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COMPUTER SIMULATIONS OF SCHOTTKY CONTACTS WITH A NON-CONSTANT RECOMBINATION VELOCITY

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Abstract—The problem of modeling Schottky contacts for computer-aided physical simulation is investigated. Boundary conditions using a current dependent carrier recombination velocity distribution are developed, and installed in the two-dimensional simulation program BAMBI.

1. INTRODUCTION

Physical device simulation programs are widely used tools in the microelectronics construction work today. The design of these programs requires deep understanding of the physics in the structure to be modeled. A very important part of this process is to create adequate models for Ohmic- and Schottky-contacts. In practice this means creating adequate boundary conditions for the differential equations which describe semiconductor behavior[1].

One of the essential contact problems is the modelling of Schottky contacts. The generally known, so called combined thermionic emission-diffusion theory[2–5] has successfully been used in many simulation programs[6–9], even in two-dimensions[10–12]. However, there are still unsolved problems connected to the carrier transport through the contact. One of these is the definition of appropriate surface recombination velocities for both type of carriers.

This paper presents the implementation of Schottky boundary conditions in the 2-D device simulator BAMBI[13,14]. We have included a current dependent carrier recombination velocity model, important under forward bias condition, and the image-force lowering of the barrier for reverse bias. Our results show no accumulation of carriers at the Schottky interface under high forward bias conditions. The influence of an increased recombination velocity under these conditions also predicts a higher forward current than the constant velocity models. Also, using our new model, a lower current is obtained under small forward bias than the current predicted by the models using a constant recombination velocity.

2. BOUNDARY CONDITIONS

The boundary conditions for the potential and the current density for electrons and holes perpendicular to the Schottky interface are:

$$\psi = \psi_{\text{app}} - \psi_s, \tag{1}$$

$$J_n = -q \cdot v_n \cdot (n_m - n_0), \tag{2}$$

$$J_p = q \cdot v_p \cdot (p_m - p_0), \tag{3}$$

where ψ_{app} is the applied voltage, n_m and p_m are the actual electron and hole concentrations at the interface and n_0 and p_0 are the zero-bias concentrations, respectively, v_n, v_p are the surface recombination velocities which will be described later, and ψ_s is the surface potential as shown in Fig. 1.

$$\psi_s = \phi_B - \frac{E_g}{2} - \frac{kT}{q} \cdot \ln\left(\frac{N_v}{N_c}\right). \tag{4}$$

The equilibrium carrier concentrations are defined in the following way:

$$n_0 = n_i \cdot \exp\left(\frac{-\psi_s}{U_T}\right) \tag{5}$$

$$p_0 = n_i \cdot \exp\left(\frac{\psi_s}{U_T}\right). \tag{6}$$

These definitions formulate current-dependent boundary condition for the Schottky interface where both the minority and majority carrier concentrations are allowed to float, and only the potential boundary condition (1) is kept constant under forward bias conditions. In case of large reverse biases, and therefore image-force lowering of the Schottky barrier, even ψ_s is allowed to change a small amount as will be described later.

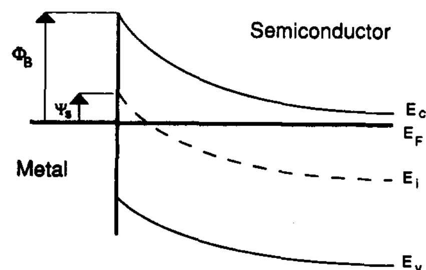

Fig. 1. Band diagram of the metal–semiconductor contact including definition of energy levels.

