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Analytical Model of the Metal-Semiconductor Contact for Device Simulation

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Abstract

We report on the implementation and first numerical results of a new analytical model of the metal-semiconductor contact in a drift-diffusion device simulator. The model covers the entire range from Schottky to Ohmic contacts and fits well with experimental I(V)-characteristics of intermediately doped silicon.

1. Introduction

Usually, in device simulation the physical system "metal-semiconductor (MS) interface" is treated in form of idealized boundary conditions. Neutrality and equilibrium are assumed for Ohmic contacts and thermionic emission for rectifying (Schottky) contacts. A model of the non-ideal contact is not only of general interest, but also desirable for certain applications, e.g. the combined Schottky-pn-structure in power diodes (MPS diodes) or the Schottky Injection Field Effect Transistor (SINFET). Obviously, such a model cannot reflect the entire complicated physics involving barrier tunneling, inelastic scattering, recombination, trapping and trap-assisted tunneling, potential fluctuations, lateral barrier height fluctuations, roughness, band-state mixing, carrier heating, image forces, and some other effects. Since barrier tunneling is commonly accepted to produce Ohmic behavior, the concept of thermionic field emission (TFE) is successful in explaining the transition from Schottky to Ohmic contacts as the doping level is increased. Schroeder [1] used a simplified version of the WKB transmittance of a parabolic barrier (neglecting quantum reflection) and derived an analytical expression of the emission current j_e suitable for a boundary condition in device simulation. We believe that because of the importance of barrier tunneling for the properties of MS contacts with arbitrary doping the substitution of the WKB approximation by a better approach should be a reasonable improvement, despite the mentioned variety of other physical effects. Details of the new model including the lengthy formulas are published elsewhere [2]. Here we concentrate on the implementation of the model in a general drift-diffusion simulator and report on first numerical results. The essentials of the model are outlined in the following section.

2. Theory

Idealizing assumptions are: parabolic potential barrier (constant doping in the barrier region, Schottky approximation, no image effect, no interfacial layer, etc.), 1D approximation for the transmission probability, and unique effective mass in the semiconductor.

The WKB approximation is by-passed by interpolating analytically between the asymptotic forms of the eigenfunctions (parabolic cylinder functions) by means of Airy functions. The maximum error at the classical turning points, where the WKB solutions diverge, is shown to be less than 0.2 %. To enable analytical integration the maximum peak of the Airy function is fitted to a Gaussian with an universal attenuation parameter for all doping concentrations. In that way good agreement is achieved with the true transmission probability up to an energy E_{max} well above the maximum of the barrier. For still higher energies the simpler WKB approximation is sufficient to account for quantum reflection there. A fully analytical model is derived if the arguments of the Gaussians are developed with respect to the energy at the maximum of the spectral current density. This maximum is solution of a transcendental equation and may be approximated by an expression similar to that given by Crowell and Rideout [3]. To avoid expensive numerical integration including Fermi integrals, we use Boltzmann statistics above and total degeneracy below the Fermi energy, respectively. The final expression then contains error functions as the most complicated ingredients.

Fig. 1 compares $j(V)$-characteristics of the MS contact calculated with the new analytical model against the results of an "exact" reference model, where the correct transmission probability in terms of parabolic cylinder functions (Conley et al. [4]) was used in a numerical integration (not changing the statistics model). Curves labeled "Schroeder" are the corresponding characteristics, if his simplified WKB transmittance [1] is used.

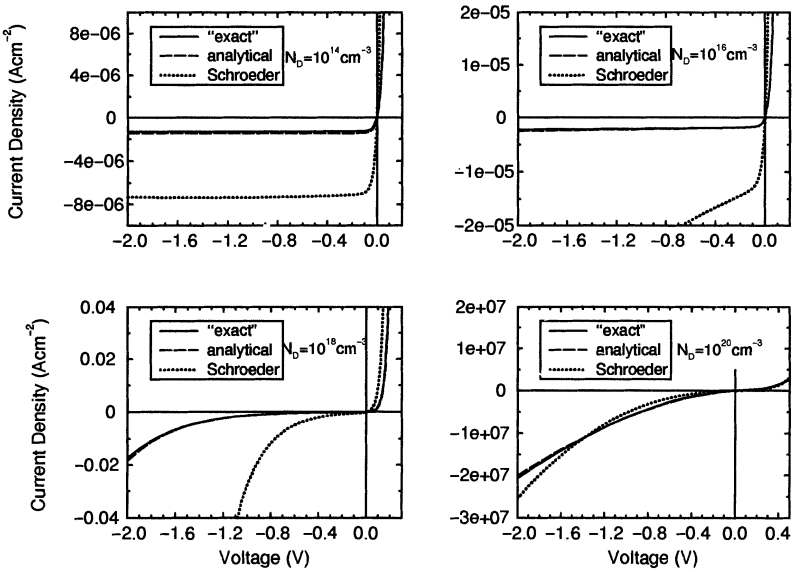

Figure 1: Calculated $j(V)$-characteristics of an Al on n-Si contact with barrier height $= 0.7\,eV$ and $m_c = 0.258\,m_0$ for different models.

3. Implementation

The implementation of the above model in a drift-diffusion device simulator requires the definition of boundary conditions for the electrostatic potential ψ and the quasi Fermi potentials φ_n and φ_p. For feasibility we assume equilibrium, i.e. $\varphi_n = \varphi_p =: \varphi$. This variable is determined by numerically balancing the drift-diffusion current and the TFE current as determined by the analytical model.

