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Network and Semiconductor Device Modeling

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Introduction

The technological progress in many application areas (telecommunication, robotics and others) is actuated by the development of the electronic components and optic. The increasing of the performance is a result of a higher complexity of integrated systems and smaller dimensions of electronic and optic devices. Both are connected with new diffculties for the design of circuits.

Circuit design consists usually of several steps: process simulation, device simulation, compact modeling for semiconductor devices, extraction and generation of model parameters, circuit simulation. The way over a compact modeling of devices (macro-modeling) was advantageous up to now since one could simulate circuits without an expensive device simulation. Thus, a simulation of integrated circuits was enabled in general. Nowadays, however, the performance of high frequency devices depends not only on their geometrical dimensions. It is significantly influenced by the surrounding circuitry. This requires additional (time consuming) iterations during the circuit design for the extraction and generation of model parameters.

Furthermore, high frequency parts of a circuit have to be modeled with a very high precision for a reliable evaluation of the circuit function. Consequently, for complex circuits with high frequency devices, it is recommended to combine circuit simulation directly with a device simulation of elements of the high frequency part. This results in coupled systems of differential-algebraic equations.

In this document, we follow an approach that includes the device model equations into the network equation system directly. Based on a detailed analysis of network and device modeling, we elaborate information about the structure of the coupled circuit and device systems.

Furthermore, we present a treatment of the coupled systems as differential algebraic systems in infinite-dimensional Hilbert spaces. Such systems are also called singular or degenerate abstract differential equations.

This work is divided into 2 parts. The first one is devoted to a detailed network analysis - network elements and topological properties of the network are discussed from a mathematical point of view.

The second part deals with modeling of semiconductor devices. After a short discussion of different models on different levels, we consider the drift diffusion equations. Particular care is taken to the boundary conditions since they play an important role for the coupling between circuit and device equations.

The Appendix collects symbols and physical constants used in this thesis.

1. Network Modeling

The numerical simulation of electric networks is closely related to the network modeling. Circuit models have to meet two contradicting demands:

- they have to describe the physical behavior of a circuit as correct as possible
- they should be simple enough to keep computing time reasonably small

A well established approach meeting both demands to a certain extent is the description of the network by a graph with branches and nodes. Branch currents, branch voltages and node potentials are introduced as variables. The node potentials are defined as voltages with respect to one reference node, usually the mass node.

The physical behavior of each network element is modeled by a relation between its branch currents *j* and its branch voltages *v*. Network elements fully described by a relation between a single branch current and a single branch voltage are called one-port or two-terminal elements. One port rejects one branch, one terminal reflects one end of a branch. Correspondingly, the other elements are called multi-port or multi-terminal elements. The describing current-voltage relations are called characteristic equations.

In order to complete the network model, the topology of the elements has to be taken into account. Assuming the electrical connections between the circuit elements to be ideally conducting and the nodes to be ideal and concentrated, the topology can be described by Kirchhoff's laws.

1.1 Network Elements

The analysis and design of circuits requires an approximation of real elements by appropriate models. The level of the models ranges from simple algebraic equations, over ordinary and partial differential equations to Boltzmann and Schroedinger equations depending on the effects to be described. Due to the high number of network elements (up to millions of elements) belonging to one circuit one is restricted to relatively simple models. In order to describe the physics as good as possible, so called compact models represent the first choice in network simulation. Complex elements such as transistors are modeled by small circuits containing basic network elements described by algebraic and ordinary dfferential equations only.

The basic network elements are ideal resistors, ideal condensers, ideal coils and ideal batteries. In order to express that we deal with ideal elements we use the terms resistor, capacitor, inductor, and voltage source, respectively.

Furthermore, we shall use current sources that play an important role for the description of more complex elements such as transistors.

The characteristic equation of a resistor may be described as

$$v(t) = r(j(t), t) \text{ or } j(t) = g(v(t), t) \tag{1.1}$$

where $j(t)$ reflects the current and $v(t)$ the voltage through the resistor at the time t. The functions r and g, respectively, can be linear and nonlinear. Typical examples are Ohms resistors and diodes. In the first case, the functions r and g are linear and time-independent. In the second case, the function g reflects an exponential function with respect to the first argument.