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BAMBI solves the basic semiconductor equations in two dimensions. The discrete form of the continuity equations for electrons and holes at a Schottky contact reads, by using eqns (2) and (3):

$$\frac{\mu_n}{k}\left[n_{\mathrm{NB}}\cdot B\left(\frac{\psi_{\mathrm{NB}}-\psi_{\mathrm{I}}}{U_{\mathrm{T}}}\right)-n_{\mathrm{I}}\cdot B\left(\frac{\psi_{\mathrm{I}}-\psi_{\mathrm{NB}}}{UT}\right)\right] - qv_n(n_{\mathrm{I}}-n_0)=0, \quad (7)$$

$$\frac{\mu_p}{k}\left[p_{\mathrm{I}}\cdot B\left(\frac{\psi_{\mathrm{NB}}-\psi_{\mathrm{I}}}{U_{\mathrm{T}}}\right)-p_{\mathrm{NB}}\cdot B\left(\frac{\psi_{\mathrm{I}}-\psi_{\mathrm{NB}}}{U_{\mathrm{T}}}\right)\right] + qv_p(p_{\mathrm{I}}-p_0)=0. \quad (8)$$

Here index I and NB denote the points on the contact and its neighbor point, respectively, ψ is the potential, n and p are the actual carrier concentrations in these points, $\mu_{n,p}$ are the electon and hole mobilities, k is the distance between the point I and NB, and B is the Bernoulli function,

$$B(x)=\frac{x}{e^x-1} \quad (9)$$

In the two continuity eqns (7) and (8) not only the carrier concentrations n_{I} and n_{NB} are unknown, but in this model also the recombination velocity, $v_{n,p}$. This extra variable will somewhat slow down the solution of the equation system, but by using a proper damping of $v_{\mathrm{n,p}}$, the system is prevented from oscillating and the average extra time consumed is less than 10% of the total cpu time. In some cases the solution of a Schottky problem using large forward bias and a constant recombination velocity is much more difficult, because the carrier concentration will have a tendency to accumulate close to the interface, than using the model described in this paper which gives a more realistic recombination velocity in the whole forward bias region. This behaviour will be demonstrated later by an example.

3. THE SURFACE RECOMBINATION VELOCITY

Several authors have combined the thermionic-emission and diffusion theories for Schottky contacts. Following the most developed theory by Crowell and Sze[2] the analytic expression for the surface recombination velocity, assuming a Maxwellian distribution of carrier velocities at the contact, is expressed in terms of a "collection" velocity defined as:

$$v_{\mathrm{c}}=\sqrt{\frac{kT}{2m^*_{n,p}\pi}}\cdot f_{\mathrm{p}}f_{\mathrm{q}}, \quad (10)$$

where f_{p} is the probability of a carrier reaching the metal without being backscattered, and f_{q} is the quantum mechanical reflection of carriers, together with effects of tunneling through the top of the barrier. These constants only effect the reverse bias velocity. Under forward bias conditions this velocity was kept constant with $f_{\mathrm{p}}, f_{\mathrm{q}}=1$.

Defining the recombination velocity $v_{n,p}$ in eqns (2) and (3) equal to a fraction of the semiconductor saturation velocity v_{sat} will give rise to an accumulation of carriers at the Schottky interface under large forward bias conditions. Setting $v_{n,p}=v_{\mathrm{sat}}$ in order to avoid this unrealistic behaviour results in a too large velocity, if reverse bias is applied to the same model. This problem can be avoided by implementing a current dependency of $v_{n,p}$. In Ref. [2] the distribution of velocities for carriers travelling into the metal is assumed to be Maxwellian. This assumption holds only under low forward bias conditions. As pointed out e.g. by Refs [2,15,16] one expects, under high forward biases, a non-Maxwellian distribution of carrier velocities.

Initially we followed the approach by Adams and Tang[15] who assume the carrier velocities to be represented by the positive part of a drifted Maxwellian distribution. The distribution function for this system reads:

$$f(v_x)=K\cdot\exp\left(\frac{-m^*_{n,p}\eta_{n,p}(v_x-v_{\mathrm{d}})^2}{2kT}\right). \quad (11)$$

Here $m^*_{n,p}$ is the effective mass for electrons or holes, K is a coefficient which cancels out during the evaluation of eqn (13), $\eta_{n,p}$ is a compensating factor for the increase in the effective mass caused by band structure changes at the Schottky interface as will be discussed later, and v_x is the carrier velocity.

