n(x_s)$ becomes lower than $n_0'(x_s)/2$), while the generalized DD simulations yield results in agreement with the expected value. Notice that the limit values for carrier concentration (i.e., $n_0'(x_s)/2$) and carrier velocity (i.e., $2v_{r0} = v_{\rm th}/2$) are not reached because of the effect of velocity saturation.

V. Conclusion

We have investigated the DD analysis of an SBC in the whole bias range (from reverse to strong forward bias). By introducing a physically sound and consistent generalization of the DD

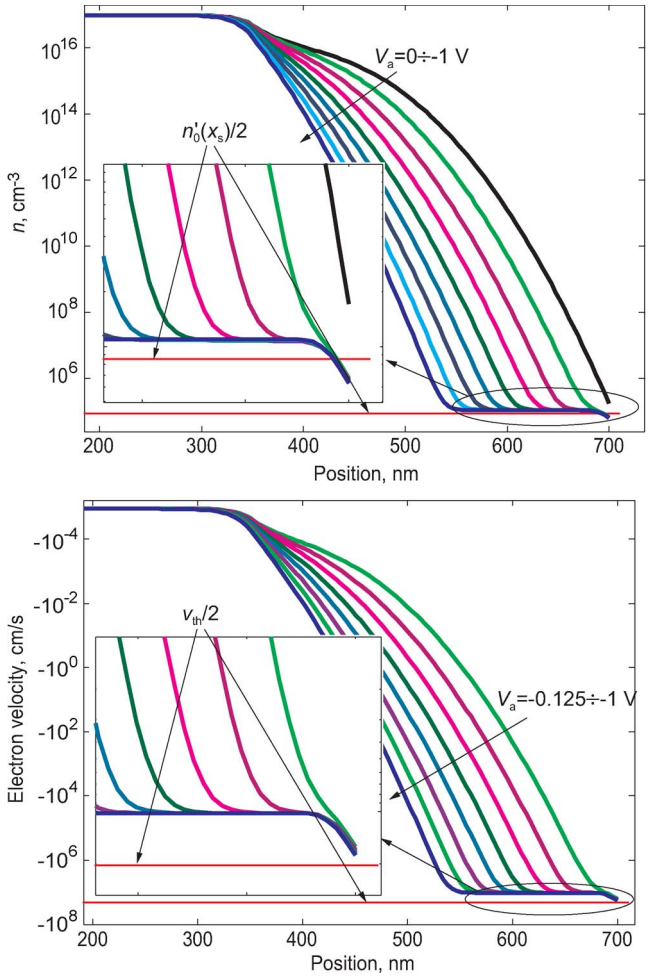

Fig. 9. Spatial and reverse-bias dependence of (from top to bottom) electron concentration and carrier velocity calculated with the DD model and the b.c. in [1].

model, we have been able to correctly implement a b.c. (in the absence of tunneling currents) accounting for the different bias dependence of carrier motion in opposite directions at the SBC. The results of the new model are in good agreement with MC simulations not only for the current value but also for the spatial distribution of the microscopic DD variables (not achieved by previous models). The generalized DD model is easily implementable into already-existing simulators.

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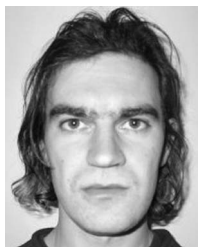

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