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BAMBI — A Transient 2D-MESFET Model with General Boundary Conditions Including Schottky and Current Controlled Contacts

Abstract — Boundary conditions using a current dependent carrier recombination velocity distribution are developed for modeling Schottky contacts by computer-aided physical simulation. In addition a boundary condition in the form of an arbitrary linear combination of voltage and current at the contact is presented. Thus, MESFET-devices with simple circuits connected to device terminals can be simulated by solving additional equations. As an example the switching behavior of a MESFET with drain resistor is investigated.

Introduction

MESFETs are a potential alternative to MOSFETs. MESFETs offer advantages in simplicity of fabrication compared to MOSFETs, because only low temperature processes are required for fabrication. Without any radiation sensitive oxide under the gate MESFETs have been reported to stand up to 100MRad [1] compared to a value of few hundred kRad for MOSFETs. In the MOS case hot carriers may be injected into the oxide. This fixed charge causes degradation of the characteristics. The effective mobility in the channel also tends to be higher in the MES case. The current flows further inside the silicon causing less interaction between carriers and the interface states. MESFETs therefore show little noise similar to JFETs. Due to these advantages concepts for complementary Silicon MESFETs have been investigated as alternative to the traditional CMOS technology [2].

Such investigations urgently ask for the help of device simulation tools with adequate models for Ohmic and Schottky contacts. This paper presents the implementation of boundary conditions for metal-semiconductor contacts and for floating contacts in
the two-dimensional transient device simulator BAMBI [3,4]. The program simulates devices with both geometry and doping profile being arbitrary. According to the drift diffusion theory [5] it solves the three basic semiconductor equations (1–3) together with the two current equations (4,5) using the method of finite-boxes [6].

\[
\begin{align*}
\Delta \psi &= -\frac{q}{\varepsilon} (p - n + N_D - N_A) \quad (1) \\
\nabla J_n &= q(\frac{\partial n}{\partial t} + R_n) \quad (2) \\
\nabla J_p &= -q(\frac{\partial p}{\partial t} + R_p) \quad (3) \\
J_n &= qD_n \nabla n - q \mu_n \nabla \psi \quad (4) \\
J_p &= -qD_p \nabla p - q \mu_p \nabla \psi \quad (5)
\end{align*}
\]

The Ohmic Contact

The analysis is based on electrostatic potential, electron and hole concentration \((\psi, n, p)\) presumed as unknowns. Poisson’s equation (1) and the two continuity equations (2,3) are numerically solved with a Dirichlet boundary condition for electrons, holes, and electrostatic potential at ohmic contacts. Assuming space charge neutrality directly under the terminal the concentrations are set equal to their thermal equilibrium values. The boundary condition for the electrostatic potential reads

\[
V_{\text{term}} = \psi - \psi_{bi} \quad (6)
\]

\[
\psi_{bi} = \pm \frac{kT}{q} \ln \left| \frac{N_D - N_A}{n_i} \right| \quad (7)
\]

where \(\psi_{bi}\) denotes the built-in potential and \(V_{\text{term}}\) the terminal voltage. Simulating contacts with external circuits, \(V_{\text{term}}\) becomes floating increasing the number of variables to be calculated by one for each floating contact. The additional equations are given by the new mixed boundary condition (8) defining the dependence between contact voltage \(V_{\text{term}}\) and contact current \(I_{\text{term}}\).

\[
\alpha \cdot V_{\text{term}} + \beta \cdot \left( I_{\text{term}} + C \frac{dV_{\text{term}}}{dt} \right) = \gamma \quad (8)
\]

This is the most general form of the boundary condition which can be handled by our method. Thus, a variety of possibilities for interpretation in mathematical as well as in electrical terms, is offered. Choosing the dimensions of \(\alpha, \beta\) and \(\gamma\) in the correct way several different definitions of the outer circuit diagram can be given using arbitrarily a serial resistive, or a parallel conductive and serial or parallel capacitive loads.

A current driven circuit shown in Fig. 1 (left side) is described by defining \(\alpha = G, \beta = 1, \gamma = I_{\text{appl}}\). The equivalent voltage driven circuit diagram of Fig. 1 (center) requires the assumption \(\alpha = 1, \beta = R, \gamma = V_{\text{appl}}\).
Interpreting $C$ as a capacity between voltage source and contact (8) has to be slightly modified by the transformation of $\gamma$: $\gamma \rightarrow \gamma + \beta C \cdot \frac{d\left(\frac{V}{A}\right)}{dt}$. For a simpler handling by the user (9) has been directly implemented.

\[ \alpha \cdot V_{term} + \beta \cdot (I_{term} - C \cdot \frac{d\left(\frac{V}{A} - V_{term}\right)}{dt}) = \gamma \]

(9)

With the values given above the outer right circuit of Fig. 1 can be simulated.

\[ I_{term} = \frac{V_{appl} - V_{term}}{R} + C \cdot \frac{d(V_{appl} - V_{term})}{dt} \]

(10)