In case of multiterminal elements j and v may form vector valued functions of time. An element with n terminals is uniquely determined by the relation between $n - 1$ branch voltages and $n - 1$ branch currents. Therefore, one chooses often one reference terminal and considers the branches between the reference terminal and all other terminals.

Capacitors store energy in their electric fields. It's charge q(t) may be expressed by

$$q(t) = q_C(v(t), t).$$

The function q_C is usually monotone. Due to the definition of the current we get the voltage-current characteristics

$$j(t) = \frac{dq_C(v(t),t)}{dt}.$$

As described for resistors, the currents, charges and voltages may be vector valued functions in case of multi-terminal elements. Typical examples are the ideal condenser and the varactor diode. Transistor modeling requires often nonlinear multi-terminal capacitors.

Inductors store energies in their magnetic fields. The flux $\phi(t)$ is represented by

$$\phi(t) = \phi_L(j(t), t).$$

Regarding the definition of voltage, we arrive at

$$v(t) = \frac{d\phi_L(j(t),t)}{dt}.$$

Also in this case, the currents, fluxes and voltages may be vector valued functions. Most of coils have a nonlinear current-flux characteristics. One can approximate them by linear functions only in a small current range. In case of large currents, the flux growths sub-linearly.

Independent voltage and current sources are distinguished by the fact that the voltage and the current are given by

$$v(t) = v_s(t) \quad \text{and} \quad j(t) = i_s(t), \text{ respectively.}$$

If we have

$$v(t) = v_s(j(t)) \qquad \text{or} \qquad j(t) = i_s(\hat{j}(t))$$

then the sources are called current controlled. Again, v, j and $\hat{j}$ may be vector valued functions. Here, the branches corresponding to j are different from those corresponding to $\hat{j}$. In case of

$$v(t) = v_s(\hat{v}(t)) \qquad \text{or} \qquad j(t) = i_s(v(t)),$$

the sources are called voltage controlled. Here, the branches corresponding to v are different from those corresponding to $\hat{v}$.

In general, we have

$$v(t) = v_s(t, j(t), \hat{v}(t)) \qquad \text{for voltage sources}$$

and

$$j(t) = i_s(t, \hat{j}(t), v(t)) \qquad \text{for current sources.}$$

1.1 Network Topology

Assuming that quantum mechanical interactions between the network elements can be neglected, the electrical behavior of the network is described by Maxwell's equations which imply Kirchhff's laws.

Considering one node with branch currents j_1, ..., j_n entering this node we may describe Kirchhoff's current law (KCL) as

$$\sum_{k=1}^{n} j_k = 0, \tag{1.2}$$

that means, the sum of all branch currents entering a node equals zero.

If we consider a loop with the branch voltages v_1, ..., v_n , then we may formulate Kirchhoff's voltage law (KVL) as

$$\sum_{k=1}^{n} v_k = 0,$$

that means, the sum of all branch voltages in a loop equals zero. Using Kirchhoff's laws, one can describe the network topology in an elegant way by the (reduced) incidence matrix A = (a_{ij}) that describes the relation between all nodes (except the mass node) and all branches of the network. It is defined as

$$a_{ij} = \begin{cases} 1 \\ -1 \\ 0 \end{cases}$$

where: 1- if the branch j leaves the node i,
- 1 - if the branch j enters the node i,
and 0 - else.

Let a connected network with n nodes and b branches be given. If $j = (j_1, j_2,\ldots, j_b)^T$ is the vector of all branch currents of the circuit, then Kirchhoff's current law implies

$$Aj = 0. \tag{1.3}$$

Consequently, the maximal number of independent node equations describing the network is given by (1.3).

The incidence matrix allows, additionally, a simple description of the relation between node potentials and branch voltages of the network. If $v = (v_1, v_2, \ldots, v_b)^T$ is the vector of all branch voltages and $e = (e_1, e_2,\ldots, e_{n-1})^T$ denotes the vector of all node potentials, then the relation

$$v = A^T e \tag{1.4}$$

is satisfied. Each individual equation of (1.4) corresponds to one branch voltage. If we apply Kirchhoff's voltage law to a loop containing both nodes of the considered branch and the mass node, we get (1.4) directly.

