

TWO DIMENSIONAL MOS-TRANSISTOR MODELING

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ABSTRACT - The advent of Very Large Scale Integration has been an incentive to concentrate persistently on device modeling. The fundamental properties which represent the basis for all device modeling activities are summarized. The sensible use of physical and technological parameters is discussed and the most important physical phenomena which are required to be taken into account are scrutinized. The assumptions necessary for finding a reasonable trade-off between efficiency and effort for a model synthesis are recollected. Methods to bypass limitations induced by these assumptions are pin-pointed. Simple and easy to use formulae for the physical parameters of major importance are presented. The necessity of a careful parameter-selection, based on physical information, is shown. Some glimpses on the numerical solution of the semiconductor equations are given. The discretisation of the partial differential equations with finite differences is outlined. Linearisation methods and algorithms for the solution of large sparse linear systems are sketched. Results of our two dimensional MOSFET model - MINIMOS - are discussed with typical applications. Much emphasis is laid on the didactic potential of such a complex high order model.

1. INTRODUCTION

The first integrated circuits which just contained a few devices became commercially available in the early 1960's. Since that time an evolution has taken place so that today the manufacture of integrated circuits with over 400.000 transistors per single chip is possible. This advent of the so-called Very-Large-Scale-Integration (VLSI) certainly revealed the need of a better understanding of the basic device physics. The miniaturization of the single transistor, which is one of the inseparable preconditions of VLSI, brought about a collapse of the classical device models, because totally new phenomena emerged and even dominated the device behaviour. One consequence of this evidence led to an unimaginable number of suggestions of how to modify the classical models to incorporate various of the new phenomena. Additionally new activities have been initiated to explore the physical principles which make a device operationable. The number of scientific publications which utilize the terms "device analysis", "device simulation" and "device modeling" (c.f./3/, /41/, /59/) grew in an incredible manner.

Introduction

At first it seems necessary to clarify these frequently used terms to facilitate the intelligibility of the subsequent chapters. Consulting a dictionary one will find among many more the following interpretations:

Analysis

- separation of a whole into its component parts, possibly with comment and judgement
- examination of a complex, its elements, and their relations in order to learn about

Simulation

- imitative representation of the functioning of one system or process by means of the functioning of another
- examination of a problem not subject to experimentation

Modeling

- to produce a representation or simulation of a problem or process
- to make a description or analogy used to help visualize something that cannot be directly observed

Therefore, analysis is at least intended to mean "Exact Analysis" and simulation must inferentially mean "Approximate Simulation" using only to some extent physically motivated models. Modeling is necessary for analysis and simulation, but with a different objective. However, any model should at least reflect the underlying physics.

The characteristic feature of early modeling was the separation of the interior of the device into different regions, the treatment of which could be simplified by various assumptions like special doping profiles, complete depletion and quasineutrality. These separately treated regions were simply connected to produce the overall solution. If analytic results are intended, any other approach is prohibitive. Fully numerical modeling based on partial differential equations /117/ which describe all different regions of semiconductor devices in one unified manner was first suggested by Gummel /52/ for the one dimensional bipolar transistor. This approach was further developed and applied to pn-junction theory by De Mari /27/, /28/ and to IMPATT diodes by Scharfetter and Gummel /93/.

A two dimensional numerical analysis of a semiconductor device was carried out the first time by Kennedy and O'Brien /62/ who investigated the junction field effect transistor. Since then two dimensional modeling has been applied to fairly all important semiconductor devices. There are so many papers of excellent repute that it would be unfair to cite only a few. Recently also the first results on three dimensional device modeling have been published. The time dependence has been investigated by e.g. /67/, /78/ and models for three space dimensions have been announced by e.g. /18/, /125/, /126/.

In spite of all these important and successful activities, the need for economic and highly user oriented computer programs became more and more apparent in the field of device modeling. Especially for MOS devices which have evolved to an incredible

standard, modeling has become inherently important because current flow controlled by a perpendicular field is an intrinsically two dimensional problem. One such program which has been applied successfully in many laboratories is called CADDET /113/. We have also tried to bridge that gap and developed MINIMOS /95/ for the two dimensional static analysis of planar MOS transistors.

In the next chapter the fundamental properties which are the basis for all device models are summarized. Much effort is laid on the documentation of various physical effects which possibly have to be taken into account when synthesizing a device model for some special application. The assumptions which are usually made to ease modeling are presented and their validity is, at least qualitatively, discussed. Simple and easy to use formulae are presented which allow phenomenological simulation of the most important physical parameters with which the modelist has to deal. In the third chapter analytical results of investigations about the semiconductor equations are presented. In the fourth chapter the numerical solution of the basic semiconductor equations is discussed. The two main methods for the solution of the differential equations (i.e. finite differences and finite elements) are briefly compared. A few linearisation schemes are presented and judged for adequacy in terms of effort and efficiency. Classical algorithms for the solution of the sparse algebraic systems which are obtained by linearisation of the discrete semiconductor equations are explained in the fifth chapter. The sixth chapter entirely deals with applications of MINIMOS.

Throughout this paper all constants and quantities are given in the following units, if not specified otherwise: lengths in cm, times in s, temperature in K, voltages in V, currents in A. The units are often omitted to gain transparency in the formulae.

2. SOME FUNDAMENTAL PROPERTIES

To accurately analyze an arbitrary semiconductor structure which is intended as a self-contained device under various operating conditions, a mathematical model has to be given. The equations which form this mathematical model are often called the fundamental semiconductor equations; these will be discussed in the first section of this chapter.

The second section will deal with assumptions which have to be made for special applications additionally to those which have already been used in the derivation of the equations and which are beyond the scope of this presentation. Furthermore, all quantities which are involved in the basic equations will be outlined more or less qualitatively. It will become apparent that the fundamental equations employ a set of physical and technological parameters. An in-depth analysis of all these parameters is far from being finished at the moment - or the results of such an analysis are of overwhelming complexity - because of inherent methodical difficulties.

The third section will deal with additional assumptions which can be made to ease and speed up models for MOS-devices.

Some Fundamental Properties

The topic of the fourth section of this chapter is the description of some suggestions for a heuristic simulation of the most important parameters (i.e. mobility, generation/recombination) based, as it were, on physical principles.

2.1 The Fundamental Semiconductor Equations

The most familiar model of carrier transport in a semiconductor device has been proposed by Van Roosbroeck /117/. It consists of Poisson's equation (2.1), the current continuity equations for electrons (2.2) and holes (2.3) and the current relations for electrons (2.4) and holes (2.5)

$$\text{div } \epsilon \text{ grad } \psi = -q \cdot (p - n + C) \quad (2.1)$$

$$\text{div } \vec{J}_n = -q \cdot (G - R) \quad (2.2)$$

$$\text{div } \vec{J}_p = q \cdot (G - R) \quad (2.3)$$

$$\vec{J}_n = -q \cdot (\mu_n \cdot n \cdot \text{grad } \psi - D_n \cdot \text{grad } n) \quad (2.4)$$

$$\vec{J}_p = -q \cdot (\mu_p \cdot p \cdot \text{grad } \psi + D_p \cdot \text{grad } p) \quad (2.5)$$

These relations form a system of coupled partial differential equations. Poisson's equation, which is one of Maxwell's laws, describes the charge distribution in the interior of a semiconductor device. The balance of sinks and sources for electron- and hole currents is characterized by the continuity equations. The current relations describe the absolute value, direction and orientation of electron- and hole currents. The continuity equations and the current relations can be derived from Boltzmann's equation by not at all trivial means. The ideas behind these considerations cannot be presented here due to limited space. The interested reader should refer to /117/ and its secondary literature or text books on semiconductor physics e.g. /12/, /56/, /94/, /101/.

However, it is of prime importance to note that the equations (2.4) and (2.5) do not characterize effects which are caused by degenerate semiconductors (e.g. heavy doping). /68/, /115/, /119/ discuss some modifications of the current relations, which partially take into account the consequences introduced by degenerate semiconductors (e.g. invalidity of Boltzmann's statistics, bandgap narrowing). These modifications are not at all simple and lead to problems especially for the formulation of boundary conditions /83/, /118/. In case of modeling MOS devices, degeneracy is, owing to the relatively low doping in the channel region, practically irrelevant. For modern bipolar devices, though, bearing in mind shallow and extraordinarily heavily doped emitters, it is an absolute necessity to account for local degeneracy of the semiconductor.

Just as further examples (2.4) and (2.5) do not describe velocity overshoot phenomena which become apparent at feature

lengths of $0.1\mu\text{m}$ for silicon and $1\mu\text{m}$ for gallium-arsenide /46/; and certainly no effects which are due to ballistic transport, the existence of which is still questionable /55/, are included. The latter start to become important for feature sizes below $0.01\mu\text{m}$ for silicon and $0.1\mu\text{m}$ for gallium-arsenide /45/. Considering the state of the art of device miniaturization, neither effect has to bother the modelists of silicon devices. For gallium-arsenide devices new ideas are mandatory for the near future /46/, /80/, /79/.

2.2 Assumptions and Discussion of Parameters

It is imperative to discuss the parameters of the semiconductor equations to get some insight into the complexity of that mathematical model and the difficulty of a more or less rigorous solution.

The permittivity ϵ in Poisson's equation in the most general case is a rank two tensor. Because all common semiconductor materials grow in cubic crystal structure and because silicon-dioxide is amorphous no anisotropy exists and the permittivity can be treated as a scalar quantity. Furthermore, one can safely assume that the permittivity is homogenous with sufficient accuracy for even degenerate semiconductors.

