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A Critical Study of Boundary Conditions in Device Simulation

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Abstract

In most approaches to device simulation a set of coupled partial differential equations must be solved. The solution is mainly determined by the applied boundary conditions. This paper critically investigates the commonly used types of boundary conditions from both the mathematical and the numerical points of view. Consistency and convergence behavior are illustrated with computational results.

1 Introduction

A considerable variety of boundary conditions has been implemented in device simulation programs. In all cases the boundary conditions must meet the requirements which are posed by the assumptions of the discretization scheme. In this paper these formulations and implementations will be analyzed from the mathematical and the numerical points of view, illustrating both correct and inconsistent approaches with examples. As far as possible, no judgement concerning the underlying physical models will be given since this is considered outside the scope of this paper. In particular the paper deals with isolating boundaries (e.g. Neumann boundary conditions), interfaces between semiconductor and dielectrica, ideal Ohmic contacts, Schottky contacts, as well as purely current–controlled contacts and mixed contacts (which account for contact resistances and mixed current control).
For the following investigations of the numerical behavior of the commonly used boundary conditions, a finite differences discretization of Scharfetter–Gummel type for the three basic semiconductor equations is assumed (drift–diffusion approach).

2 Conditions for Isolating Boundaries

In general boundary conditions for isolating boundaries are characterized by prescribing the derivatives of variables with respect to the outer normal vector $\vec{n}$

$$\frac{\partial f(\vec{x})}{\partial \vec{n}} = g(\vec{x}, \ldots) \ ,$$

where $f(\vec{x})$ is the space dependent unknown variable and $g(\vec{x},\ldots)$ is a function depending on space $\vec{x}$ and other arbitrary parameters.

2.1 Neumann Boundary Conditions

Neumann boundary conditions are applied to artificial boundaries in order to guarantee that the domain under consideration is self contained. They can be written as

$$\frac{\partial \psi}{\partial \vec{n}} = 0$$
$$\frac{\partial n}{\partial \vec{n}} = 0$$
$$\frac{\partial p}{\partial \vec{n}} = 0 \ .$$

The implementation of Neumann boundary conditions can be carried out in a straight forward way: The differential quotient is replaced by the one–sided difference quotient whereby the lateral effect is neglected. This first order approximation of the Neumann boundary condition works well in most cases. In the following example of a simple resistor (geometry in Fig. 1) however, a significant discretization error is introduced by taking the derivative at the first midpoint of the grid line instead of the value at the boundary and by neglecting the lateral effects. This can be seen in Fig. 2 where the values for div $\vec{J}$ are plotted at each point. Due to the law of Gauss

$$\text{div } \vec{J} = 0$$

should be fulfilled at each point, however, it is not fulfilled at the points along the Neumann boundaries between the contacts and at the singularity of the re–entrant corner. By insertion of a grid line close to the boundaries this discretization error can be reduced drastically.

It should be pointed out that the formulation of the Neumann boundary condition is only consistent for the semiconductor equations if the outer normal derivatives of C, μ_n, μ_p, and U_T (under non–isothermal conditions) vanish. This is of major importance at corners with adjacent Neumann boundary conditions and at points with a change from Dirichlet to Neumann conditions. Furthermore inconsistent Neumann boundary conditions can be crucial for convergence especially in floating regions of a device which are *per se* difficult to handle from the numerical point of view.

For convergence reasons Neumann boundary conditions are sometimes replaced by Dirichlet boundary conditions. If this is done very carefully (e.g. between source/drain contact and gate contact at the oxide surface in a MOS device) the solution is influenced only locally as it can be seen in Fig. 3 (Neumann boundaries) and Fig. 4 (Dirichlet boundaries). The thickness of the oxide block between gate and drain contact is 0.35μm. The computed current flow in the semiconductor is not affected by this systematic error as long as the thickness of the oxide block is of sufficient magnitude.

2.2 Interface between Semiconductor Region and Insulator

At the interface between semiconductor region and insulator Dirichlet boundary conditions are applied for the current densities, i.e. no current will flow into the oxide ($\vec{J}_{n,p} \cdot \vec{n} = 0$). Again the term accounting for interface generation/recombination effects will be neglected.
By the law of Gauss the interface condition for the potential reads

$$\varepsilon_{sem} \cdot \frac{\partial \psi}{\partial \vec{n}} - \varepsilon_{ox} \cdot \frac{\partial \psi}{\partial \vec{n}} = Q_{int} \ ,$$

which is of Neumann type (Q_i is the interface charge). The implementation of this interface condition can be done by means of so–called "mirror imaging" [1]. For reasons of consistency and accuracy it must be implemented at least as a 2nd order boundary condition to account for currents flowing parallel to the interface.

