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An analytical model of non-ideal ohmic and Schottky contacts for device simulation

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Abstract

The paper presents a new and computationally simple model for the currents through metal-semiconductor contacts including both thermionic emission and tunneling effects. The model allows the simulation of devices with non-ideal contacts where commonly used boundary conditions are not applicable.

1 Introduction

Both low resistance (ohmic) and rectifying (Schottky) contacts are essential parts of many semiconductor devices. Accordingly, models for ohmic as well as Schottky contacts have been established in many device simulation programs. These models are introduced as boundary conditions for the numerical solution of the semiconductor transport equations. The usual Schottky contact model is derived from a given barrier height and a thermionic emission current across the Schottky barrier, while the conventional model for ohmic contacts simply states charge neutrality and vanishing voltage drop at the contact boundary [1]. Some simulators allow the inclusion of an additional but constant specific contact resistance.

A comprehensive overview on metal-semiconductor contacts is given in [2]. The fundamental statement is that Schottky contacts are present at high barrier heights and low doping concentrations, while contacts with a low barrier or high doping exhibit ohmic behavior. This means that the common Schottky contact model looses its validity with increasing doping density, because additional tunneling currents come into play which are not covered by the model. The usual ohmic contact model on the other hand is not valid at lower doping, if depletion regions are present near the contact, or if the bias dependence of the contact resistance is of importance. If the doping varies over many decades under the contact (as is the case in certain power diodes), the contact behavior changes from ohmic to Schottky [3], and none of both models can be used for the simulation. Thus the need for a contact model arises which bridges the gap and includes thermionic emission (dominant in Schottky contacts) as well as tunneling (dominant in ohmic contacts) and is thus valid over the whole range of interesting doping concentrations. Traditional models of tunneling at metal-semiconductor contacts [2, 4, 5, 6] either do not fully cover all necessary modes of operation or require cost intensive numerical integrations, which makes them far too expensive for device simulation purposes. For device simulation a simple, explicit formula is needed which comprises the essential physical effects but is easy to evaluate.

In the paper, a new analytical model for the contact current and the specific contact resistance is derived by introduction of novel approximations for the quantum-mechanical transmission probability and the Fermi distribution. An equivalent recombination velocity can be derived as well.

2 Derivation of the contact boundary condition

Boundary conditions for the semiconductor transport equations should be consistently based on general interface conditions for the electron distribution function at hetero interfaces by evaluation of corresponding integrations (moments of the interface condition) with respect to k-space [7, 8]. In order to carry out the moment integrations, assumptions on the form of the distribution function have to be made. In the literature concerned with metal-semiconductor contacts, it is common practice to assume a semiconductor electron distribution that is composed of two halves of the equilibrium distribution having the metal or the semiconductor quasi-Fermi energies for the incoming or outgoing velocities, respectively [2, 4, 5, 6, 9]. This interface distribution is then connected to the bulk distribution (shifted Maxwellian or similar) by equating the current transported by each distribution and keeping the semiconductor quasi-Fermi energy. Although this procedure is questionable (details will be discussed elsewhere), it is used here too in order to obtain an analytical approximation for an accepted model.

Under the assumptions stated above, the first order moment of the boundary condition reduces to the following expression for the current density through the contact:

$$J_n = -\frac{q}{4\pi^3}\frac{\hbar}{m_n}\int_0^\infty dk_x\, k_x\, T(k_x)\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dk_y\, dk_z\,\left[f_M(\vec{k}) - f_s(\vec{k})\right]. \tag{1}$$

$T(k_x)$ is the transmission probability, while f_M and f_s are the metal and semiconductor equilibrium distributions, respectively. Because of a possible degeneration of the semiconductor in ohmic contacts, Fermi-Dirac distributions must be used. A parabolic band structure with an effective mass m_n of appropriate orientation to the crystallographic axes [5] has been assumed. Eq. (1) is identical to the formula in [9] after transforming the integration variables to k-space.

In the following, approximations are introduced for both the tunneling probability and the Fermi distribution in order to enable an analytical evaluation of (1).

2.1 Transmission probability

The contact model is based on a tunneling transmission probability which has been given by Crowell and Rideout in [5].

The energy band model of the contact under consideration is depicted in fig. 1. The metal-semiconductor interface is located at $x = 0$, with the metal at $x < 0$ and the semiconductor at $x \geq 0$. The barrier height is ϕ_B, while W_0 is the top energy of the barrier. The Fermi level is indicated by the dashed line. At the interface, the Fermi level is discontinuous, thus accounting for a voltage drop V_c across the contact.