The electrically active net doping concentration C in Poisson's equation is the most important technological parameter. To obtain this quantity by mathematical analysis /37/ is at least as cumbersome as to accurately analyze some semiconductor device, because the physics of the technological processes which determine the doping concentration still lacks basic understanding. The need of modeling in this area is drastically increasing in view of VLSI devices. One-dimensional process modeling is fairly well established nowadays, but two-dimensional simulation is just appearing /37/, /112/. Some glimpses of modeling doping profiles with handy analytical expressions are given in e.g. /97/. One assumption which is usually made with satisfactory success (at room temperature) is the total ionization of all dopants (2.6).

$$C = N_D - N_A = N_D^+ - N_A^- \quad (2.6)$$

As long as the Fermi level is separated several thermal voltages from the impurity level, this assumption holds quite nicely. For modern bipolar transistors, however, it certainly becomes questionable for the emitter region (degenerate material).

The electron density n and the hole density p are commonly assumed to obey Boltzmann's statistics (2.7).

$$n = n_i \cdot e^{(\psi - \psi_n)/U_T} \quad p = n_i \cdot e^{(\psi_p - \psi)/U_T} \quad (2.7)$$

This assumption principally neglects degeneracy; but moderate degeneracy can be included /40/ by introducing an effective, doping dependent intrinsic number (2.8).

$$n_i = n_i(T, N) \quad (2.8)$$

$$n_i(T, N) = n_i(T) \cdot e^{52.7 \cdot (\ln(N/10^{17})) + \sqrt{(\ln(N/10^{17}))^2 + 0.5}} / T$$

$$n_i(T) = 3.88 \cdot 10^{16} \cdot T^{1.5} \cdot e^{-7000/T}$$

$$N = N_D + N_A$$

The temperature dependence of the intrinsic number is based on the influence of the effective carrier masses and the bandgap. More elaborate formulae for these effects which might be imperative for low temperature applications can be found in /47/. The formula for bandgap narrowing in (2.8) was first suggested by Slotboom /99/. For a doping concentration of $1.3 \cdot 10^{17} \text{ cm}^{-3}$ the intrinsic number has already increased by twenty percent.

The mobility of electrons μ_n and holes μ_p is in principle a rank two tensor function of many arguments. One ends up with a so called "mobility" after averaging and combining various physical mechanisms which are still not analyzed thoroughly enough to be modeled satisfactorily /57/.

Another assumption which is unfortunately not at all free of doubts is the validity of the Einstein-Nernst relations (2.9).

$$D_n = \mu_n \cdot U_T \quad D_p = \mu_p \cdot U_T \quad (2.9)$$

Some guidelines on how to extend these relations for degenerate material are given in e.g. /6/. It is important to remember that the current relations (2.4) and (2.5) do not differentiate between lattice temperature and electron temperature. Therefore, if one has to deal with hot electrons in a precise manner, the current relations have to be updated; in particular the mathematical structure of the diffusion current term has to be refined.

The last parameter which remains to be dealt with for a qualitative characterization is the net generation/recombination rate (G-R) in (2.2) and (2.3). This quantity has to describe a number of physical processes which are responsible for generation/recombination of electron-hole pairs. These processes and their interactions are also not analyzed to a satisfactory level so that one has to use heuristic expressions for a model which is at least plausible in the underlying physics. Some suggestions for these formulae will be given in section 2.4.

2.3 Additional Assumptions for MOS-Models

The fundamental semiconductor equations describe the internal behavior of any semiconductor device. However, for certain devices these equations may be simplified without significant loss of accuracy. As the MOSFET is a minority carrier device, the current is given mainly by the continuity equation of one carrier type. If avalanche is neglected, only little carrier generation occurs in the MOSFET.

Therefore, the eqs. (2.2)-(2.3) may be rewritten as

$$\text{div } \vec{J}_n = 0 \quad (2.10)$$

$$\vec{J}_p = 0 \quad (2.11)$$

for the n-channel device and

$$\text{div } \vec{J}_p = 0 \quad (2.12)$$

$$\vec{J}_n = 0 \quad (2.13)$$

for the p-channel device. However, it should be kept in mind that these assumptions are valid only if the avalanche effect is negligible (see chapter 6).

The channel width of a MOSFET is usually (often) much larger than the depletion widths. As a consequence the partial derivatives in that direction can be neglected and the semiconductor equations reduce to two dimensions. The neglect of the derivative of the potential in source-drain direction is a proper assumption only for long-channel devices. The so called "gradual-channel approximation" was the basis of a lot of one-dimensional models. These models fail to predict accurately the behavior of modern miniaturized devices.

If the avalanche effect should be included, the assumptions (2.10)-(2.13) are no longer valid and both continuity equations have to be solved with inhomogeneity terms. As a consequence, the ionization-generated majority carriers (holes for an n-channel MOSFET) flow to the substrate as they are repelled from the source and drain junctions. There are several options to account for the voltage drop which is induced by the substrate current: (a) a truly three-dimensional analysis; (b) extension of the simulation over the entire bulk area; (c) extension of the two-dimensional simulation over the depletion region and using an (effective) bulk resistor (Fig. 2.1). If one wants to avoid excessive computing time associated with (a), option (c) is to be preferred because it allows inclusion of current spread into the third dimension and, also, consumes less computing time than (b). In that way the voltage drop across the parasitic bulk resistor simulates a more positive bulk bias and, if large enough, is able to forward-bias the parasitic bipolar npn transistor (according to source, bulk, and drain). This causes a larger drain current and facilitates the breakdown which then will occur at smaller drain voltages [91].

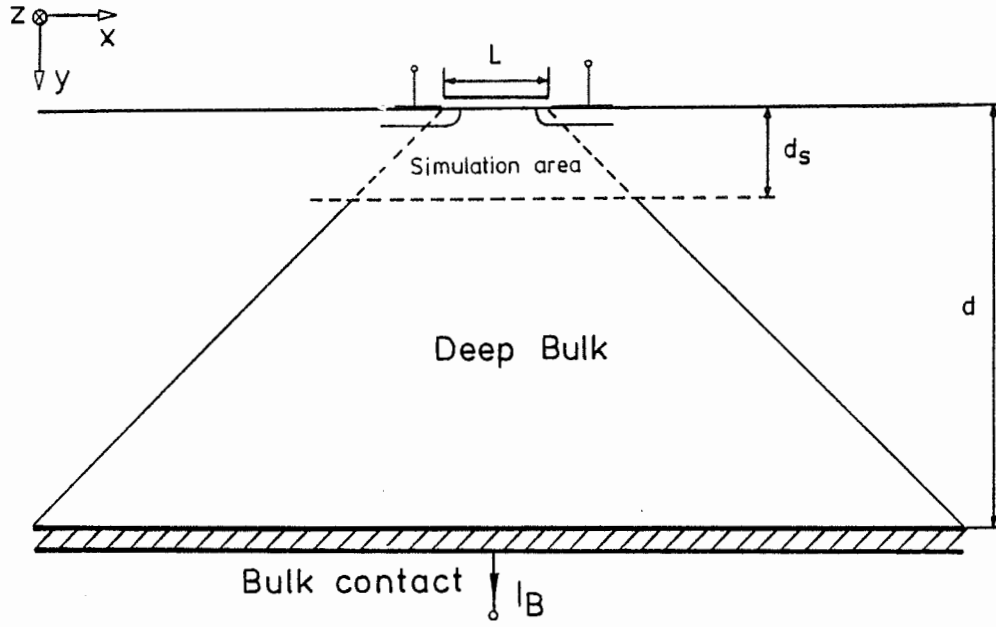


Fig. 2.1: Current flow in deep bulk

In the following we should like to suggest an easy method to estimate the value of the bulk resistor. It is assumed that the current spreads at an angle of 45 degrees /10/ into both directions perpendicular to its flow (x- and z- direction in Fig. 2.1). This assumption is arbitrary but not implausible, and, furthermore, if we neglect any diffusion current, we obtain the following expression for the electric field in the deep substrate.

$$\frac{d\psi}{dy} = \frac{I_B}{KA} = \frac{I_B}{K(L+2y)(W+2y)} \quad (2.14)$$

with K standing for the conductivity of the substrate and A the area of the current flow. L and W are channel length and channel width, respectively. Integrating this equation along y from the end of the simulation area d_s to the bulk contact we obtain

$$R_{Bulk} = \frac{\int_{d_s}^d \frac{d\psi}{dy} dy}{I_B} = \frac{1}{2K(W-L)} \left(\ln\left(\frac{L+2d}{L+2d_s}\right) - \ln\left(\frac{W+2d}{W+2d_s}\right) \right) \quad (2.15)$$

For $L=W$ this equation simplifies to

$$R_{Bulk} = \frac{d-d_s}{K(L+2d)(L+2d_s)} \quad (2.16)$$

This calculation is fairly crude compared to the elaborate solution of the basic equations. However, any more precise calculation would be very complicated and the present method is sufficient to investigate the influence of the parasitic bulk resistance at least qualitatively.

2.4 Models of Physical Parameters

a) Formulae for Mobility Modeling

The mobility of carriers is, as already mentioned, an eminently complex quantity. Additionally it is an important parameter, because all errors in the mobility lead to a proportional error of the current through the multiplicative dependence. This is certainly one of the primary results any model should yield reliably. The formulae which will be given below describe phenomenologically the mobility in silicon; the subscripts n and p denote electrons and holes, respectively.