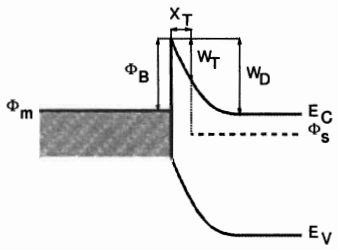

Figure 2: Schematic band diagram

The simplifying assumption of equilibrium is caused by the problem that the TFE current depends on the variable V_{app}, the potential drop over the barrier, which is a non-local variable and hence not available in a device simulator. This is why we approximate it by $V_{app} = \Phi_m - \Phi_s = V_{contact} - \varphi$ (see Fig. 2).

To be able to derive the boundary condition for ψ we have to identify the position in the barrier until which the current is determined by the TFE current and from which it can be treated as a pure drift-diffusion current. In Fig. 2 this point is shown at the depth X_T under the contact. It can be determined from the TFE model by the condition that tunneling remains negligible at lower energies. From the parabolic barrier assumption we can then derive a corresponding energy W_T and using this arrive at the following formula for ψ at the point X_T: $\psi = \varphi + \Phi_{bi} + (W_T - W_D)/q$, Φ_{bi} is the built-in potential. Unfortunately, $W_T - W_D$ depends again on V_{app} and is hence not available. Using the same approximation as above we arrive at: $\psi = \varphi + \Phi_{bi} + (W_T - W_D)_{eq}/q$, $W_{T,eq}$ and $W_{D,eq}$ are the equilibrium values of the energies W_T and W_D shown in Fig. 2. Note, that the expression for ψ reduces to the common boundary conditions in the two extreme cases of a pure Ohmic ($W_{T,eq} = W_{D,eq}$) and the Schottky case ($W_{T,eq} = 0$).

4. Examples

Fig. 3 compares simulation results with the drift-diffusion simulator SIMUL [5] against experimental data of a Kelvin structure (Ti on n-Si with ⟨100⟩-orientation, barrier height – $0.50\,eV$, $N_D = (1.8 - 2.2) \times 10^{18}\,cm^{-3}$). Such a contact represents an intermediate case be-

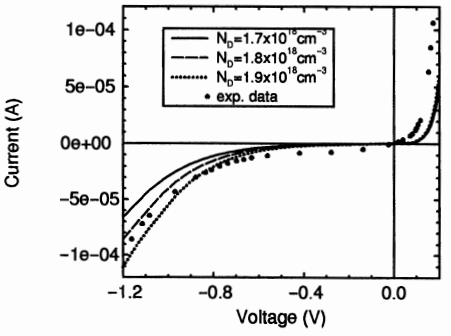

Figure 3: Comparison of simulations with a measured $I(V)$-characteristic of Ti/n-Si with $N_D = (1.8 - 2.2) \times 10^{18}\,cm^{-3}$ and an area of $3.4 \times 10^{-7}\,cm^2$ (dots). Simulated curves are based on the parameter set: $m_c = 0.19\,m_0$, $\Phi_B = 0.50\,eV$, $m_M = m_0$, and $E_{F,M} = 11.7\,eV$.

tween Ohmic and Schottky, and the data are not influenced by an unknown bulk resistance. The reverse bias branch can be well fitted with the transverse effective mass $m_t = 0.19\, m_0$ ($\langle 100 \rangle$-orientation!) for doping concentrations in the range $N_D = (1.8 - 1.9) \times 10^{18}\, cm^{-3}$.

Note that no ideality factor was used to remove the deviations at low reverse and forward biases, which are presumably caused by recombination inside the barrier region.

As another example we show the behavior of a *nin* structure (e.g. the Schottky part of a combined Schottky-pn-structure) with a variation of the surface doping concentration. The structure under consideration is $10\,\mu m$ long with a bulk value of $10^{14}\, cm^{-3}$. The one contact is Ohmic with a surface concentration of $N_D = 10^{20}\, cm^{-3}$ and the other is varied in steps from $10^{18}\, cm^{-3}$ to $2 \times 10^{19}\, cm^{-3}$ as shown in Fig. 4a.

The simulated $j(V)$-characteristics in Fig. 4b show the transition from a Schottky diode like behavior to a resistive behavior.

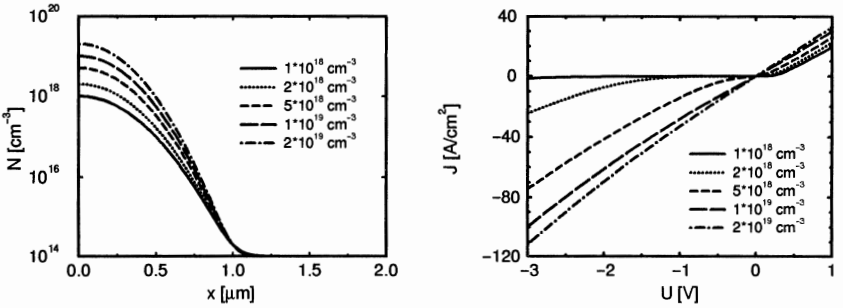

Figure 4: *nin* structures for varying surface doping. a) Doping versus spatial coordinate for the varying well. b) $j(V)$-characteristics.

Acknowledgements

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References

[1] D. Schroeder, Proc. 4th Int. Conf. on Sim. of Sem. Dev. and Proc., Zürich 1991, p. 313
[2] A. Schenk, submitted to Solid-State Electronics
[3] C. R. Crowell and V. L. Rideout, Solid-State Electronics **12**, 89 (1969)
[4] J. W. Conley, C. B. Duke, G. D. Mahan, and J. J. Tiemann, Phys. Rev. **150** (2), 466 (1966)
[5] SIMUL 1.1 manual, S. Müller, K. Kells, J. Litsios, U. Krumbein, A. Schenk, and W. Fichtner, Integrated Systems Laboratory, ETH Zurich, Switzerland, 1993