The semiconductor conduction band edge according to [5] is assumed to be parabolic:

$$W_c(x) = W_0 + qE_{max}\,x + \frac{q^2 N_D}{2\varepsilon_s}\,x^2, \tag{2}$$

where E_{max} is the maximum electric field at the contact, and qN_D is the effective space charge responsible for the band bending in the x-direction. In one dimension, N_D is the donor doping concentration. Assumption (2) is discussed in [4, 5, 10]. Image force effects are accounted for by a respective lowering of ϕ_B [2, 11]. The diffusion potential V_D in fig. 1 is defined by the maximum electric field at the interface:

$$qV_D = \frac{\varepsilon_s E_{max}^2}{2N_D}. \tag{3}$$

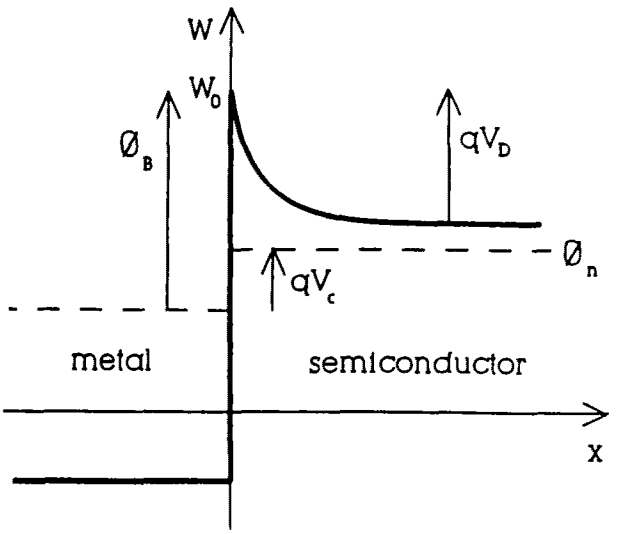

Figure 1: Energy band model of the contact

The quantum-mechanical transmission probability for an electron with energy $W < W_0$ in the WKB approximation has been computed by Crowell and Rideout for the band model of fig. 1 to give [5]:

$$T(W) = \exp\left(-\frac{\varepsilon_s E_{max}^2}{2N_D W_{00}}\left[\sqrt{c} - (1-c)\,Artanh\sqrt{c}\right]\right), \tag{4}$$

where

$$W_{00} = \frac{q\hbar}{2}\sqrt{\frac{N_D}{m^*\varepsilon_s}} \tag{5}$$

and

$$c = \frac{2N_D}{\varepsilon_s E_{max}^2}(W_0 - W) \tag{6}$$

have been introduced as abbreviations. For energies $W > W_0$, a transmission probability of unity is assumed, leading to classical thermionic emission [2]. It is assumed that the tunneling effective mass m^* is not a function of energy [5]. Crowell and Rideout investigated the contact current using (4) in a numerical integration of (1).

For device simulation purposes, the transmission probability has to be simplified to arrive at an analytically integrable expression. It is easily verified that (4) can be reasonably well approximated by

$$T(W) \approx \exp\left(-\frac{(W_0 - W)^2}{W_{00} q V_D}\right). \tag{7}$$

This new approximation will be used subsequently for an analytical evaluation of the tunneling current expression.

2.2 Fermi-Dirac distribution

Insertion of the transmission probability into (1) yields the current density across the barrier. Using the exact definition of the Fermi distribution, a closed solution of the integral is not

known. In order to arrive at an analytically tractable integral, a new approximation of the Fermi distribution is introduced:

$$f(x) = \frac{1}{1+e^x} \approx \begin{cases} 1 - e^x + \frac{1}{2}e^{3x/2} & \text{for } x < 0 \\ e^{-x} - \frac{1}{2}e^{-3x/2} & \text{for } x \geq 0 \end{cases} . \tag{8}$$

This expression approximates the original function quite well since it preserves the main features (symmetry, asymptotic behavior, value and slope at $x = 0$) while having a small overall error.

2.3 The contact current

In a first approximation, only the leading terms in (8) are kept. Comparison with the results of the exact formula shows that the additional terms in general have a negligible effect. Evaluation of the term involving f_s in (1) for energies below W_0 using (7) and (8) yields the tunneling current of electrons going from semiconductor to metal

$$J_s = \frac{q m_n k T}{2\pi^2 \hbar^3} \frac{1}{2} \sqrt{\pi W_{00} q V_D} \exp\left(-\frac{\phi_B - qV_c}{kT} + \frac{W_{00} q V_D}{4(kT)^2}\right) \times$$
$$\times \left[\operatorname{erf}\left(\frac{\sqrt{W_{00} q V_D}}{2kT}\right) - \operatorname{erf}\left(\sqrt{\frac{qV_D}{W_{00}}}\right)\right] \quad (\phi_B - qV_c > qV_D), \tag{9}$$