To model mobility at least plausibly, several scattering mechanisms have to be taken into account, the basis of which is lattice scattering. This effect can be described by a simple power law /57/, /94/ in dependence of temperature (2.17).

$$\mu_L(T) = A \cdot T^{-g} \quad (\text{cm}^2/\text{Vs}) \quad (2.17)$$

$$\begin{aligned} A_n &= 7.12 \cdot 10^8 & A_p &= 1.35 \cdot 10^8 \\ g_n &= 2.3 & g_p &= 2.2 \end{aligned}$$

The pure lattice mobility is reduced through the scattering processes at ionized impurities. (2.18) is a well established formula which models temperature dependent ionized impurity scattering /17/ and electron-hole scattering /40/. The latter is extremely important in low doped regions where high injection takes place.

$$\mu_{LI}(N, T) = \mu_L(T) \cdot a + \mu_{\min} \cdot (1 - a) \quad (\text{cm}^2/\text{Vs}) \quad (2.18)$$

$$a = \frac{1}{1 + (T/300)^b \cdot (N/N_0)^c}$$

$$N = 0.67 \cdot (N_D^+ + N_A^-) + 0.33 \cdot (n + p)$$

$$\begin{aligned} \mu_{\min n} &= 55.24 & \mu_{\min p} &= 49.7 \\ b_n &= -3.8 & b_p &= -3.7 \\ c_n &= 0.73 & c_p &= 0.7 \\ N_{0n} &= 1.072 \cdot 10^{17} & N_{0p} &= 1.606 \cdot 10^{17} \end{aligned}$$

Similar expressions which have been partly deduced from measurement and/or theory have been presented in /5/, /29/, /33/, /65/, /93/.

To properly simulate the mobility in MOS transistors, one has to deal with surface roughness and field dependent surface scattering. /22/, /88/, /105/ presented interesting measured results on inversion layer mobility; /111/, /110/ gave some excellent ideas on how to treat theoretically these and other scattering mechanisms; /124/ suggested a heuristic formula for field dependent surface scattering which is applicable for two-dimensional simulations, but whose adequacy is questioned in /111/. However, we have developed (2.19) which models phenomenologically with best fit to measurement surface roughness as well as field dependent surface scattering /96/.

$$\mu_{LIS}(y, E_p, E_t, N, T) = \mu_{LI}(N, T) \cdot \frac{y + y_r}{y + b \cdot y_r} \quad (\text{cm}^2/\text{Vs}) \quad (2.19)$$

$$y_r = y_0 / (1 + E_p / E_{p0})$$

$$b = 2 + E_t / E_{t0}$$

$$E_p = \max(0, (E_x \cdot J_x + E_y \cdot J_y) / (J_x^2 + J_y^2)^{1/2})$$

$$E_t = \max(0, (E_x \cdot J_y - E_y \cdot J_x) \cdot J_x / (J_x^2 + J_y^2))$$

$$y_{0n} = 5 \cdot 10^{-7} \quad y_{0p} = 4 \cdot 10^{-7}$$

$$E_{p0n} = 10^4 \quad E_{p0p} = 8 \cdot 10^3$$

$$E_{t0n} = 1.8 \cdot 10^5 \quad E_{t0p} = 3.8 \cdot 10^5$$

In regions with a high electric field component parallel to current flow, drift velocity saturation has to be taken into account. (2.20) combines, also phenomenologically, this physical effect and the lattice-impurity-surface mobility using a Mathiessen-type rule with a weakly temperature dependent saturation velocity /16/, /57/, /58/.

$$\mu_{tot}(y, E_p, E_t, N, T) = (\mu_{LIS}(\dots))^{\theta} + (v_s / E_p)^{\theta} \quad (2.20)$$

$$v_{sn} = 1.53 \cdot 10^9 \cdot T^{-0.87}$$

$$v_{sp} = 1.62 \cdot 10^8 \cdot T^{-0.52}$$

$$\theta_n = -2$$

$$\theta_p = -1$$

b) Formulae for Modeling Generation/Recombination

To simulate satisfactorily transfer phenomena of majority carrier current and minority carrier current in just a simple diode, it is an absolute necessity to model carrier recombination and generation as carefully as possible. (2.21) represents the well known Shockley-Read-Hall term for modeling thermal generation/recombination. The carrier lifetimes can be simulated as being doping dependent /25/, /75/.

$$(G - R)_{th} = \frac{n_i^2 - p \cdot n}{\tau_n(p + p_1) + \tau_p(n + n_1)} \quad (1/\text{cm}^3\text{s}) \quad (2.21)$$

$$\tau_n = 3.95 \cdot 10^{-5} / (1 + N / 7.1 \cdot 10^{15}) \quad \tau_p = 3.52 \cdot 10^{-5} / (1 + N / 7.1 \cdot 10^{15})$$

Surface generation/recombination /53/ can be treated in a fairly similar manner by (2.22).

$$(G - R)_s = \frac{n_i^2 - p \cdot n}{(p + p_1)/s_n + (n + n_1)/s_p} \cdot \delta(y) \quad (1/\text{cm}^3\text{s}) \quad (2.22)$$

$\delta(y)$: Dirac-Delta function, $y=0$ denotes an interface

$$s_n = 100$$

$$s_p = 100$$

Impact ionization can be modeled by an exponentially field dependent generation term /20/, /21/. The constants in (2.23) are essentially taken from /116/.

$$G_a = \frac{|\vec{J}_n|}{q} \cdot A_n \cdot \exp \left(- \frac{B_n |\vec{J}_n|}{\vec{E} \cdot \vec{J}_n} \right) + \frac{|\vec{J}_p|}{q} \cdot A_p \cdot \exp \left(- \frac{B_p |\vec{J}_p|}{\vec{E} \cdot \vec{J}_p} \right) \quad (1/\text{cm}^3\text{s}) \quad (2.23)$$

$$\begin{aligned} A_n &= 7 \cdot 10^5 & A_p &= 1.588 \cdot 10^6 \\ B_n &= 1.23 \cdot 10^6 & B_p &= 2.036 \cdot 10^6 \end{aligned}$$

It should be noted that this form of simulating avalanche is relatively crude compared to more exact considerations, but the underlying physical principles are so complex that a trade-off in accuracy and complexity leads to that type of formula. The ionization probabilities $\alpha_{n,p}$ for silicon as a function of the electric field have been measured by various authors: Mc Kay /73/, /74/, Miller /76/, Chynoweth /20/, /21/, Lee /63/, Moll /81/, /82/, Ogawa /84/, Van Overstraeten /116/, Grant /48/, Dalal /26/. Their results are summarized in Fig. 2.2 for electrons and in Fig. 2.3 for holes. Additionally, the measured results are compared to theoretical results of Baraff /9/ (material constants from Sze /106/, /107/). Also drawn in Fig. 2.2 and Fig. 2.3 are theoretical limits published by Okuto /85/, /86/, which imply that all the energy the carriers can obtain from the electric field is used to generate additional carriers. Furthermore, the energy loss per single ionization has been taken to be 1.6eV for electrons and 1.8eV for holes (see also /54/). A more concise treatment of the ionization probabilities has been undertaken theoretically by /4/, /19/, /64/, /98/, /108/, /109/, /111/, /114/, /123/ and experimentally by /89/, /102/.

To analyze high injection conditions, Auger recombination has to be included as an antagonism to avalanche generation. Already the use of a simple formula like (2.24) in general gives satisfactory results /23/, /25/, /38/, /40/.

$$(G - R)_{\text{Aug}} = (n_i^2 - p \cdot n) (C_n \cdot n + C_p \cdot p) \quad (1/\text{cm}^3\text{s}) \quad (2.24)$$

$$C_n = 2.8 \cdot 10^{-31} \quad C_p = 9.9 \cdot 10^{-32}$$

Finally, all generation/recombination phenomena have to be combined to one total quantity. The usual way to do so is to simply sum up all terms (2.25). However, that means that no interaction of the different phenomena does exist.

$$(G-R)_{\text{tot}} = (G-R)_{\text{th}} + (G-R)_s + (G-R)_{\text{Aug}} + G_a \quad (2.25)$$