By defining:

$$v_{\mathrm{d}}=\frac{I_{n,p}}{q(n,p)}, \quad (12)$$

as a drift velocity, it is possible to model the amount of the Maxwellian shift. Here $I_{n,p}$ is the current density and n,p is the electron/hole concentration inside the interface. Integrating and normalizing the function (11) using:

$$v_{n,p}=\frac{\int_0^\infty v_x f(v_x)\,\mathrm{d}v_x}{\int_0^\infty f(v_x)\,\mathrm{d}v_x}, \quad (13)$$

yields the current dependent recombination velocity expression:

$$v_{n,p}=v_{\mathrm{d}}+\sqrt{\frac{2kT}{m^*_{n,p}\pi\eta_{n,p}}}\times\frac{\left\{\exp\left[-v_{\mathrm{d}}^2\left(\frac{m^*_{n,p}\eta_{n,p}}{2kT}\right)\right]\right\}}{1+\mathrm{erf}\left(v_{\mathrm{d}}\sqrt{\frac{m^*_{n,p}\eta_{n,p}}{2kT}}\right)}. \quad (14)$$

Equation (14) is bounded from above by the semiconductor saturation velocity v_{sat} which limits v_{d}, and from below by the condition $v_{\mathrm{d}}=0$. This condition gives:

$$v_{n,p}|_{(\psi_{\mathrm{applied}}=0)}=\sqrt{\frac{2kT}{m^*_{n,p}\pi\eta_{n,p}}}. \quad (15)$$

Changes in the band structure will increase the effective carrier mass at the Schottky interface and,

according to Stratton[17], the carrier temperature is lowered by a factor of 0.7 under forward bias condition. Comparing eqn (15) with the collection velocity eqn (10) shows that $\eta_{n,p} = 4$ yields equality between these expressions at zero voltage. Physically this predicts a ratio $T/m^*_{n,p} = 0.25$ at the Schottky interface.

Baccarani and Mazzone[18], who made Monte-Carlo simulations of the velocity distribution, predict a mean velocity for electrons flowing into the metal of two times the velocity v_c predicted by Crowell and Sze. From eqn (15) we see that settting $\eta_{n,p} = 1$ yields the velocity obtained by Baccarani and Mazzone. Even Berz[16] found the velocity to be two times v_c, although she used half the carrier concentration, and therefore achieved the same current density as Crowell and Sze. These different results showed that the same constant recombination velocity could not be used under different forward bias conditions. Since the last two simulations were made under high forward bias conditions, our velocity model would fit the latest two predicted values, even if using $\eta_{n,p} = 4$ in eqn (15), a fitting with Crowell and Sze's velocity for zero bias was made. This is because in this region of eqn (14) the term v_d has started to be the dominating factor, and therefore our velocity model will follow the higher velocity proposals until equality will be reached with v_{sat} in the semiconductor.

In reality $\eta_{n,p}$ will also be depending on the difference in work functions between the metal and the semiconductor, and hence on the barrier height. In our numerical model these effects have been neglected. $\eta_{n,p} = 4$ has been kept in all our simulations, since this follows the Crowell and Sze proposals for low and reverse bias, and it also fits with Baccarani and Mazzones velocity under high forward bias conditions. The introduction of the effective Richardson "constant" done by Crowell and Sze also predicts a variable current depending factor. For numerical approaches, where it is possible to use eqn (14), the model described in this paper is superior.

A comparison between eqn (14) using $\eta_{n,p} = 4$ (solid line) and the formulation proposed by [15] (dashed line) is shown in Fig. 2. In both models the recombination velocity increases, when the forward bias is increased, to the line $v_{n,p} = v_d$ and then continues until $v_{n,p} = v_{sat}$ is reached. The limit for v_{sat} is determined by the physical parameters in the bulk material. The discrepancy between these two formulations occur in the domain where $v_{n,p}$ is slightly smaller than v_d. Here the previously proposed model shows a slight increase in $v_{n,p}$ just before joining the $v_{n,p} = v_d$-line and in this point, as shown in Fig. 2, a discontinuous derivative occurs. The model proposed in this paper gives a smooth function, with a continuous derivative, for every point in the actual domain. This is very important, especially in a 2-D model like this, since the recombination velocity is calculated uniquely for every iteration step in every point at the Schottky contact and if the recombination velocity for any of these points is close to the point where the described problem occurs, a solution is difficult to find.