$$J_s = \frac{q m_n k T}{2\pi^2 \hbar^3} \frac{1}{2} \sqrt{\pi W_{00} q V_D} \left\{ \exp\left(-\frac{\phi_B - qV_c}{kT} + \frac{W_{00} q V_D}{4(kT)^2}\right) \times \right.$$
$$\times \left[\operatorname{erf}\left(\frac{\sqrt{W_{00} q V_D}}{2kT}\right) - \operatorname{erf}\left(\frac{\sqrt{W_{00} q V_D}}{2kT} - \frac{\phi_B - qV_c}{\sqrt{W_{00} q V_D}}\right)\right]$$
$$+ \left(\frac{\phi_B - qV_c}{kT} - 1\right)\left[\operatorname{erf}\left(\frac{\phi_B - qV_c}{\sqrt{W_{00} q V_D}}\right) - \operatorname{erf}\left(\sqrt{\frac{qV_D}{W_{00}}}\right)\right]$$
$$\left. + \frac{\sqrt{W_{00} q V_D}}{\sqrt{\pi}\, kT}\left[\exp\left(-\frac{(\phi_B - qV_c)^2}{W_{00} q V_D}\right) - \exp\left(-\frac{qV_D}{W_{00}}\right)\right]\right\} \quad (\phi_B - qV_c < qV_D). \tag{10}$$

The corresponding result for the current J_M of electrons tunneling from metal to semiconductor is identical to (9-10) with $\phi_B - qV_c$ replaced by ϕ_B. The total contact current is then obtained by $J_n = J_s - J_M + J_{TE}$, where J_{TE} represents the classical thermionic emission part [2] of the current. It should be noted that the model includes the temperature dependence of the contact current.

3 Results of the model

Exemplary results for contacts on n-Si at $T = 300K$ are presented in figures 2-4.

3.1 I-V characteristics

The relation of the current density to the voltage drop V_c for an Al-Si contact with a barrier height of 0.7 V is displayed in figures 2 and 3 on a logarithmic as well as a linear scale. Note the rectifying behavior at lower doping and the transition to nearly symmetric (ohmic) curves at increased doping concentrations. On the scale of fig. 3, the contact with a doping of $10^{20} cm^{-3}$ appears as an ideal contact of zero voltage drop.

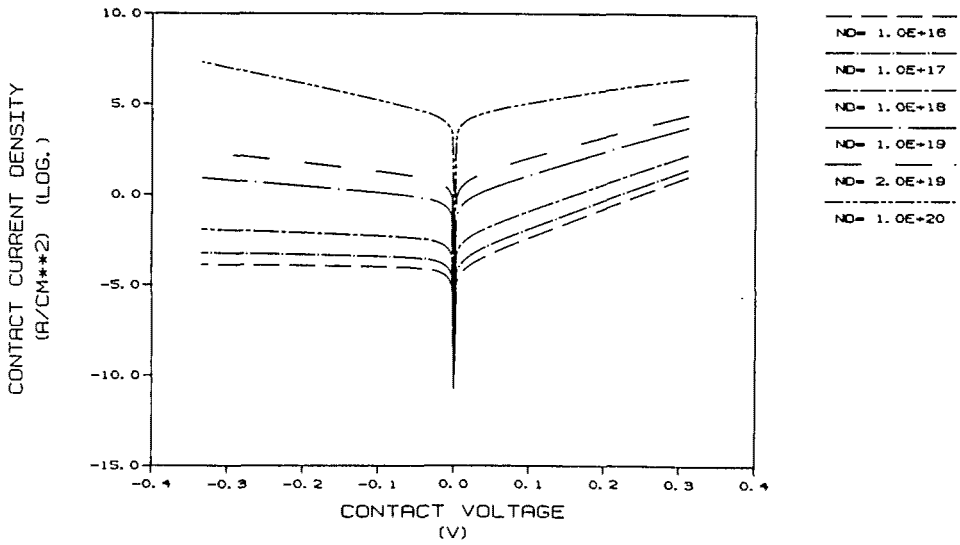

Figure 2: Contact current density versus contact voltage (logarithmic).