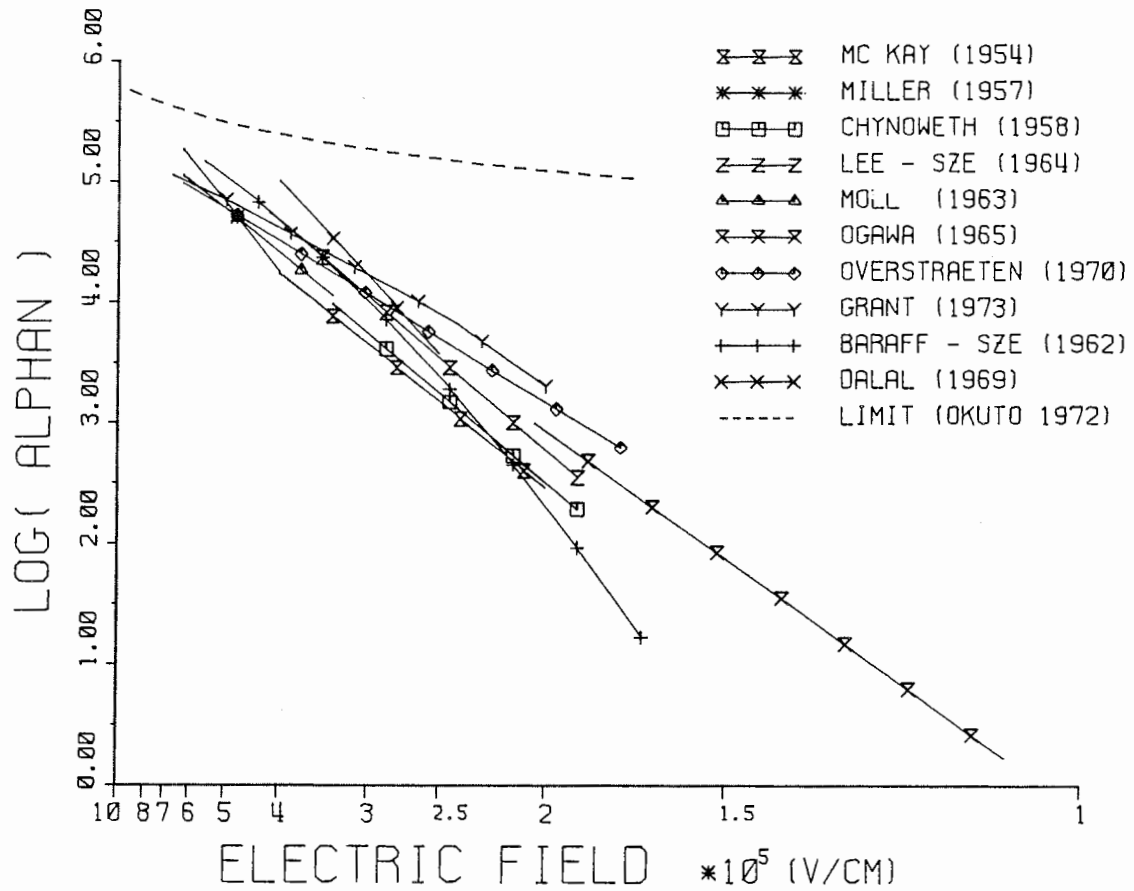


Fig. 2.2: Ionization probabilities for electrons

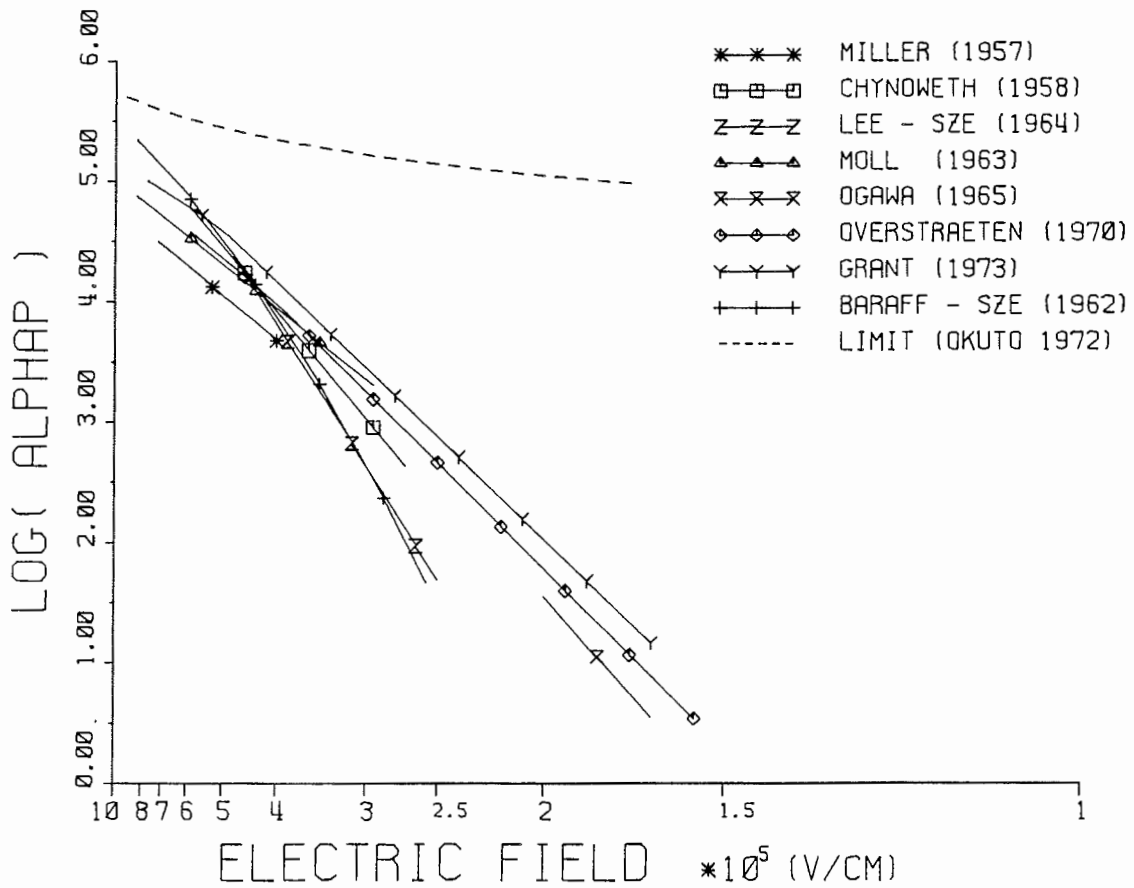


Fig. 2.3: Ionization probabilities for holes

3. ANALYTICAL INVESTIGATIONS ABOUT THE SEMICONDUCTOR EQUATIONS

In this chapter we present some of the existing analytical results for the fundamental semiconductor equations. Particularly, we are interested in the possible boundary conditions, dependent variables and an appropriate scaling approach. We shall discuss the structure of solutions to the semiconductor equations, because these results are of importance in both the theoretical and practical context, since - as we shall see in the next chapter - the knowledge of the structure and smoothness properties of solutions is indeed essential for the development of a numerical solution method.

3.1 Domain and Boundary Conditions

Most of the existing programs which solve the semiconductor equations are restricted to a rectangular device geometry. This is not essential as far as the analysis of the equations is concerned. In this chapter we shall assume that the equations (2.1)-(2.5) are posed in a domain D of R^n ($n=1,2,3$) with a piecewise smooth boundary ∂D . Equations (2.1)-(2.5) are subject to a mixed set of Dirichlet and Neumann boundary conditions. That means ∂D consists of three parts $\partial D = \partial D_1 \cup \partial D_2 \cup \partial D_3$. ∂D_1 denotes the part of the boundary where the device is surrounded by insulating material. There one assumes the boundary conditions:

$$\frac{\partial \psi}{\partial \vec{n}} \Big|_{\partial D_1} = \frac{\partial n}{\partial \vec{n}} \Big|_{\partial D_1} = \frac{\partial p}{\partial \vec{n}} \Big|_{\partial D_1} = 0 \quad (3.1)$$

Here \vec{n} denotes the unit normal vector on ∂D which exists anywhere except at a finite number of points (arbitrarily defined corners of the simulation geometry). ∂D_2 denotes the part of the boundary corresponding to the ohmic contacts. There ψ , n and p are prescribed. The boundary conditions can be derived from the applied bias ψ_D and the assumptions of thermal equilibrium and vanishing space charge:

$$\psi = \psi_D + \psi_{\text{built-in}}, \quad n \cdot p = n_i^2, \quad n - p - C = 0 \quad (3.2)$$

The last two conditions in (3.2) can be rewritten as:

$$\begin{aligned} n &= (\sqrt{C^2 + 4 \cdot n_i^2} + C) / 2 \\ p &= (\sqrt{C^2 + 4 \cdot n_i^2} - C) / 2 \end{aligned} \quad (3.3)$$

Modeling MOS devices one has also to account for controlled insulator-semiconductor interfaces. ∂D_3 denotes the part of the boundary which corresponds to such an interface. There we have the interface conditions:

$$\begin{aligned} \vec{J}_n \cdot \vec{n} \Big|_{\partial D_3} &= \vec{J}_p \cdot \vec{n} \Big|_{\partial D_3} = 0 \\ \epsilon_{\text{sem}} \cdot \frac{\partial \psi}{\partial \vec{n}} \Big|_{\text{sem}} &= \epsilon_{\text{ins}} \cdot \frac{\partial \psi}{\partial \vec{n}} \Big|_{\text{ins}} \end{aligned} \quad (3.4)$$

Again $\vec{n}|$ denotes the normal vector on ∂D . ϵ_{sem} and ϵ_{ins} denote the permittivity constants for the semiconductor and the insulator respectively. $\partial\psi/\partial\vec{n}|_{\text{sem}}$ and $\partial\psi/\partial\vec{n}|_{\text{ins}}$ denote the onesided limits of the derivatives perpendicular to the interface approaching the interface. Within the insulator the Laplace equation: $\text{div grad } \psi = 0$ holds.

3.2 Dependent Variables

For analytical purposes it is often useful to use other variables than n and p to describe the system (2.1)-(2.5). Two other sets of variables which are frequently employed are $(\psi, \varphi_n, \varphi_p)$ and (ψ, u, v) which relate to the set (ψ, n, p) by:

$$n = n_i \cdot e^{(\psi - \varphi_n)/U_t}, \quad p = n_i \cdot e^{(\varphi_p - \psi)/U_t} \quad (3.5)$$

$$n = n_i \cdot e^{\psi/U_t \cdot u}, \quad p = n_i \cdot e^{-\psi/U_t \cdot v} \quad (3.6)$$

(3.5) can be physically interpreted as the application of Boltzmann statistics. However (3.5) also can be regarded as a purely mathematical change of variables so that the question of the validity of the Boltzmann statistics does not need to be considered. The use of $(\psi, \varphi_n, \varphi_p)$ a priori excludes negative carrier densities n and p , which may be present as undesired nonphysical solutions of (2.1)-(2.5) if we use (ψ, n, p) or (ψ, u, v) as dependent variables. As we will see later in this chapter the advantage of the set (ψ, u, v) is that the continuity equations (2.2), (2.3) and current relations (2.4), (2.5) become self-adjoint. This also has an important impact on the use of iterative schemes for the solution of the evolving linear systems (cf. chapter 5). However, owing to the enormous range of the values of u and v , the sets (ψ, n, p) or $(\psi, \varphi_n, \varphi_p)$ have to be preferred for actual computations. We personally favour the set (ψ, n, p) .