3 Boundary Conditions for Contacts

Since the semiconductor equations form an elliptic system in the stationary case the solution in the inner of the integration area is determined by the Dirichlet boundary conditions.

3.1 Ideal Ohmic Contacts

The most common Dirichlet boundary condition is the so–called ideal Ohmic contact. In this case all variables have a given value at the boundary. The conditions for the carrier concentrations are based on the assumption of space charge neutrality

$$n - p - C = 0$$

which leads to

$$\begin{aligned} \psi &= \psi_{applied} + \psi_{bi} \\ n &= \frac{\sqrt{C^2 + 4 \cdot n_i^2} + C}{2} \\ p &= \frac{\sqrt{C^2 + 4 \cdot n_i^2} - C}{2} \ . \end{aligned}$$

The built–in potential ψ_{bi} can be explained physically, however, it is also of major importance for the mathematical consistency of the formulation: ψ_{bi} cancels lateral currents in the contact plane. Lateral currents would interfere with the assumption of space charge neutrality which is equivalent to the assumption of an infinite surface recombination velocity. The Ohmic contact provides the best possible convergence behavior due to good conditioning of the system, as long as the boundary conditions are consistent, i.e. no contacts exist which have a common point but different values for the potential.

3.2 Schottky Contacts

The general formulation of Schottky contacts consists of Dirichlet boundary conditions for the electrostatic potential and the current densities. Usually the boundary conditions read

$$\begin{aligned} \psi &= \psi_{applied} - \psi_{Schottky} \\ \vec{J}_n \cdot \vec{n} &= -q\vec{v}_n \cdot (n - n_0) \\ \vec{J}_p \cdot \vec{n} &= q\vec{v}_p \cdot (p - p_0) \ , \end{aligned}$$

where $\psi_{Schottky}$ contains the built–in potential and the barrier height ϕ_B. n_0 and p_0 are the equilibrium carrier concentrations and $\vec{v}_{n,p}$ denotes the surface recombination velocity of electrons and holes, respectively. All physical considerations which make the boundary condition suitable for simulation purposes have to be described using $\psi_{Schottky}$ and $\vec{v}_{n,p}$ (e.g. [2]). Thus $\psi_{Schottky}$ is independent of the doping and is constant along the contact:

$$\psi_{Schottky} = \phi_B - \frac{E_g}{2q} + \frac{kT}{2q} \ln\left(\frac{N_v}{N_c}\right) \ .$$

E_g denotes the bandgap, k the Boltzmann constant, T the absolute temperature and $N_{v,c}$ the density of states in the valence band and the conduction band, respectively. However, several basic rules regarding n_0 and p_0, $\vec{v}_{n,p}$ and $\psi_{Schottky}$ have to be obeyed for a consistent formulation.

The most common approach assumes an infinite surface recombination velocity for n_0 and p_0 (e.g. [3]). These formulations are obviously inconsistent. If the electrostatic potential depends on $\psi_{Schottky}$ then the concentrations must depend on $\psi_{Schottky}$ as well. Otherwise the current will not vanish in equilibrium.
Another approach [4] applies a factor $e^{\pm\phi_B}$ to the equilibrium concentrations. This is even formally incorrect since the exponent should read $\pm\phi_B/U_T$ in order to be dimensionless. Numerical experiments using this (corrected) approach resulted in high currents even in equilibrium. Furthermore this approach can also be shown to be contrary to physics by considerations regarding the band diagram structure.
The formulation in [2] is only consistent for doping profiles which are constant along the contact. Otherwise lateral currents will arise in the contact plane. For a generally valid formulation the built–in potential must be taken into account. This could be done e.g. by replacing the boundary condition for the electrostatic potential

$$\psi = \psi_{applied} - \psi_{Schottky}$$

by

$$\psi = \psi_{applied} - \psi_{Schottky} + \psi_{bi} - \psi_{bi}^{ref} \ ,$$

where ψ_{bi}^{ref} denotes the built–in potential at which the barrier height ϕ_B has been measured. Note that for a constant doping along the contact and for correct ψ_{bi}^{ref}

$$\psi_{bi} - \psi_{bi}^{ref} = 0$$

holds thus leading back to the original formulation.