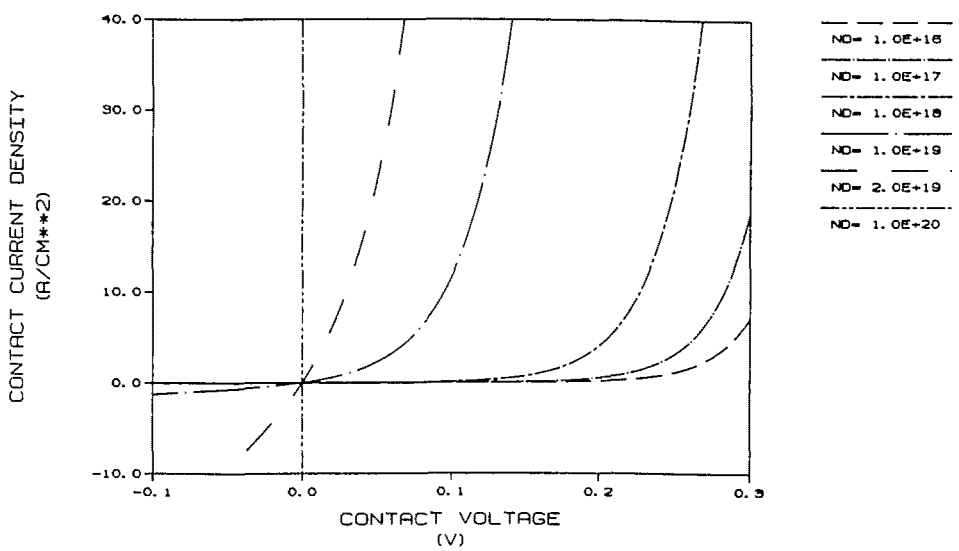

Figure 3: Contact current density versus contact voltage (linear).

3.2 Specific contact resistance

The specific contact resistance ρ_c is derived from J_n by [12]

$$\frac{1}{\rho_c} = \left.\frac{\partial J_n}{\partial V_c}\right|_{V_c=0}. \tag{11}$$

A bias dependent contact resistance can be introduced by definition of a secant contact resistance rather than a tangential one as in (11).

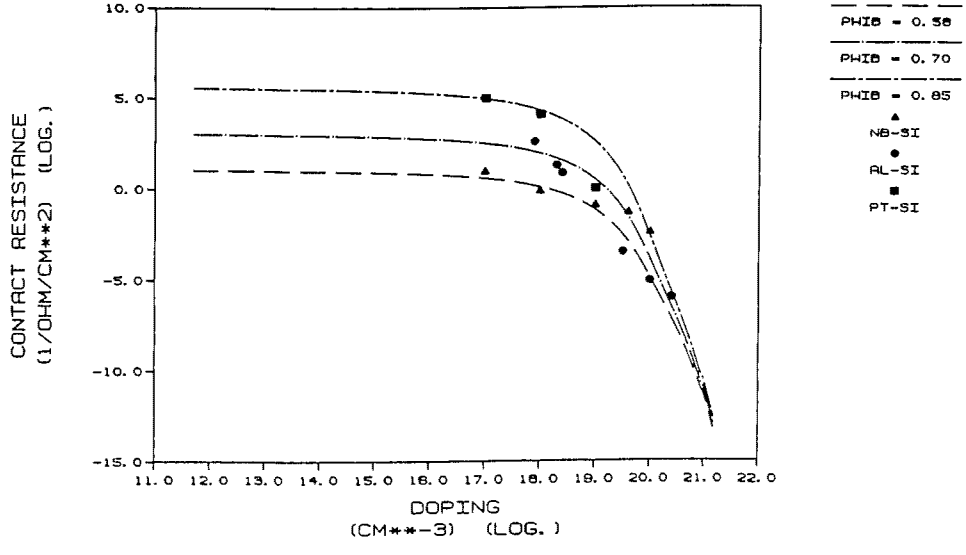

Figure 4: Specific contact resistance versus doping concentration ($T = 300K$).

Fig. 4 shows the specific contact resistance according to (11) for selected contact materials as a function of doping concentration together with respective experimental data. Experimental data and barrier heights of 0.58 eV, 0.7 eV, and 0.85 eV for Nb-Si, Al-Si, and Pt-Si have been taken from [13], [12], and [11], respectively. Although no parameter adjustment has been made, the agreement is quite reasonable. Note the drastic decrease of the resistance due to the onset of tunneling as the doping increases above $10^{18} cm^{-3}$.

3.3 Recombination velocity

The contact current can be equivalently expressed in terms of the recombination velocity by division of the current components by certain electron concentrations [2]. With pure thermionic emission, the concentration at the top of the barrier and a related equilibrium concentration is commonly used. This concept can be generalized to include the case of tunneling. The most consistent way is to take the electron concentration at a distance of the order of the tunneling length from the interface. Since the derivation of the tunneling length goes beyond the scope of the present paper, these results will be presented elsewhere.

4 Conclusion

A contact model has been presented that is valid for nondegenerate and degenerate semiconductor as well as forward and reverse bias. It is easy to evaluate (even on a pocket calculator) and thus suited for quick estimations, optimization loops, or for implementation in a device simulation program as a new boundary condition for the electron continuity equation. The capability of the model to include doping, bias, and temperature dependence of contact current, contact resistance, or recombination velocity into device simulations has been illustrated.

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