The numerical treatment of mixed boundary conditions (8) or (9) is illustrated by Fig. 2. Both equations include the two variables $V_{term}$ and $I_{term}$ in which $V_{term}$ is the additional unknown and $I_{term}$ has to be expressed by $\psi_i, n_i, p_i$. The terminal current is given by integrating electron-, hole- and displacement current densities $J_n, J_p$ and $J_d$ over the area of the contact $A$:

\[ I_{term} = \int_A \left( J_n + J_p + J_d \right) \cdot dA \]

(10)

Using the well known finite difference scheme first suggested by Scharfetter and Gummel [7] the boundary conditions (8) and (9) finally yield the discrete expressions:

\[ \alpha \cdot V_{term_T} + \beta \cdot \left( \sum_k (J_{n_k} + J_{p_k} + J_{d_k}) + C \cdot \frac{V_{term_T} - V_{term_{T-\Delta T}}}{\Delta T} \right) = \gamma \]

(11)

\[ \alpha \cdot V_{term_T} + \beta \cdot \left( \sum_k (J_{n_k} + J_{p_k} + J_{d_k}) - \left[ \frac{1}{\Delta T} \left( \frac{V}{\Delta T} - \frac{V_{term_T} - V_{term_{T-\Delta T}}}{\Delta T} \right) \right] \right) = \gamma \]

(12)
\[
\begin{align*}
J_{nk} &= q D_n \frac{w_k}{d_k} [n_{II_k} B(\Delta_k) - n_{I_k} B(-\Delta_k)] \\
J_{pk} &= q D_p \frac{w_k}{d_k} [p_{II_k} B(\Delta_k) - p_{I_k} B(-\Delta_k)] \\
J_{dk} &= \frac{w_k}{d_k} \left( \psi_{II_k} - \psi_{I_k} \right) T - \left( \psi_{II_k} - \psi_{I_k} \right) T^2 \Delta T \\
\Delta_k &= \frac{\psi_{II_k} - \psi_{I_k}}{V_T}, \quad B(x) = \frac{x}{e^x - 1}
\end{align*}
\]

where \( I \) denotes the point at the contact and \( II \) the next neighbour (Fig. 2), \( J_{n,p,d} \) denote the three current contributions at the midpoints, \( T \) the actual time, \( \Delta T \) the actual time step, \( d_k \) the distance between point \( I \) and point \( II \) and \( w_k \) the weighting factor for the integration. \( D_n \) and \( D_p \) are the coefficients for electron- and hole diffusion, \( \epsilon \) is the dielectric permittivity, \( q \) the electronic charge and \( V_t \) the thermal voltage.

Solving the discrete form of the mixed boundary condition (11) and (12), respectively, together with a discrete representation of Poisson’s equation and both continuity equations (2,3) yields a numerical solution for electrostatic potential, electron and hole concentration \( \psi_i, n_i, p_i \) at each free node in a finite-boxes mesh and the terminal voltage \( V_{term} \) for each floating contact. Since (13) and (14) are nonlinear in the unknown variable \( V_{term} \) a linearization technique is required. For current or mixed boundary problems the discretized nonlinear equation system is therefore solved simultaneously by a coupled Newton’s method.

The Schottky Contact

![Diagram of the energy bands at a Schottky contact](Fig. 3)

When metal is in contact with a semiconductor, potential barriers \( \Phi_{bn} \) for electrons and \( \Phi_{bp} \) for holes will be formed at the Metal Semiconductor (MS) interface (Fig. 3). The Fermi levels in the two materials must coincide what causes a depletion layer similar to that of the one-sided abrupt (e.g., \( p^+-n \)) junction. According to the thermionic...
emission–diffusion theory of Crowell and Sze [8] the boundary conditions at the MS-interface read:

\[ \psi_i = V_{app} - \psi_s \quad (18) \]
\[ J_n = -q \cdot v_n \cdot (n_i - n_0) \quad (19) \]
\[ J_p = q \cdot v_p \cdot (p_i - p_0) \quad (20) \]

\( n_i \) and \( p_i \) are the surface concentrations of electrons and holes, \( \psi_i \) the surface potential at the MS-interface, \( V_{app} \) the applied voltage and \( \psi_{bi} \) the doping dependent built-in voltage (7).

(18) defines the surface potential with the help of the barrier dependent potential value \( \psi_s \) (Fig. 3) according to the potential variation within the depletion layer. \( \psi_s \) is defined by (21,22)

\[ \psi_s = \Phi_{bn} - \Phi_i \quad (21) \]
\[ \psi_s = \Phi_i - \Phi_{bp} \quad (22) \]

where \( \Phi_i \) is the intrinsic energy level.

The boundary conditions (19) and (20) model the carrier flow through the MS-interface with surface recombination terms using effective surface recombination velocities \( v_n \) and \( v_p \) for electrons and holes, respectively [9].