The velocities $\vec{v}_{n,p}$ depend on the solution. They add another non–linearity to the problem. Since $\vec{v}_{n,p}$ are positive and bounded the numerical treatment does not give rise to many problems. With a fix–point iteration good convergence can be obtained, however, limiting the changes (damping) from one iteration step to the next will enhance convergence even more.
From the numerical point of view a smooth transition from the Schottky contact to the Ohmic contact exists even if no physical model exists at present.

3.3 Current–Controlled Contacts

Current–controlled (mixed) contacts provide another class of boundary condition. In the most general case both the carrier concentrations and the potential are unknown [5]. This means that for each unknown an additional condition must be defined, resulting in an extra equation in the discretized system. Even purely current–controlled contacts need an additional condition in order to determine the integration constant stemming from the relation between carrier concentrations and current densities. This integral boundary condition may provide major convergence problems, especially if the contact currents are not computed in a proper, numerically stable way [6].

Again, the problem of lateral currents in the contact plane arises if the boundary condition is "distributed". From the rigorous mathematical point of view these distributed boundary conditions are inconsistent: either lateral currents occur if the contact is seen as one entity, or the potential distribution is discontinous if each point is seen as a single contact. This results in the fact that no estimation of the discretization error is possible if this condition is used. It is even not guaranteed that the original differential operator is solved.

4 Summary

Some basic mathematical properties have been analyzed which have to be fulfilled for self–consistent formulations of the boundary conditions in device simulation. This paper has discussed commonly used approaches as found in literature which are often inconsistent. It has pointed out the mathematical assumptions which must be fulfilled for correct formulations, especially of Schottky contacts and current–controlled contacts. Furthermore remarks on the convergence behavior and implementation have been made.

Acknowledgement

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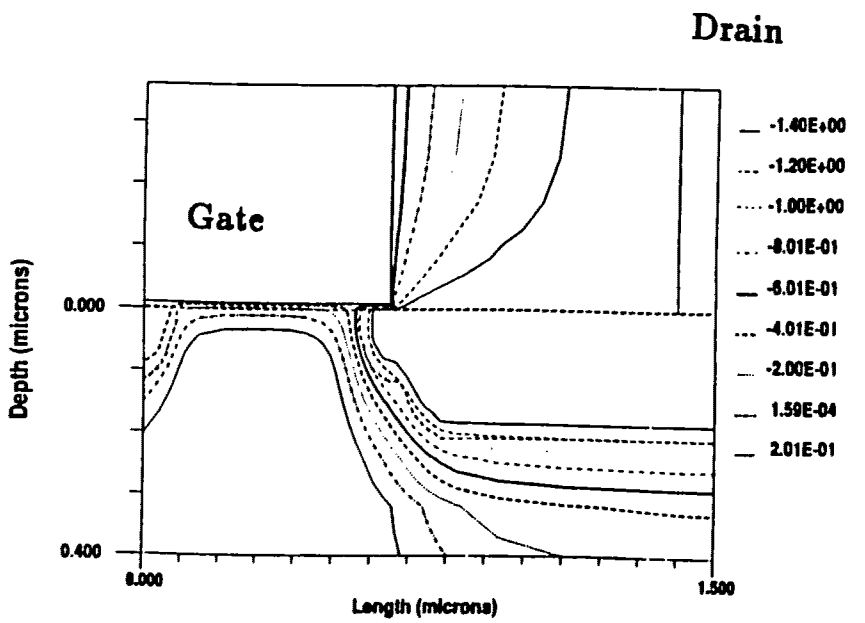