3.3 Scaling

Since the dependent variables in the system (2.1)-(2.5) are of different order of magnitude and show a strongly different behaviour in regions with small and large space charge the first step towards a structural analysis of (2.1)-(2.5) has to be an appropriate scaling. A standard way of scaling (2.1)-(2.5) has been given by De Mari /27/. There ψ is scaled by the thermal voltage U_t , n and p are scaled by n_i (similar to Mock /77/) and the independent variables are scaled such that all multiplying constants in Poisson's equation become unity. Although physically reasonable this approach has the disadvantage that n and p in general are still several orders of magnitude larger than ψ . A scaling which reduces ψ , n and p to the same order of magnitude has been given by Vasiliev'a and Butuzov /121/. This approach makes the system (2.1)-(2.5) accessible to an asymptotic

analysis which is given together with applications in /69/, /70/ and /71/. There n and p are scaled by the maximum absolute value of the net doping C and the independent variables are scaled by the characteristic length of the device. More precisely the following scaling factors are employed.

quantity	symbol	value	
\vec{x}	1	$\max(\vec{x}-\vec{y}), \vec{x}, \vec{y}$ in D	
ψ	U_t	$k \cdot T / q$	(3.7)
n, p	α	$\max C $	

After scaling the equations become:

$$\lambda^2 \cdot \text{div grad } \psi = n - p - C \quad (3.8)$$

$$\text{div} (\text{grad } n - n \cdot \text{grad } \psi) = -R$$

$$\text{div} (\text{grad } p + p \cdot \text{grad } \psi) = -R$$

Here, for simplicity only, μ_n and μ_p have been assumed to be constant. It should be noted that the following analysis also holds if the usual smooth dependence of μ_n and μ_p on n, p and $\text{grad } \psi$ e.g. /97/ is assumed. Since the independent variable \vec{x} has been scaled, equations (3.8) are now posed on a domain D^S with maximal diameter equal to one. The small constant λ^2 multiplying the Laplacian in (3.8) is the minimal Debye length of the device:

$$\lambda^2 = \frac{\epsilon \cdot U_t}{l^2 \cdot q \cdot \alpha} \quad (3.9)$$

l and α are defined in (3.7). Thus for high doping ($\alpha \gg 1$) λ^2 will be small. For instance for a silicon device with characteristic length $25 \mu\text{m}$ and $\alpha = 10^{20} \text{cm}^{-3}$ we compute for λ^2 at approximate room temperature $T=300\text{K}$: $\lambda^2 = 4 \cdot 10^{-10}$.

R denotes the scaled generation/recombination rate, which is in general a (not necessarily mildly) nonlinear function of n, p and $\text{grad } \psi$. Thus different models of R may influence analysis results quite drastically. This is obviously to be expected as in many operating conditions the device behaviour depends strongly on the net generation/recombination R .

3.4 The Singular Perturbation Approach

(3.8) represents a singularly perturbed elliptic system with perturbation parameter λ . The advantage of this interpretation is that we can now obtain information about the structure of solutions of (3.8) by using asymptotic expansions: In the subdomains of D^S where the solutions behave smoothly we expand them into power series of the form:

$$w(\vec{x}, \lambda) = \sum_{i=0}^{\infty} w_i^{\sim}(\vec{x}) \cdot \lambda^i, \quad w = (\psi, n, p)^T \quad (3.10)$$

which implies a smooth dependence on λ . C - the scaled doping - is smooth in these subdomains and exhibits a sharp transition across the pn-junctions in the device. For the case of an abrupt junction this behaviour is represented by a discontinuity across an $n-1$ dimensional manifold $\Gamma: (\vec{x}=\vec{x}(s), s \text{ of } \mathbb{R}^{n-1})$ in the device. Thus Γ is a point in 1 dimension, a curve in 2 dimensions and a surface in 3 dimensions. Of course one curve or surface has to be used for each junction. Since the procedure is the same for each of the junctions it is demonstrated only for one junction. In the case of an exponentially graded doping profile C consists of two parts:

$$C = C^{\sim} + C^{\wedge} \quad (3.11)$$

where C^{\sim} and C^{\wedge} are discontinuous, C^{\sim} is piecewise smooth and C^{\wedge} is exponentially decaying to zero away from Γ . In the vicinity of Γ the expansion (3.10) is not valid and has to be supplemented by a "layer" term according to the singular perturbation analysis:

$$w(\vec{x}, \lambda) = \sum_{i=0}^{\infty} [w_i^{\sim}(\vec{x}) + w_i^{\wedge}(s, t/\lambda)] \cdot \lambda^i, \quad w = (\psi, n, p)^T \quad (3.12)$$

Here the following coordinate transformation has been employed: For a point in the vicinity of Γ s denotes the parameter value at the nearest point on Γ and t denotes its distance perpendicular to Γ . Thus the solution of the semiconductor equations exhibits internal layers at pn-junctions.

The w_i^{\sim} and w_i^{\wedge} in (3.12) can now be determined separately and the structure of the solution is given by its partition into the smooth part $\sum w_i^{\sim} \cdot \lambda^i$ and its rapidly varying part $\sum w_i^{\wedge} \cdot \lambda^i$. w_0^{\sim} has to satisfy the reduced equations:

$$0 = n_0^{\sim} - p_0^{\sim} - C^{\sim} \quad (3.13)$$

$$\text{div} (\text{grad } n_0^{\sim} - n_0^{\sim} \cdot \text{grad } \psi_0^{\sim}) = -R^{\sim} \quad (3.14)$$

$$\text{div} (\text{grad } p_0^{\sim} + p_0^{\sim} \cdot \text{grad } \psi_0^{\sim}) = -R^{\sim} \quad (3.15)$$

For the sake of simplicity but without loss of generality the mobilities μ_n and μ_p have been assumed to be constant. (3.13)-(3.15) is subject to the boundary conditions (3.1)-(3.4). Of course the condition of vanishing space charge is redundant with (3.13). Since C^{\sim} is discontinuous at Γ and (3.13)-(3.15) represents a second order system of two equations four "interface conditions" have to be imposed at Γ . They are of the form:

$$n_0^{\sim} \cdot e^{-\psi_0^{\sim}} \Big|_{\vec{x}=\vec{x}^-} = n_0^{\sim} \cdot e^{-\psi_0^{\sim}} \Big|_{\vec{x}=\vec{x}^+} \quad (3.16)$$

$$p_0 \cdot e^{\psi_0} \Big|_{\vec{x}=\vec{x}-} = p_0 \cdot e^{\psi_0} \Big|_{\vec{x}=\vec{x}+} \quad (3.17)$$

$$\vec{J}_{n_0} \cdot \vec{n} \Big|_{\vec{x}=\vec{x}-} = \vec{J}_{n_0} \cdot \vec{n} \Big|_{\vec{x}=\vec{x}+} \quad (3.18)$$

$$\vec{J}_{p_0} \cdot \vec{n} \Big|_{\vec{x}=\vec{x}-} = \vec{J}_{p_0} \cdot \vec{n} \Big|_{\vec{x}=\vec{x}+} \quad (3.19)$$

where $w|_{\vec{x}-}$ and $w|_{\vec{x}+}$ denote the onesided limits of w as \vec{x} tends to Γ from each side. \vec{n} denotes the unit normal vector on Γ . \vec{J}_{n_0} and \vec{J}_{p_0} are the zeroth order terms of the smooth parts of the (scaled) electron and hole current densities.

$$\vec{J}_{n_0} = \text{grad } n_0 - n_0 \cdot \text{grad } \psi_0 \quad (3.20)$$

$$\vec{J}_{p_0} = \text{grad } p_0 + p_0 \cdot \text{grad } \psi_0$$

(3.13)-(3.15) together with (3.16)-(3.19) and the boundary conditions (3.1)-(3.4) define the reduced problem whose solution is an $O(\lambda)$ approximation to the full solution away from Γ . As we will see in the next chapter the reduced problem is a useful tool for the development and analysis of numerical methods, since it (especially the conditions (3.16)-(3.19)) has to be solved implicitly by any discretisation method which requires a reasonable number of grid points.

The equations for the rapidly varying parts w_i reduce to ordinary differential equations. That means that only derivatives with respect to the "fast" variable t/λ occur. Since the rate of decay of w_i depends heavily on ψ the width of the layer grows with the applied voltage; a fact which is absolutely well known by device physicists, but which becomes nicely apparent by the singular perturbation approach.