Under reverse bias the recombination velocity is kept constant. The reduction of $v_{n,p}$ under reverse bias by f_p and f_q has not been taken into account in this numerical model. This reduction, in the order of $f_p \times f_q = 0.5$[2] effects the current less than a change in barrier height in the order of kT/q, and it is therefore negligible compared to image-force lowering of the barrier.

4. BARRIER LOWERING

Under reverse bias conditions the image-force lowering of the barrier is taken into account following the outline by Crowell and Sze[2]. The effective barrier height ϕ_b as a function of the electric field E reads:

$$\phi_b(E) = \phi_0 - \Delta\phi_b(E), \tag{16}$$

where ϕ_0 is the zero bias barrier height and $\Delta\phi_b$ is the barrier lowering given by:

$$\Delta\phi_b = \left(\frac{qE}{4\pi\epsilon_s}\right)^{1/2} \tag{17}$$

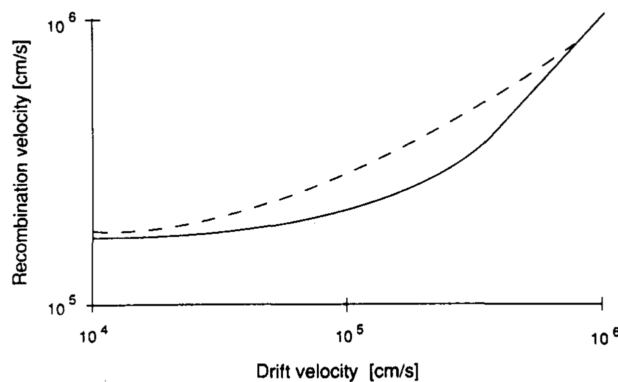

Fig. 2. Comparison of the proposed recombination velocity function as calculated from eqn (14) (—), and as suggested by Adams and Tang[15] (---). The drift velocity is calculated from eqn (12)

Since ϕ_b is directly proportional to ψ_s in eqn (4), ψ_s is replaced by $\psi_s - \Delta\psi_s$ in eqns (5) and (6), where $\Delta\psi_s$ is proportional to $(\psi_{applied})^{1/4}$. The permittivity is set to the static value $\epsilon_s = \epsilon_0 \times 11.7$ since Sze, Crowell and Kahng[19] have predicted a constant silicon permittivity up to a frequency $\approx 3 \times 10^{14}$ Hz. Under forward bias the barrier height is assumed to be constant, since the electric field is very small, and effects from image force lowering can therefore be neglected.

5. RESULTS

We present results calculated with the current dependent recombination velocity for Schottky contacts, and comparisons between this model and simulations made by using a constant recombination velocity.

The forward bias region can be divided into three areas:

(1) for very small biases, where the velocity described by Crowell and Sze is valid. In this region the constant velocity will predict a slightly too large current,

(2) for biases around flat band voltage, where there is no difference between the constant velocity and the velocity calculated by our model, and

(3) for large biases, approximately larger than 0.6 V, where the constant velocity is not sufficiently large to transport the carriers across the barrier and therefore no adequate solution is possible to find if not a variable velocity model which calculates a recombination velocity depending on the current density, is used.