1.2 The Modified Nodal Analysis

Let a connected electrical network be given. The nodal analysis is based on the network equations (1.3)

$$Aj = 0 \tag{1.5}$$

and (1.4)

$$v = A^T e \tag{1.6}$$

as well as the characteristic equations of all network elements. As described in the section before, they may be written as

$$f\left(\frac{dq_C(v,t)}{dt}, \frac{d\phi_L(j,t)}{dt}, v, j, t\right) = 0. \tag{1.7}$$

The system (1.5)-(1.7) is a differential algebraic system, that means a coupled system of differential and algebraic equations in the network variables j, v and e. The dimension of this system equals $2b+n-1$. The approach leading to this system is called **sparse tableau analysis**.

The so called **modified nodal analysis** (MNA) requires a much smaller number of unknowns. In this case, one replaces the branch currents of all current defining elements in (1.5) by their characteristic equations, and all branch voltages by node voltages using (1.6). It is not difficult to see, that the resulting system represents a differential-algebraic equation.

In order to design an effective solution scheme, it is important to look at the structure of the equations. Other physical systems, like multibody systems, in mechanics, can be described by differential-algebraic equations, which are Euler equations of a variational principle (see e.g. [ESF98, RR99]). This gives them a structure, which is exploited by modern numerical schemes. In electrical network simulation, the structure is not so evident. Therefore, simulation methods could not be based on a particular structure until a few years ago. Our detailed investigations in [Tis99] lead to a structure based description of the network equations. It has been extended for a more general class of networks in [ET00, EFM+03].

We will explain this structure here for networks containing resistors, capacitors, inductors and independent sources. Since we want to present the essential idea we will neglect the case of controlled sources. The treatment of controlled sources requires a lot of technical details which are presented in [ET00].

For the vector j_R of branch currents and the vector v_R of branch voltages of all resistors, we obtain

$$j_R = \tilde{g}\,(v_R, t).$$

Here, the function $\tilde{g}$ represents the composition of the functions g for each resistor. Since we are not interested in the individual functions g anymore, we will use g instead of $\tilde{g}$ in the following, that means $j_R = g\,(v_R, t)$. Analogously, for the branch currents j_C/j_L and the branch voltages v_C/v_L of all capacitors/inductors, we have

$$j_C = \frac{dq_C(v_C,t)}{dt}, \qquad v_L = \frac{d\phi_L(j_L,t)}{dt}.$$

Finally we get

$$v_V = v_s(t) \text{ and } j_I = i_s(t)$$

for the branch voltages v_V of all voltage sources and the branch currents j_I of all current sources.

The essential idea for getting structure information is a numbering of the network branches in such a way that the incidence matrix forms a block matrix with blocks describing the different types of network elements. The blocks are then given as follows:

$$A = (A_R, A_C, A_L, A_V, A_I), \tag{1.8}$$

where the index stands for resistive, capacitive, inductive, voltage source and current source branches, respectively. Replacing the branch currents of all current defining elements in (1.5) by their characteristic equations, and all branch voltages by node voltages using (1.6), we obtain the system

$$\begin{aligned} A_C \frac{dq_C(A_C^T e,t)}{dt} + A_R\, g(A_R^T e,t) + A_L\, j_L + A_V\, j_V &= -A_I\, i_s(t), \\ \frac{d\phi_L(j_L,t)}{dt} - A_L^T e &= 0, \\ A_V^T e &= v_s(t) \end{aligned}$$

with the unknowns $e(t)$, $j_L(t)$, and $j_V(t)$.

Consequently, the classical modified nodal approach results in a differential algebraic equation system of the form

$$A_C C(A_C^T e,t)A_C^T \frac{de}{dt} + A_C \frac{\partial q_C}{\partial t}(A_C^T e,t)$$

$$+ A_{Rg}(A_R^T e,t) + A_L j_L + A_V j_V = -A_I i_s(t), \tag{1.9}$$

$$L(j_L,t)\frac{dj_L}{dt} + \frac{\partial \phi_L}{\partial t}(j_L,t) - A_L^T e = 0, \tag{1.10}$$

$$A_V^T = v_s(t) \tag{1.11}$$

if the functions $q_C(v, t)$ and $\phi_L(j, t)$ are sufficiently smooth and

$$C(v,t) := \frac{\partial q_C}{\partial v}(v,t), \qquad L(j,t) := \frac{\partial \phi_L}{\partial j}(j,t).$$

Denoting the number of nodes by n, the number of inductive branches by n_L and the number of voltage source branches by n_V, the dimension of the system is $n - 1 + n_L + n_V$.