The quasi-equilibrium concentrations \( n_0 \) and \( p_0 \) are the surface concentration for zero bias (\( V_{appl} = 0 \)). With (18) the surface potential \( \psi_i \) becomes \( \psi_i = \psi_s \) yielding

\[ n_0 = n_i \cdot \exp \left( \frac{-\psi_s}{kT} \right) \quad (23) \]
\[ p_0 = n_i \cdot \exp \left( \frac{\psi_s}{kT} \right) \quad (24) \]

where \( n_i \) denotes the intrinsic concentration.

The recombination velocities \( v_{n,p} \) at a MS-junction are upper bounded by the saturation velocities of the carriers within the semiconductor and lower bounded by the collection velocity \( v_c \) (25). The value of \( v_c \) has been derived by Crowell and Sze, assuming a Maxwellian distribution of carrier velocities at the contact.

\[ v_c \mid_{V_{appl} \leq 0} = \sqrt{\frac{kT}{2m^* \pi}} \cdot f_b f_q \quad (25) \]

\( m^* \) is the effective mass for electrons or holes, \( f_b \) is the probability of a carrier reaching the metal without being backscattered and \( f_q \) is the probability for quantum mechanical reflection of carriers together with tunneling effects.
Defining \( v_{n,p} \) equal to a fraction of \( v_{sat} \) under forward bias conditions causes unrealistic accumulation of carriers at the MS-interface. Setting \( v_{n,p} = v_{sat} \) in order to avoid this accumulation for high forward bias, will result in an unrealistic depletion of carriers at the contact if zero or low bias is applied. As pointed out by Adams [10] one expects a non-Maxwellian distribution of velocities of carriers travelling into the metal.

Our investigations followed the approach by Adams [10] who assumed the carrier velocities to be represented by the positive part of a drifted Maxwellian distribution (26):

\[
f(v_x) = K \cdot \exp\left(\frac{-m_{n,p}^* \gamma_{n,p} (v_x - v_d)^2}{2kT}\right)
\]

(26)

Taking the mean value (27)

\[
v_{n,p} = \frac{\int_0^\infty v_x f(v_x) dv_x}{\int_0^\infty f(v_x) dv_x}
\]

(27)

yields the current dependent expression (28)

\[
v_{n,p} = v_d + \sqrt{\frac{2kT}{\pi m_{n,p}^* \gamma_{n,p}}} \cdot \frac{\exp\left(-v_d^2 \cdot \frac{m_{n,p}^* \gamma_{n,p}}{2kT}\right)}{1 + \text{erf}\left(v_d \sqrt{\frac{m_{n,p}^* \gamma_{n,p}}{2kT}}\right)}
\]

(28)

Here \( v_d = \frac{J_{n,p}}{q\gamma_{n,p}} \) is the drift velocity, \( \gamma_{n,p} \) is a compensating factor for the increase of the carrier effective mass caused by band structure changes at the MS interface (Stratton[11]), and \( K \) is a normalization constant.

Since the drift velocity is upper bounded by the saturation velocity in the semiconductor, (28) is valid in all practical cases. Comparing the lower bound of (28) for \( V_{app} = 0 \) with the expression for the collection velocity yields the fitting parameter \( \gamma_{n,p} = 4 \). Physically this would predict a ratio \( \frac{m_{n,p}^*}{m_{n,p}} \) at the MS-interface of 0.25 times the ratio within the semiconductor.

Fig. 4: Recombination velocity vs. drift velocity

Fig. 4 shows the recombination vs. drift velocity. Under reverse bias \( v_{n,p} \) are kept constant by neglecting their reduction by \( f_b \) and \( f_q \).
**Application Example**

As a major application the switching behavior of an n–channel Silicon MESFET is presented. Fig. 5 shows the geometry and Fig. 6 the simulated circuit. The gate voltage is switched abruptly from a turn–off voltage $V_G = -2\, \text{V}$ to a turn–on voltage $V_G = 0.2\, \text{V}$. This voltage jump is transmitted to the drain terminal (Fig. 7) resulting in a drain voltage peak of $V_D = 6.78\, \text{V}$ which is at least higher than the supply voltage. The drain current therefore flows out of the device first (Fig. 8). It changes sign after $t = 40\, \text{ps}$ corresponding to the decreasing drain voltage which reaches the value of the supply voltage at the same time. The depleted region under the MES gate (Fig. 9) is reduced from both sides (Fig. 10) but the source current is obviously dominating (Fig. 8,10) due to the limiting drain resistor. During the first $40\, \text{ps}$ the current enters the device through the gate terminal and passes the depletion region as displacement current towards drain and source. After $40\, \text{ps}$ the depletion region is reduced so far (Fig. 11) that an electron convection current starts to flow directly from drain to source. Finally in steady–state condition we observe a broad current pass at that side of the device being opposite to the MES gate (Fig. 12).

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**Fig. 5:** Geometry of the simulated MESFET

**Fig. 6:** Simulated circuit

**Fig. 7:** Drain voltage during turn on

**Fig. 8:** Contact currents during turn on
Fig. 9: Electron distribution before turn on

Fig. 11: Electron distribution after 40ps

Fig. 10: Electron current density after 1ps (logarithmic scale)

Fig. 12: Steady state electron current density after turn on

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