The first two diodes presented here are n-type devices. They have a barrier height = 0.8 eV and, for the sake of simplicity, a constant doping $N_D = 5 \times 10^{15}$ cm^{-3}, and their geometry is presented in Fig. 3. Figures 4 and 5 show a comparison in majority carrier distributions between these two simulated forward biased components, one using a constant recombination velocity $b_n = 2 \times 10^6$ cm/s, $v_p = 1 \times 10^6$ cm/s (Fig. 4), and one using the velocity model described in this paper (Fig. 5). When applying a sufficiently large forward bias, here 0.55 V it becomes obvious that the constant velocity is too low, because of the accumulation of carriers close to the interface. Consequently a bottleneck for carrier transport occurs at the contact in this case (Fig. 4).

Using the constant velocity model and biases greater than 0.8 V caused convergence problems when trying to find a solution for the carrier concentration at the Schottky interface. The carrier concentration might be increased more than three orders of magnitude above the normal concentrations, because of the too low recombination velocity, and this behavior prevents the program from finding a solution in the large forward bias region.

A simulated I–V curve of a Schottky diode using a nn^+ doping structure (Fig. 6), with an Iridium contact (barrier height = 0.89 eV) and with the variable velocity model is compared with measured data in Fig. 7. A discrepancy occurs for very high bias, here more than 1.0 V. This is probably caused by the

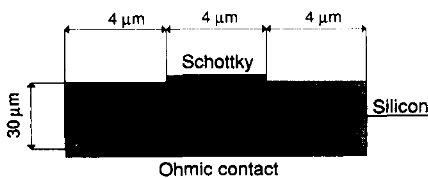

Fig. 3. Schematic of the investigated diode structure used in Figs 4 and 5.

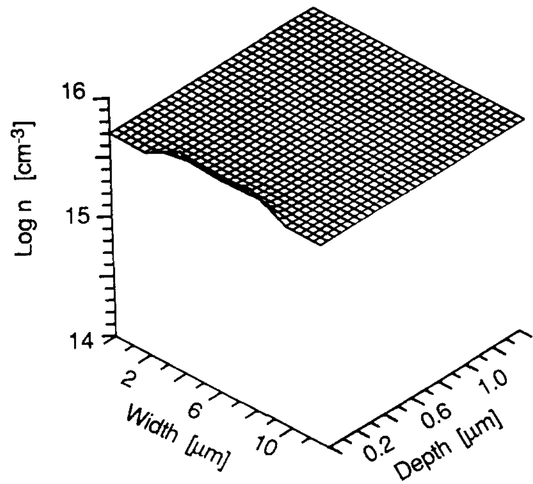

Fig. 4. Electron density distribution n at 0.55 V forward bias of the n-type Schottky diode described in Fig. 3. The bulk is assumed to be homogeneously doped $N_D = 5 \times 10^{15}$ cm^{-3} and $\Phi_B = 0.8$ eV. The recombination velocities are $v_n = 2 \times 10^6$ cm/s and $v_p = 1 \times 10^6$ cm/s. Note the accumulation of electrons unable to pass the Schottky contact because of the small recombination velocity.

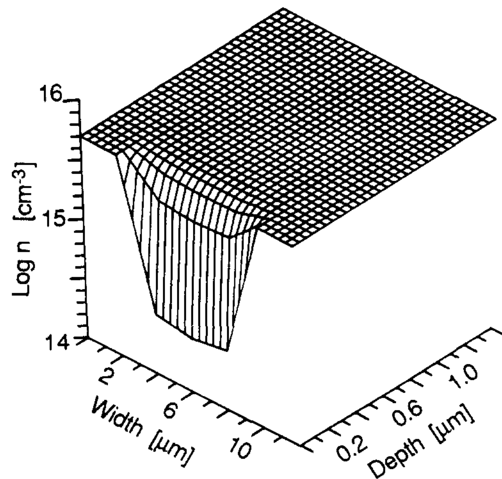

Fig. 5. Electron density distribution during the same conditions as in Fig. 4 but using eqn (14) to calculate the recombination velocity distributions. No electron accumulation will occur at the contact at large forward bias.