In the charge oriented MNA approach, one introduces additionally charges q and fluxes ϕ as unknown variables. This implies the equivalent system

$$A_C \frac{dq}{dt} + A_R g(A_R^T e,t) + A_L j_L + A_V j_V = -A_I i_s(t), \tag{1.12}$$

$$\frac{d\phi}{dt} - A_L^T e = 0, \tag{1.13}$$

$$A_V^T e = v_s(t) \tag{1.14}$$

$$q = q_C(A_C^T e,t), \tag{1.15}$$

$$\phi = \phi_L(j_L,t). \tag{1.16}$$

At a first glance, the charge oriented system (1.12)-(1.16) seems to be disadvantageous since its dimension is significantly larger than the dimension of system (1.9)-(1.11). However it is, for several reasons, the main approach used in circuit simulators. For a detailed discussion of these reasons we refer to [GF99a, Gun01a]. We only want to mention a few aspects here. Replacement circuit models for semiconductor elements are often formulated by (1.15)-(1.16). This way charge and flux conservation is guaranteed automatically.

Numerical methods applied to system (1.9)-(1.11) require the differentiation of the functions q_C and ϕ_L. Solving the resulting system of nonlinear equations requires the second derivatives of these functions, i.e., we need more smoothness. This plays a significant role for the numerical solution since models are usually not twice differentiable. Additionally, it is

computationally more expensive. Furthermore, charge and flux conservation is only fulfilled approximately.

Finally, the simple form of the equations (1.15) and (1.16) involves only function evaluations for the determination of q and ϕ. Consequently, from the computational point of view, the dimension of the charge oriented system equals the dimension of the classical system. In fact, one has to apply a numerical method to the system

$$A_C \frac{dq_C(A_C^T e,t)}{dt} + A_R g(A_R^T e,t) + A_L j_L + A_V j_V = -A_I i_s(t), \tag{1.17}$$

$$\frac{d\phi_L(j_L,t)}{dt} - A_L^T e = 0, \tag{1.18}$$

$$A_V^T e = v_s(t) \tag{1.19}$$

directly (without the differentiation done in (1.9)-(1.11)). Note, that the system (1.17)-(1.19) represents a DAE with a proper stated leading term [Mar02a, Mar02b] if the matrices *C(v, t) and L(j, t)* are positive definite for all voltages *v*, currents *j* and time points *t*. These conditions seem to be natural from the physical point of view. For two-terminal capacitors, this means that a positive change of the voltage yields a current in forward direction. The current flows in reverse direction if the voltage change is negative.

2. Semiconductor Device

Modeling

Considering the literature, one finds an enormous amount of books and papers dealing with semiconductor device modeling. We refer here only to [Sel84, GG86, GG89, MRS90,Wac91]. These contributions provide a comprehensiv overview of the topic and focus onto the mathematical background.

Semiconductor device models describe the electron transport in the semiconductor. In consideration of the degree of simplification one distinguishes between quantum level transport and semi-classical transport completed with balance equations. The first one yields the Schrödinger equation and the second one leads to the Boltzmann equation. Simplifying the Boltzmann equation further by the method of moments [Sch90], one obtains the so called energy balance equations (considering four moments) or the drift diffusion equations (considering only two moments).

From the practical point of view, the interest in semiconductor device modeling is to replace as much laboratory testing as possible by numerical simulation in order to minimize the costs. Thus, mathematical models requiring expensive simulations are not preferable. For most semiconductor technologies, the drift diffusion equations seem to represent a reasonable compromise between computational efficiency and an accurate description of the underlying physics.