Figure 3: Electrostatic potential of a MOS transistor with Neumann boundaries

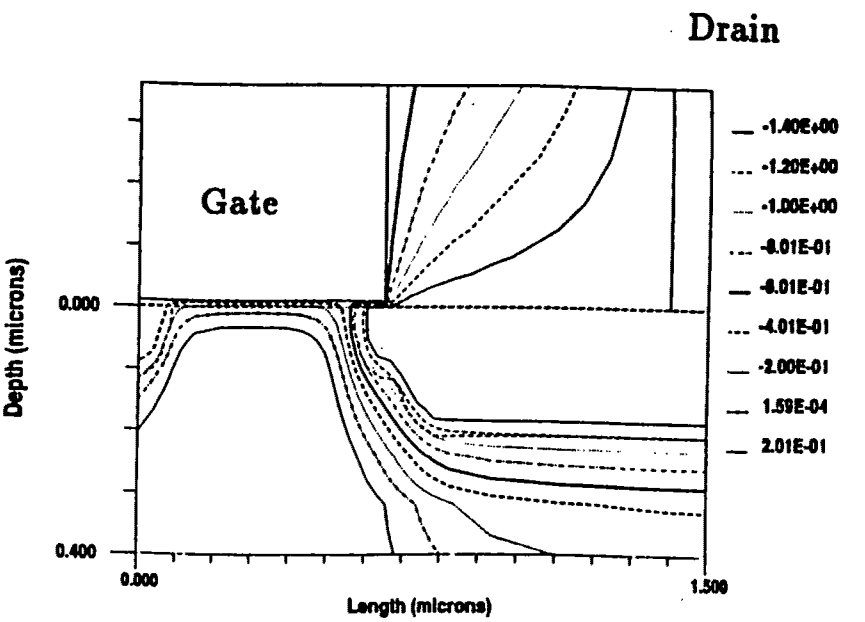

Figure 4: Electrostatic potential of a MOS transistor with Dirichlet boundaries

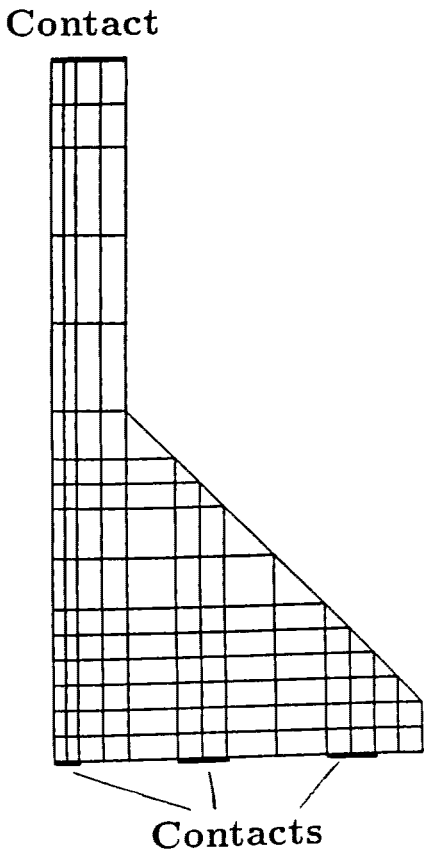

Figure 1: Geometry of a simple resistor

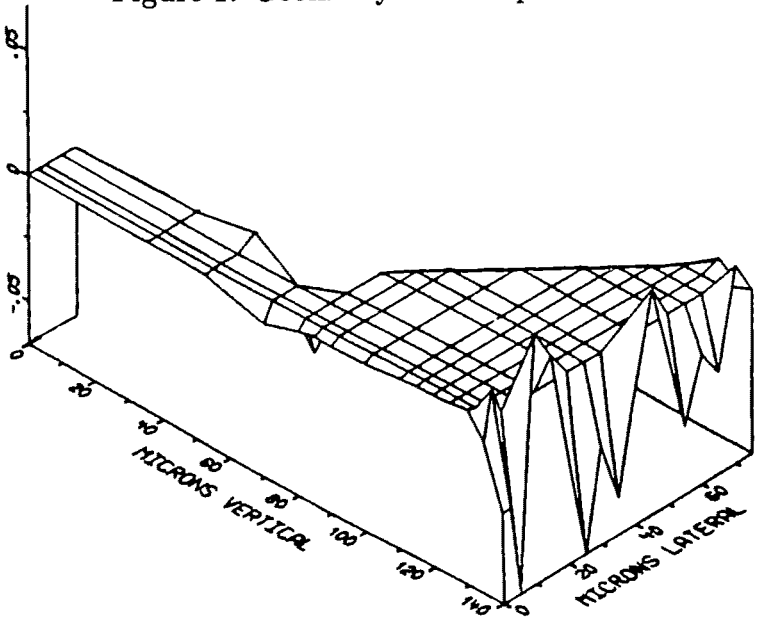

Figure 2: Residuals for the law of Gauss