4. NUMERICAL SOLUTION OF THE SEMICONDUCTOR EQUATIONS

In this chapter we discuss some of the problems occurring in the numerical solution of the semiconductor equations and the analysis of existing numerical methods. From the viewpoint of numerical analysis there are essentially three major topics to be considered. The first one is the type of discretisation to be used. There exist programs for both Finite Element and Finite Difference discretisations of the system (2.1)-(2.5). As outlined in the previous chapter the solution exhibits a smooth behaviour in some subregions of the domain whereas in others it varies rapidly. Thus a nonuniform mesh is mandatory and adaptive mesh refinement is desirable. So the second topic is the question how to set up the mesh refinement algorithm i.e. which quantities have to be used to control the mesh. Each type of discretisation will lead to a large sparse system of nonlinear equations and so the solution of this system is the third topic.

For the sake of simplicity in nomenclature we shall only consider the two-dimensional case in this chapter. However, all results given in the following can be generalized to three dimensions in a straightforward manner. So, the equations are posed in a domain D of \mathbb{R}^2 and $\vec{x} = (x,y)^T$ denotes the independent variable.

4.1 Discretisation Schemes

Using Finite Elements or Finite Differences one has to take into account that Poisson's equation (2.1) is of a different type than the continuity equations. Poisson's equation - in the scaling of Markowich /69/ using the variables (ψ, u, v)

$$\lambda^2 \cdot \text{div grad } \psi = e^{\psi} \cdot u - e^{-\psi} \cdot v - C \quad (4.1)$$

is a singularly perturbed elliptic problem whose right hand side has a positive derivative with respect to ψ . Thus it is of a standard form (as discussed in e.g. /42/) except for the discontinuous or exponentially graded term C . Equations of that type are generally well behaved and it suffices to apply a usual discretisation scheme. In the case of Finite Differences using the index convention given in Fig. 4.1 equation (4.1) is discretized by:

$$\lambda^2 \cdot (\text{div grad } \psi)_{ij} = n_{ij} - p_{ij} - C(x_i, y_j) \quad (4.2)$$

$$E_{i+1/2,j}^x = (\psi_{i+1,j} - \psi_{i,j}) / h_i \quad (4.3)$$

$$E_{i,j+1/2}^y = (\psi_{i,j+1} - \psi_{i,j}) / k_j$$

$$h_i = x_{i+1} - x_i, \quad k_j = y_{j+1} - y_j$$

$$\begin{aligned} (\text{div grad } \psi)_{i,j} = & 2 \cdot (E_{i+1/2,j}^x - E_{i-1/2,j}^x) / (h_i + h_{i-1}) + \\ & + 2 \cdot (E_{i,j+1/2}^y - E_{i,j-1/2}^y) / (k_j + k_{j-1}) \end{aligned} \quad (4.4)$$

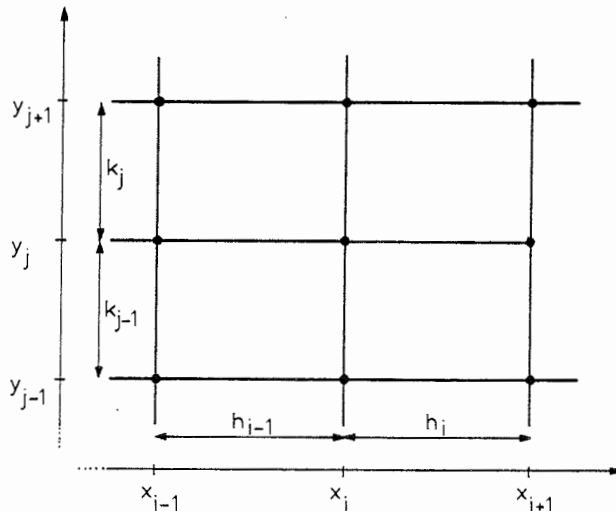


Fig. 4.1: The index convention used

If one of the neighbouring gridpoints (x_{i+1}, y_j) , (x_{i-1}, y_j) , (x_i, y_{j+1}) , (x_i, y_{j-1}) does not exist - as possible in a terminating line approach /1/, /2/ or in the Finite Boxes approach /44/ - (4.4) has to be modified. In the case of Finite Elements classical shape functions can be used (i.e. linear shape functions for triangular elements, bilinear shape functions for rectangular elements).

It turns out that the discretisation of the continuity equations is more crucial than the discretisation of Poissons's equation. The usual error analysis of discretisation methods provides an error estimate of the form:

$$\max |w_h - w| \leq c \cdot H \quad (4.5)$$

w_h denotes the numerical approximation to $w(x, y) = (\psi, n, p)^T$. H denotes the maximal gridspacing. The constant c will in general depend on the higher order derivatives of w . The singular perturbation analysis /70/ shows that derivatives of ψ , n and p in (3.12) are of magnitude $O(\lambda^{-3}) - O(\lambda^{-4})$ locally near the junction (λ is defined in (3.9)). /70/ shows also that, even if a nonuniform mesh is used, the amount of gridpoints required to equidistribute the error term in (4.5) can be proportional to λ^{-2} which is of course prohibitive. Therefore a discretisation scheme is needed where the constant c in (4.5) does not depend on the higher derivatives of the rapidly varying terms ψ , n and p . For the case of Finite Differences such a scheme was given by Scharfetter and Gummel /93/. They approximate:

$$J_n = \text{grad } n - n \cdot \text{grad } \psi \quad (4.6)$$

$$\text{div } J_n = \partial J_n^x / \partial x + \partial J_n^y / \partial y = R \quad (4.7)$$

by:

$$J_{n_{i+1/2}, j}^x = \frac{1}{2} \cdot (\psi_{i+1, j} - \psi_{i, j}) \cdot (n_{i+1, j} - n_{i, j}) / h_i - (n_{i, j} + n_{i+1, j}) / 2 \cdot (\psi_{i+1, j} - \psi_{i, j}) / h_i \quad (4.8)$$

$$J_{n_{i, j+1/2}}^y = \frac{1}{2} \cdot (\psi_{i, j+1} - \psi_{i, j}) \cdot (n_{i, j+1} - n_{i, j}) / k_j - (n_{i, j} + n_{i, j+1}) / 2 \cdot (\psi_{i, j+1} - \psi_{i, j}) / k_j$$

$$\frac{1}{2}(s) = s \cdot \coth(s)$$

$$2 \cdot (J_{n_{i+1/2}, j}^x - J_{n_{i-1/2}, j}^x) / (h_i + h_{i-1}) + 2 \cdot (J_{n_{i, j+1/2}}^y - J_{n_{i, j-1/2}}^y) / (k_j + k_{j-1}) = R_{i, j} \quad (4.9)$$

The continuity equation for holes is discretized analogously. Scharfetter and Gummel gave a physical reasoning for the derivation of their scheme. Markowich et al. /70/ proved

that in one dimension the Scharfetter-Gummel scheme is uniformly convergent. That means that the error constant c in (4.5) does not depend on the derivatives of ψ , n and p in (3.12) and therefore not on λ . For two dimensions /70/ shows that the choice $\gamma(s) = s \cdot \coth(s)$ is necessary for uniform convergence. Exponentially fitted schemes like the Scharfetter-Gummel scheme have been analyzed by Kellogg /61/, /60/ and Doolan /32/ (for different classes of problems). The reason for the uniform convergence of these schemes is that inside the pn-junction layers the interface conditions (3.16)-(3.19) are satisfied automatically if $|\text{grad}\psi|$ is large and the gridspacing is not $O(\lambda)$.

The results for Finite Difference schemes suggest that a similiar approach (like the exponentially fitted schemes) should be used in the case of Finite Elements. This fact has been intuitively observed by Engel /39/ for the one-dimensional case. A modeling group at IBM has tried to make use of the Scharfetter-Gummel scheme for Finite Elements in two and three space dimensions /14/, /13/, /24/. However, we have the impression that their approach needs still quite a bit of analysis, although it has been used effectively by other modelists too e.g. /87/. Macheck /66/ has tried to develop a more rigorous discretisation for Finite Elements using exponentially fitted shape functions. He uses classical bilinear shape functions for ψ and

$$\begin{aligned}\alpha_1(x,y) &= [1 - \psi_1(x,y)] \cdot [1 - \psi_2(x,y)] \\ \alpha_2(x,y) &= \psi_1(x,y) \cdot [1 - \psi_2(x,y)] \\ \alpha_3(x,y) &= \psi_1(x,y) \cdot \psi_2(x,y) \\ \alpha_4(x,y) &= [1 - \psi_1(x,y)] \cdot \psi_2(x,y)\end{aligned}\tag{4.10}$$

for u , and

$$\begin{aligned}\beta_1(x,y) &= [1 - \sigma_1(x,y)] \cdot [1 - \sigma_2(x,y)] \\ \beta_2(x,y) &= \sigma_1(x,y) \cdot [1 - \sigma_2(x,y)] \\ \beta_3(x,y) &= \sigma_1(x,y) \cdot \sigma_2(x,y) \\ \beta_4(x,y) &= [1 - \sigma_1(x,y)] \cdot \sigma_2(x,y)\end{aligned}\tag{4.11}$$

for v , where

$$\begin{aligned}\psi_1(x,y) &= f(x, \frac{\partial \psi}{\partial x}) \\ \psi_2(x,y) &= f(y, \frac{\partial \psi}{\partial y})\end{aligned}\tag{4.12}$$

$$\begin{aligned}\sigma_1(x,y) &= f(x, -\frac{\partial \psi}{\partial x}) \\ \sigma_2(x,y) &= f(y, -\frac{\partial \psi}{\partial y})\end{aligned}$$

$$\text{with: } f(x,a) = (\exp(ax) - 1) / (\exp(a) - 1)\tag{4.13}$$

The advantage of these shape functions is that they accommodate nicely the layer behaviour of the solution. They degenerate into the ordinary bilinear shape functions when the electric potential is constant. In order to be able to switch from coarse to fine grid spacing in different subdomains transition elements have to be used /66/. However, no theoretical investigations have been carried out so far to analyse the uniform convergence properties of this method.