However with the increased miniaturization of semiconductor devices, one comes closer and closer to the limits of validity of the drift diffusion equations. The reason for this is, on one hand, that in ever smaller devices the free carriers can not longer be modeled as a continuum. On the other hand, the drift diffusion equations are derived through a limiting process where the mean free path of a particle tends to zero. Through miniaturization this mean free path becomes larger and larger in comparison to the size of the device. In addition, quantum mechanical effects play a more and more important role in novel device structures.

Nevertheless, the drift diffusion equations remain an important tool since microscopic effects not described by them appear only locally. Thus, the most likely approach will be to use more sophisticated models only locally, and to use the drift diffusion equations in the parts of the device where they are sufficient to describe the physics (usually in the bulk of the semiconductor).

Therefore, we concentrate in Section 2.1 on the drift diffusion equations considered as an important model description for the device part in coupled network and device simulation.

Regarding the coupling between network and device simulation, the type of contacts between the semiconductor and the network has to be taken into account. Usually, they consist of layers of metal, insulator, or other semiconductors. This implies that the boundary conditions for the transport equations in the bulk of the semiconductor have to be formulated in such a

way that the physical processes at the interfaces are described appropriately.
We will discuss them in Section 2.2, but for a more detailed description we refer to [Sch90, Sze81].

2.1 The Drift Diffusion Model for Semiconductor Devices

In this part we describe the drift diffusion model for semiconductor devices including a brief derivation. For a more detailed discussion see e.g. [Sel84, Sze81].

First, we introduce Ω to be a nonempty, open and bounded domain with a regular boundary $\Gamma = \partial\Omega$ in $\boldsymbol{R}^N$ with $1 \leq N \leq 3$ such that $\overline{\Omega}$ describes the range of the semiconductor inclusive its contacts.

2.1.1 Current-Density Equations

The conductivity of semiconductors is strongly connected to the number of its free charge carriers. As charge carriers, we have to consider not only electrons but also holes. If a semiconductor atom lacks one of its valence electrons, then it may attract an electron from another atom. This can be considered as a movement of a hole from one atom to another one. Correspondingly, holes are considered as positive charge carriers, whereas electrons are negative charge carriers.

As the name of the drift-diffusion model already expresses, the current in a semiconductor is mainly driven by drift and diffusion. The drift current is caused by an electric field E that is present due to the existence of free charge carriers.

It is given by

$$q\mu_n n \mathrm{E} \qquad \text{and} \qquad q\mu_p p \mathrm{E}$$

for electrons and holes, respectively. Here, q represents the elementary charge. The variables n and p denote the concentrations of electrons and holes, respectively. The electron and hole mobilities, μ_n and μ_p are bounded, strictly positive functions depending on semiconductor material, doping, temperature and the electric field E.

The dffusion current is caused by a movement of charge carriers that aims to compensate inhomogeneous concentrations. The diffusion current is proportional to the gradient of the charge carrier concentration.
More precisely, we have

$$qD_n \, grad \, n \qquad \text{and} \qquad -qD_p \, grad \, p.$$

D_n and D_p are called carrier diffusivities. In general, they are bounded, strictly positive functions depending on semiconductor material, doping and temperature.

In thermal equilibrium, the mobilities μ_p, μ_n and the diffusivities D_n, D_p related by

$$D_n = \frac{kT}{q}\mu_n \qquad \text{and} \qquad D_p = \frac{kT}{q}\mu_p$$

for non-degenerate semiconductors. Here, *T* denotes the temperature and *k* is the Boltzmann constant. The last equations are called Einstein relations.

Since the electric field E is related to the electrostatic potential V by

$$\mathrm{E} = -grad \, V; \tag{2.1}$$

we obtain for the current densities of electrons and holes

$$J_n = -q\mu_n n grad \, V + qD_n \, grad \, n, \tag{2.2}$$

$$J_p = -q\mu_p p grad \, V - qD_P \, grad \, p. \tag{2.3}$$

Note that one has to consider an additional current, if a magnetic field is applied to the semiconductor. However, this is usually negligible for devices included in integrated circuits.