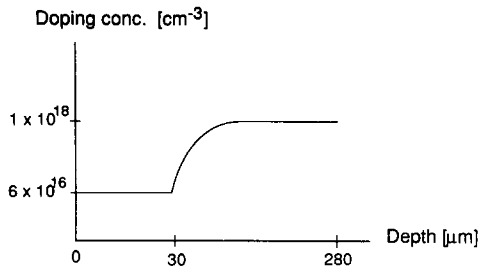

Fig. 6. The doping density profile for the diode presented in Fig. 7. The depth is measured from the Schottky contact.

fact that the velocity distribution no longer could be described there as a shifted Maxwellian distribution. Details connected to the processing of the compared device are described in Ref. [9].

6. CONCLUSIONS

A more exact numerical determination of the forward bias current has been presented in the case of Schottky diodes. Our model gives us the possibility to define a recombination velocity expression for all forward bias cases, predicting a proper current for both low and high biases. Also, it gives the possibility to define the recombination velocity equal to the recombination velocity defined by Crowell and Sze[2] under reverse bias conditions, and still making simulations under forward bias conditions possible.

Limitations to the proposed model is mainly connected with the assumption of a drifted Maxwellian distribution just inside the contact, where under high forward biases, the distribution will probably not be Maxwellian. Also, according to Berz[16] the assumption of normal transport equations in the region close to the contact is not valid.

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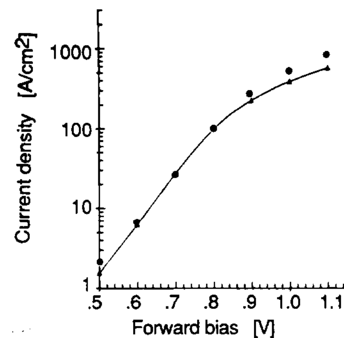

Fig. 7. The upper forward bias part of the I–V curve showing a comparison between simulated (—) and measured (●) values.

REFERENCES

1. S. Selberherr *Analysis and Simulation of Semiconductor Devices*, p. 41. Springer, Wien (1984).
2. C. R. Crowell and S. M. Sze, *Solid St. Electron.* **9,** 1035 (1966).
3. M. A. Green and J. Shewchun, *Solid-St. Electron.* **16,** 1141 (1973).
4. F. Masszi, L. Stolt, P. A. Tove and K. Tarnay, *Physica Scripta,* **24,** 456 (1981).
5. J. G. Simmons and G. W. Taylor, *Solid-St Electron.* **26,** 705 (1983).
6. C. T. Chuang *Solid-St. Electron.* **27,** 299 (1984).
7. S. F. Guo, *Solid-St. Electron.* **27,** 537 (1984).
8. B. Elfsten and P. A. Tove, *Solid-St. Electron.* **28,** 721 (1985).
9. F. Masszi, P. A. Tove, K. Bohlin and H. Norde, *IEEE Trans. Electron Devices,* **ED-33,** 469 (1986).
10. M. R. Pinto, C. S. Rafferty and R. W. Dutton, Technical Report DAAG-29-83-K-0125, Integrated Circuits Laboratory, Stanford University (1984).
11. F. Masszi, N. Masszi, K. Bohlin, J. Nylander and P. A. Tove, Proceedings 12th Nordic Semiconductor Meeting, Jevnaker, Norway, pp. 100–103 (1986).
12. J. O. Nylander, F. Masszi and P. A. Tove, *COMPEL* **7,** 135 (1988).
13. A. F. Franz and G. A. Franz *IEEE Trans Comput. aided Design* **CAD-4,** 177 (1985)
14. A. F. Franz and G. A. Franz, User's guide, TU Vienna (1985).
15. J. Adams and Ting-Wei Tang *IEEE Electron Device Lett.* **EDL-7,** 525 (1986).
16. F. Berz, *Solid-St. Electron.* **28,** 1007 (1985).
17. R. Stratton, *Phys. Rev.* **126,** 2002 (1962).
18. G. Baccarani and A. M. Mazzone, *Electron. Lett.* **12,** 59 (1976).
19. S. M. Sze, C. R. Crowell and D. Khang, *J. appl. Phys.* **35,** 2534 (1964).