4.2 Grid Construction

Since subregions of strong variation of ψ , n and p alternate with regions where these quantities behave smoothly (i.e. their gradients are small) different meshsizes are mandatory in these subregions. Thus the discretisation scheme should be able to switch locally from a coarser to a finer grid. However, the question arises which criteria should be used to generate the mesh. If the user of a simulation program has to define his elements or nodes a priori as input parameters, this could perhaps be done by experience /15/. If - as it is the case for modern user oriented programs - an adaptive mesh selection is desired mathematically formulated criteria are a "sine qua non". Generally such criteria should satisfy two conditions. Firstly they should not cause the program to construct more gridpoints/elements than necessary to achieve a certain accuracy. Secondly they should guarantee that a prescribed relative accuracy δ is really achieved once they are satisfied. A usual way to design adaptive mesh refinement procedures is to equidistribute the local truncation error of the discretisation scheme. In the case of Finite Differences this error is proportional to the meshsize and the third and fourth derivatives of ψ , n and p . Markowich /70/ however showed that it is practically not possible to equidistribute this quantity. In the case of a simple MOS-transistor $O(\delta^{-2}\lambda^{-2})$ gridpoints would be required. On the other hand the singular perturbation analysis shows that the solution of the difference scheme approximates the solution of the reduced problem (3.13)-(3.15) even if this criterion is not satisfied inside the layer regions (inversion layer and space charge regions). Therefore the quantity to be equidistributed is the discretisation error of Poisson's equation (i.e. the partial derivatives of the space charge times the meshsizes). This equidistribution can be relaxed inside the pn-junction layers by e.g. simply limiting the number of gridpoints there.

4.3 Linearisation Schemes

Each discretisation scheme (Finite Differences or Finite Elements) will lead to a large sparse system of nonlinear equations to be solved. The theory of iterative methods to solve these equations is to a large extent independent of the used discretisation and so it is convenient to view the whole problem as solving a nonlinear system of equations iteratively by solving linear systems. The existing numerical methods can essentially be divided into two classes: The first approach, a block nonlinear iteration algorithm, is due to Gummel /52/ and uses the

fact that the current relations are linear in the variables u and v (as defined in (3.6)). In these variables the equations become (again we use the scaling of /66/):

$$\lambda^2 \cdot \text{div grad } \psi = e^{\psi} \cdot u - e^{-\psi} \cdot v - C \quad (4.14)$$

$$\text{div } \vec{J}_n = R, \quad \vec{J}_n = e^{\psi} \cdot \text{grad } u \quad (4.15)$$

$$\text{div } \vec{J}_p = -R, \quad \vec{J}_p = -e^{-\psi} \cdot \text{grad } v \quad (4.16)$$

Gummels approach works as follows: Given $(\psi, u, v)^k$ ψ^{k+1} is computed by solving:

$$\lambda^2 \cdot \text{div grad } \psi^{k+1} = e^{\psi^{k+1}} \cdot u^k - e^{-\psi^{k+1}} \cdot v^k - C \quad (4.17)$$

subject to the appropriate boundary conditions. Then u^{k+1} and v^{k+1} are computed from:

$$\text{div } \vec{J}_n^{k+1} = R(\text{grad } \psi^{k+1}, u^k, v^k), \quad \vec{J}_n^{k+1} = e^{\psi^{k+1}} \cdot \text{grad } u^{k+1} \quad (4.18)$$

$$\text{div } \vec{J}_p^{k+1} = -R(\text{grad } \psi^{k+1}, u^k, v^k), \quad \vec{J}_p^{k+1} = -e^{-\psi^{k+1}} \cdot \text{grad } v^{k+1} \quad (4.19)$$

together with the boundary conditions for u and v . (4.18) and (4.19) are two decoupled linear equations for u^{k+1} and v^{k+1} . Poissons's equation (4.17) is nonlinear in this setting and therefore it has to be solved iteratively itself in each step by a Newton like method. Since Newton's method is an inner iteration within the overall iteration process (4.17)-(4.19) it may not be necessary to let this inner iteration "fully converge" /49/.

The advantage of Gummels's method is obvious. (4.17)-(4.19) can be solved sequentially which decreases the required amount of storage and computing time drastically for each step. However, bad convergence properties can be observed in the case of high currents. This is explained by viewing (4.17)-(4.19) as iterating the map $M: (u^k, v^k) \rightarrow (u^{k+1}, v^{k+1})$ where the evaluation of M involves the solution of (4.17). Then the norm of the linearisation of M (as an operator acting in the appropriate spaces) at the fixpoint $M(u^*, v^*) = (u^*, v^*)$ is proportional to the current densities /72/.

The second approach to the solution of the nonlinear equations (2.1)-(2.5) is a damped modified Newton method. To solve the general equation $F(x)=0$ one computes the sequence $\langle x^k \rangle$ by:

$$M^k \cdot \delta^k = -F(x^k), \quad x^{k+1} = x^k + t^k \cdot \delta^k \quad (4.20)$$

For the usual Newton method $M^k = F'(x^k)$ and $t^k = 1$ holds.

Bank and Rose /8/ have given criteria for the choice of the damping parameters t^k which guarantee global convergence. Moreover they investigate how well d^k has to approximate the classical Newton step in order to get a certain rate of convergence. They obtain that the rate of convergence is p ($1 < p < 2$) if:

$$|M^k \cdot d^k + F(x^k)| = O(|F(x^k)|^p) \quad (4.21)$$

holds asymptotically for $k \rightarrow \infty$. Alternatively Bank and Rose /7/ suggested $M^k = \lambda^k I + F'(x^k)$ where λ^k is proportional to $|F(x^k)|$. Franz /44/ tested this method with good success. However, he additionally chooses damping parameters t^k according to Deuflhard /30/, /31/.

5. SOLUTION OF LINEAR SYSTEMS

For any of the linearization procedures which have been outlined in the last chapter a large sparse linear equation system (5.1) has to be solved repeatedly.

$$A \cdot x = b \quad (5.1)$$

A has been derived by linearizing discretized PDEs. Hence A has only five to nine nonzero entries per row and block (a block is formed by the three discretized equations); A is very sparse. For the solution of these special types of linear systems of equations two classes of methods, can, in principle, be used: direct methods which are based on elimination and iterative methods. An excellent survey on that subject has been published recently by Duff /34/. Classical Gaussian elimination is not feasible for our systems of equations because the rank of A in (5.1) is very large and A has many coefficients which are zero. Therefore, modifications of the classical Gaussian elimination algorithm have to be introduced to account for the zero entries. There exist quite a few activities on that subject (c.f. /35/) and powerful algorithms which treat the nonzero coefficients only are available (so called sparse matrix codes). Another serious drawback of direct methods lies in the fact that the upper triangular matrix which is created by the elimination process has to be stored for back substitution. This matrix has usually more nonzero entries than the matrix A. Therefore, memory requirement of direct methods is substantial. One advantage of the linear systems obtained from the discretised semiconductor equations is that no pivoting in order to maintain numerical stability is needed. In spite of all drawbacks of direct methods, their major advantage is high accuracy of the solution. However, we feel that for the semiconductor problems iterative algorithms are to emphasize. Nevertheless we and many others have observed difficulties with respect to the convergence speed of iterative methods, so that the direct methods, which require an exactly predictable amount of computer resources, will always stay in consideration.

The fundamental idea of relaxation methods (which are the best established iterative methods) is the splitting of the coefficient matrix A (5.1) into three matrices D, E, F (5.2).

$$A = D - E - F \quad (5.2)$$

D denotes the diagonal entries of A; -E denotes a lower triangular matrix which consists of all sub-diagonal entries of A; and -F denotes an upper triangular matrix which consists of all super-diagonal entries of A.

With an arbitrary non singular matrix B which has the same rank as A the linear system (5.1) can be rewritten to (5.3):

$$B \cdot x + (A-B) \cdot x = b \quad (5.3)$$

One obtains an iterative scheme by setting:

$$B \cdot x^{k+1} = b - (A-B) \cdot x^k \quad (5.4)$$

(5.4) can be solved for x^{k+1} :

$$x^{k+1} = (I - B^{-1} \cdot A) \cdot x^k + B^{-1} \cdot b \quad (5.5)$$

The scheme (5.5) will converge if condition (5.6) holds:

$$\rho(I - B^{-1} \cdot A) < 1 \quad (5.6)$$

(5.6) is a necessary and sufficient condition where ρ denotes the spectral radius [20]. Any relaxation method can be derived by differently choosing the matrix B from the splitting of A (5.2). The simplest scheme, the point-Jacobi method, uses D for B. Matrix D is a diagonal matrix and, therefore, is easily invertible. The Gauss-Seidel method uses D-E for B. The matrix D-E is a lower triangular matrix. Therefore one has only to perform a forward substitution process for its inversion. The successive overrelaxation method (SOR) uses a parameter ω within the range]0,2[. The iteration matrix B is defined:

$$B = D/\omega - E \quad (5.7)$$

Since B is again a lower triangular matrix, its inversion is instantly reduced to a substitution.