2.1.2 Continuity Equations

The continuity equations describe particle conservation and are given by

$$-q\partial_t n + \mathrm{div} \, J_n = qR, \tag{2.4}$$

$$q\partial_t p + \mathrm{div} \, J_p = -qR. \tag{2.5}$$

Here, *R* describes the generation/recombination rate. There are several physical mechanisms causing generation and recombination of electrons and holes. The main ones are phonon transitions, photon transitions, Auger (three particle) transitions and impact ionization.

Corresponding to the different mechanisms, different models have been developed in order to describe the generation and recombination process.
The mostly used models are:

Shockley-Read-Hall recombination

$$R_{RSH} = \frac{np - n_i^2}{T_p(n + n_i) + T_n(p + n_i)},$$

Optic recombination

$$R_{OPT} = C^{OPT}(np - n_i^2),$$

Auger recombination

$$R_{AU} = (C_n^{AU} n + C_p^{AU} p)(np - n_i^2);$$

and impact ionization

$$R_{II} = -\alpha_n \frac{\|J_n\|}{q} - \alpha_p \frac{\|J_p\|}{q}.$$

Here, n_i represents the intrinsic charge density. If the semiconductor is in equilibrium, then np is constant and n_i is defined by

$$n_i^2 = np$$

The factors τ_n and τ_p reflect the average lifetimes of electrons and holes, respectively. The constants C^{OPT}, C_p^{AU} and C_n^{AU} have to be determined by experiments. α_n and α_p are the ionization rates for electrons and holes, respectively. They may be approximated by

$$\alpha_n = \alpha_n^{\infty} \cdot \exp\left(-\left(\frac{E_n^{crit}}{E}\right)^{\beta_N}\right),$$

$$\alpha_p = \alpha_p^{\infty} \cdot \exp\left(-\left(\frac{E_n^{crit}}{E}\right)^{\beta_P}\right).$$

with constants α_n, α_p, β_n, β_p, E_n^{crit}, E_p^{crit}.

If all effects are present, then one simply adds up all rates such that

$$R = R_{RSH} + R_{OPT} + R_{AU} + R_{II.}$$

2.1.3 Poisson Equation

The transport equations (2.2)-(2.5) constitute equations for the concentrations of electrons and holes (n and p) as well as the densities of electron and hole current (J_n and J_p). Additionally, the existence of these charge carriers causes an electrical field. In order to obtain a self-consistent formulation, the transport equations have to be completed by an equation that determines this electrical field. This is given by the third Maxwell equation, which relates the electric field to the electric charges.

It reads

$$\text{div D} = e \tag{2.6}$$

where D is the electric displacement and e is the charge density. The electric charge is the source of the electric displacement.

The electric field E is related to D by

$$\text{D} = \varepsilon \text{ E} \tag{2.7}$$

with the permittivity constant ε of the medium if the medium is homogeneous.

Inserting (2.7) and (2.1) into (2.6), we get

$$\text{div } (-\varepsilon \text{ grad V}) = e$$

In a semiconductor, the local charge is composed of electrons, holes, donor atoms and acceptor atoms. Thus, the charge *e* is given by

$$e = q(p - n + N_D^+ - N_A^-),$$

where q is the elementary charge, N_D^+ the donor concentration and N_A^- the acceptor concentration.

Finally, we arrive at the Poisson equation

$$\text{div}\,(-\varepsilon gradV) = q(p - n + N_D^+ - N_A^-). \tag{2.8}$$

The impurity atoms are assumed to be fixed in the semiconductor, i.e. N_D^+ and N_A^+ are independent of time and, thus, given as functions of the position. This assumption is justified if the impurity concentrations are sufficiently small. But it holds no longer true in case of high power transistors and high power diodes.

2.1.4 Complete Drift-Diffusion Model

Summarizing the model equations (2.2), (2.3), (2.4), (2.5) and (2.8), we get the drift-diffusion model equations

$$\text{div}\,(\varepsilon gradV) = q(n - p - N), \tag{2.9}$$

$$-\partial_t n + \frac{1}{q}\,\text{div}\,J_n = R, \tag{2.10}$$

$$\partial_t p + \frac{1}{q}\,\text{div}\,J_p = -R \tag{2.11}$$

$$J_n = q(D_n gradn - \mu_n n gradV), \tag{2.12}$$

$$j_p = q(-D_p gradp - \mu_p p gradV). \tag{2.13}$$

The unknowns are the electrostatic potential V, the electron and hole concentrations, n and p, as well as the current densities of electrons and holes, J_n and J_p. Note, that J_n and J_p are given by (2.12)-(2.13). Thus, inserting (2.12) and (2.13) into (2.10) and (2.11) yields to a system in the primary variables V, n and p only.

The doping concentration $N := N_D^+ - N_A^-$ represents a given function depending only on the position variable x. The sizes ε and q are constants. The mobilities μ_n and μ_p as well as the diffusivities D_n and D_p are bounded, strictly positive functions. They may depend on position x (due to dependency on doping) and on the gradient of the potential grad V (due to dependency on the electric field E. Finally, the generation/recombination rate R may depend on n, p, J_n, J_p and grad V corresponding to the applied model.

The system (2.9)-(2.13) represents a system of five coupled partial differential equations. The Poisson equation (2.9) is of elliptic type. Regarding the current density equations (2.12) and (2.13), the continuity equations (2.10) and (2.11) are of parabolic type.

Note that we assume a constant temperature. It is justified for applications with low performance devices. In case of high performance devices, one has to consider the temperature T as a variable. The drift diffusion equations have to be completed by an energy balance equation (see e.g. [Wac95, Jun01, AGH02]). It is a future task to combine such energy models with the network equations.

2.2 The Boundary Conditions

Semiconductors have essentially three different types of adjoining materials. The contacts between the network and the semiconductor are usually layers of metal. The second kind of bounding materials are insulators (e.g. oxide). Finally, they may be bounded by other semiconductors. Such semiconductor-semiconductor interfaces are called heterojunction. Here, we are interested in devices with one semi-conducting material only and we do not consider heterojunction.

The following sections are devoted to a brief explanation of the boundary conditions connected with different types of interfaces. For a more detailed description, the books [Sze81, Sel84, Sch90] are recommended.

2.2.1 Metal-Semiconductor Contacts

Many semiconductor devices have low resistance or rectifying contacts. The corresponding models are called Ohmic and Schottky contacts, respectively. They have been established in many device simulation programs and we want to consider such contacts here. Note that, in [Sch90], a new model was presented for non-ideal contacts including tunneling effects (regarded in Ohmic contact models) as well as thermionic emissions (regarded in Schottky contact models) and generalizing both types of metal contact models. This results, in general, in mixed boundary conditions which are coupled in a highly nonlinear manner.

Ohmic Contacts

Ohmic contacts are characterized by a high doping of the semiconductor. This implies a large band bending and a very thin barrier at the metalsemiconductor interface. In this case, tunneling of electrons is the dominant transport mechanism. It leads to high current densities at low voltage dropsand, consequently, to a low resistance of the contact.

Since tunneling is not included in the drift diffusion equations describing electron transport in the semiconductor volume, one should place the actual boundary for the simulation domain at the end of the tunneling region. At high doping concentrations, the tunneling length comprises the total depletion region, and the boundary is placed at the depletion layer edge. Consequently, we have charge neutrality at the actual boundary that means

$$n - p - N = 0.$$

Furthermore, the electrostatic potential at the boundary is given by

$$V = V_{ap} + V_{bi}, \tag{2.14}$$

where V_{ap} is the applied voltage and V_{bi} is the so called built-in potential of the semiconductor. The built-in potential depends on semiconductor material, doping concentration, and temperature.

For very high doping (ideal ohmic contact), the resistance tends to zero which implies [Sch90]

$$np = n_i^2$$

with the intrinsic concentration n_i depending on material and temperature.

This leads to Dirichlet boundary conditions for the electron and hole concentrations

$$n = \frac{1}{2}\left(\sqrt{N^2 + 4n_i^2} + N\right), \tag{2.15}$$

$$n = \frac{1}{2}\left(\sqrt{N^2 + 4n_i^2} - N\right). \tag{2.16}$$

Schottky Contacts

Schottky contacts have a rectifying behavior. This is caused by low semiconductor doping which leads to a slow weak band bending and a thick barrier at the interface. Therefore, thermionic emission of electrons is the dominant transport mechanism here.

In this case, the carriers crossing the interface have to overcome the barrier height ϕ_B arising from the band bending. This implies

$$V = V_{ap} + V_{bi} + V_B \tag{2.17}$$

where V_{ap} , V_{bi} are as in (2.14) and

$$qV_B = \phi_B$$

In zero order approximation, the barrier height ϕ_B is a constant, dependent on the combination of the materials.

Denoting γ as the unit outer normal vector on the contact, the boundary condition for the continuity equations read as

$$J_n \cdot \gamma = -qv_n(n - n_0), \tag{2.18}$$

$$J_p \cdot \gamma = qv_p(p - p_0), \tag{2.19}$$

where v_n and v_p are the recombination velocities depending on material and temperature. The quantities n_0 and p_0 are the quasi-equilibrium concentrations. They depend on barrier height and temperature.

Note that we have Dirichlet boundary conditions for the potential *V* and, consequently, mixed boundary conditions for the concentrations *n* and *p*.

2.2.2 Semiconductor-Insulator Interface

As a consequence of Maxwell's third law (2.6), we obtain as boundary condition for the Poisson equation

$$\varepsilon \frac{\partial V}{\partial \gamma} - \varepsilon i \frac{\partial V_i}{d\gamma} = \sigma,$$

where ε and ε_i are the dielectric constants of the semiconductor and the insulator, respectively, and σ is the surface charge at the interface.

Regarding the existence of surface recombination, we obtain

$$J_n \cdot \gamma = -qR_{surf} \quad \text{and} \quad J_p \cdot \gamma = qR_{surf} \tag{2.20}$$

with

$$R_{surf} = \frac{np - n_1^2}{\frac{1}{s_p}(n + n_1) + \frac{1}{s_n}(p + p_1)}$$

for the continuity equations. Here, *n* and *p* denote the electron and hole concentration at the contact, respectively. The recombination velocities s_n and s_p as well as the concentrations n_1, p_1, and the intrinsic carrier concentration n_i are parameters depending on the material of the semiconductor and the effective doping. By γ we denote the outer unit normal vector. If surface recombination can be neglected, then we arrive at

$$J_n \cdot \gamma = 0, \qquad J_P \cdot \gamma = 0. \tag{2.21}$$

Summary

The further miniaturization of optic and electronic components demands a refined network analysis describing certain semiconductor elements by contributed models. Using the instationary drift-diffusion model, the device equations represent a system of elliptic and parabolic differential equations. The network is described by a differential-algebraic system. Both systems are mutually coupled via boundary conditions and integral relations.

The coupled system can be analyzed as an abstract differential algebraic system in infinite-dimensional Hilbert spaces. For the one-dimensional case (with respect to space), network topological criteria for the index of the coupled system are described. Furthermore it is shown that the index does not exceed 2. This corresponds exactly to the results for networks with compact models instead of distributed models. It is still an open question whether the results remain true for a higher-dimensional case.

Appendix

1. Symbols

$\boldsymbol{R}$	set of real numbers
C	capacitance
D	diffusivity
D	electric displacement
J	current density
L	inductance
N	doping concentration
N_D^+	donor concentration
N_{A-}	acceptor concentration
R	1. resistance (network element) 2. generation/recombination rate (drift-diffusion model)
T	1. temperature 2. end of a time interval
V	electrostatic potential
V_{bi}	built-in potential
e	nodal potential
j	current
n	electron density
n_i	intrinsic density
p	hole density
q	charge
t	time
x	position variable
Ω	domain
ε	permittivity
μ	-permeability -mobility
γ	outer unit normal vector
σ	surface charge
ϕ	flux
ϕ_B	barrier height

2. Physical constants

Boltzmann constant	k	$1.38066 \cdot 10^{-23}$ J/K

Elementary charge	q	$1.60218 \cdot 10^{-19}$ C
Thermal voltage at 300 K	$\frac{kT}{q}$	0.0259 V
Permeability in vacuum	μ_0	$1.25663 \cdot 10^{-8}$ H/cm
Permittivity in vacuum	ε_0	$8.85418 \cdot 10^{-14}$ F/cm

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