The major advantage of these iterative methods lies in their simplicity. They are very easy to program and demand only low memory requirement. As already noted, they converge if condition (5.6) holds. However, this is generally difficult to prove. A sufficient condition for convergence is that A is positive definite (5.8) which is the normal case for five-point-star discretized PDEs.

$$x^T \cdot A \cdot x > 0 \text{ for all } x \neq 0 \quad (5.8)$$

It should be noted again here that the current relations and continuity equations are not self adjoint if (ψ, n, p) are used as variables (see (2.10), (2.11)). However, the transformation:

$$n = e^{\psi} \cdot u, \quad p = e^{-\psi} \cdot v \quad (5.9)$$

results in a similarity transformation of the iteration matrix in (5.6). Thus the spectral radius of the iteration matrix is not influenced and the same convergence properties are obtained as if the system had been discretized in its self adjoint form with (ψ, u, v) as variables.

Some point-iterative schemes can be accelerated quite remarkably with the conjugate gradient method or the Chebyshev method. An excellent survey on these topics can be found in /50/, /51/.

Various activities can be observed for the development of more powerful algorithms with the advantages of iterative schemes. One of the best known algorithms which has been established in semiconductor device analysis is Stone's strongly implicit procedure /104/. Stone's idea was to modify the original coefficient matrix A by adding a matrix N (whose norm is much smaller than the norm of A) so that a factorization of $(A+N)$ involves less computational effort than the standard decomposition of A . Assuming this has been done, the development of an iterative procedure is then fairly straightforward because the equation can be written as:

$$(A+N) \cdot x = (A+N) \cdot x + (b-A \cdot x) \quad (5.10)$$

which suggests the iterative procedure:

$$(A+N) \cdot x^{k+1} = (A+N) \cdot x^k + (b-A \cdot x^k) \quad (5.11)$$

When the right hand side is known and if $(A+N)$ can be factorized easily, (5.11) gives an efficient method for directly solving for x^{k+1} . Furthermore, one would intuitively expect a rapid rate of convergence if N is sufficiently small compared to A . We will refrain from explaining in detail Stone's suggestion of how to choose the perturbation matrix N because this has been done thoroughly in many publications e.g. /43/, /100/, /104/. A major disadvantage of Stone's method is that it is only applicable for linear systems obtained by a classical Finite Difference discretisation. It is not applicable for systems obtained by the Finite Boxes approach /44/ or the general Finite Element approach.

There exist a few algorithms which are similar to Stone's method in terms of underlying ideas. The most attractive are the method of Dupont et al. /36/, the "alternating direction implicit" methods e.g. /11/, /43/, /122/ and the Fourier methods /103/, /120/. However, most of these sophisticated algorithms lack general applicability.

No matter which iterative method is used one has to deal with the question of an appropriate termination (convergence) criterion. Usually (5.12) is applied with a properly chosen relative accuracy ϵ :

$$|x^{k+1} - x^k| < \epsilon \cdot |x^{k+1}| \quad (5.12)$$

Since increments still accumulate when (5.12) is already satisfied we suggest to use (5.13) instead of (5.12):

$$|x^{k+1} - x^k| < \epsilon \cdot |x^{k+1}| \cdot (1 - \rho(G)) \quad (5.13)$$

$\rho(G)$ can be estimated as $\lim_{k \rightarrow \infty} |x^{k+1} - x^k| / |x^k - x^{k-1}|$.

One disadvantage of all strongly implicit methods and also the direct methods is that they cannot be implemented efficiently on a computer with a pipe-line architecture (vector processor). Some comments on that subject have been given in /34/.

6. AN EXAMPLE

The main power of a fully numerical model lies in its ability to provide the distributions of all physical quantities in the interior of a device. However, one has to bear in mind that the only possible check of numerical calculations is an elaborate comparison of experimental and theoretical results. The particular example in this chapter is intended to highlight the didactic potential of the fully numerical model MINIMOS.

Fig. 5.1 shows the doping profiles of two devices the geometrical channel length of which is $1.6\mu\text{m}$. The oxide thickness is 30nm ; the junction depth is about $.44\mu$ and the lateral subdiffusion is about $.23\mu\text{m}$. The profile on the right hand side has just an additional channel implantation in order to suppress the punch through effect. We shall discuss now some of the internal physical quantities of these two devices for an operating condition with 0V at source, gate and substrate; and 7V at drain. The picture on the right hand side of the next figures (Fig. 5.2, Fig. 5.3 and Fig. 5.4) corresponds to the doping profile on the right hand side of Fig. 5.1.

Fig. 5.2 shows the contour lines of the electrical potential for both devices. We nicely can observe a saddle point in the picture on the left hand side, which is the typical indication of punch through in weak inversion. This phenomenon has been reported for many years by all authors working on multy dimensional MOS models. The picture on the right hand side exhibits a well pronounced barrier between source and the channel region, thus indicating a proper subthreshold behaviour.

Fig. 5.3 shows the electron distribution in a logarithmic scale. The punch through channel is fully suppressed by the deep channel implant. It also seems worthwhile to note that the qualitative behavior of the electron density at the surface is identical for both devices.

In Fig. 5.4 the lateral component of the electron current density is given for both devices. The punch through channel is even better visible than in the last figure. The tongue-like appearance of the lateral component of the electron current density in the picture on the right hand side is typical for devices functioning properly in the subthreshold region. It should be mentioned, although it is trivial, that the scale of these pictures differs more than four orders of magnitude.

At the chosen bias point (0V at gate, 7V at drain) no significant impact ionization takes place in both devices. The reason for this fact can be found in the absolute current level which is simply too low [90/, [92/. To demonstrate the influence of impact ionization we have chosen the bias point with 0V at source and substrate, 1V at gate and 7V at drain. All figures in the following (Fig. 5.5-Fig. 5.8) correspond to this operating condition. The pictures on the right hand side of these figures are the simulation results obtained with ionization coefficients set to zero.

Fig. 5.5 shows the electric potential. Almost no barrier exists between source and channel, whereas an acceptable barrier is still simulated when neglecting impact ionization. In Fig. 5.6 the ionization rate is plotted in a quasi logarithmic scale ($\log(10^{18}+GA)-18$). The peak value reads about $2.5 \cdot 10^{27}$ pairs per cm^3 and second.

The carrier densities are given in Fig. 5.7 and Fig. 5.8. A large increase of the carrier densities due to avalanche generation can be seen from these figures. This increase results not only from carrier generation but also from the rigid source-substrate barrier lowering (cf. Fig. 5.5).

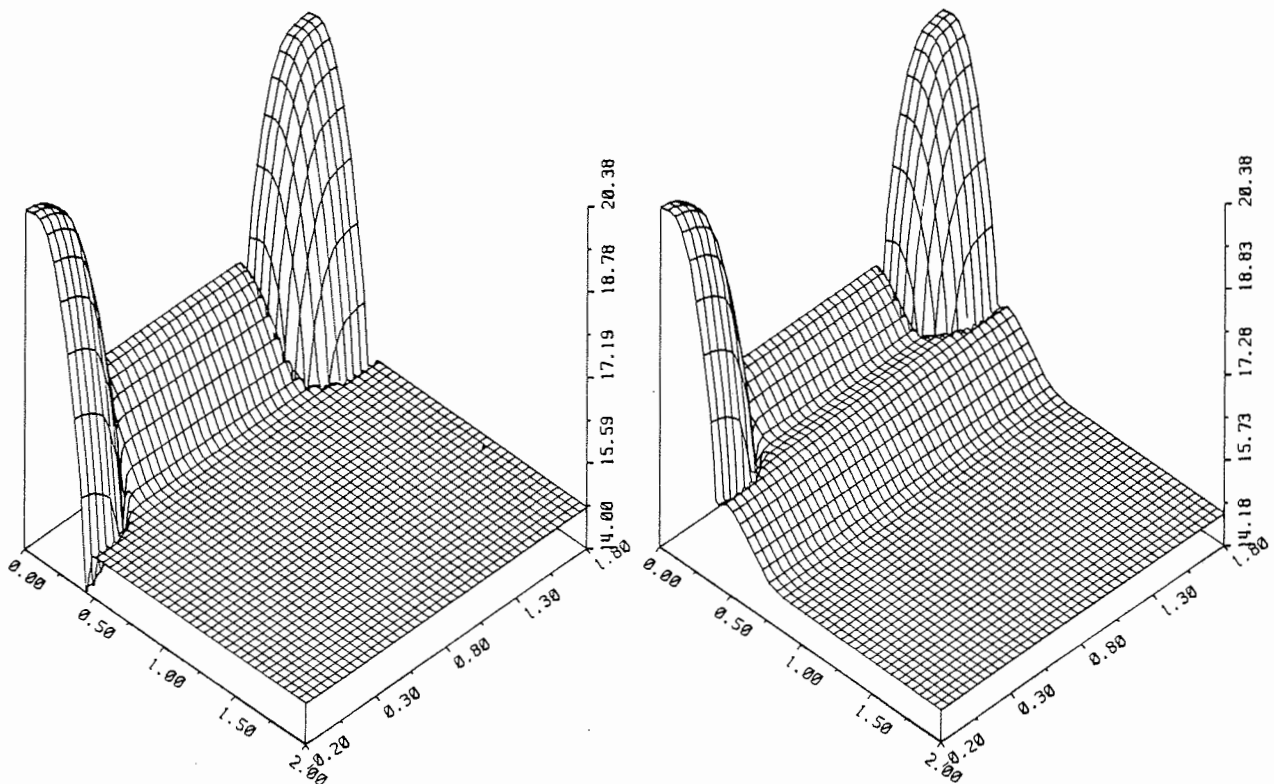


Fig. 5.1: Device 1 - Doping profile - Device 2

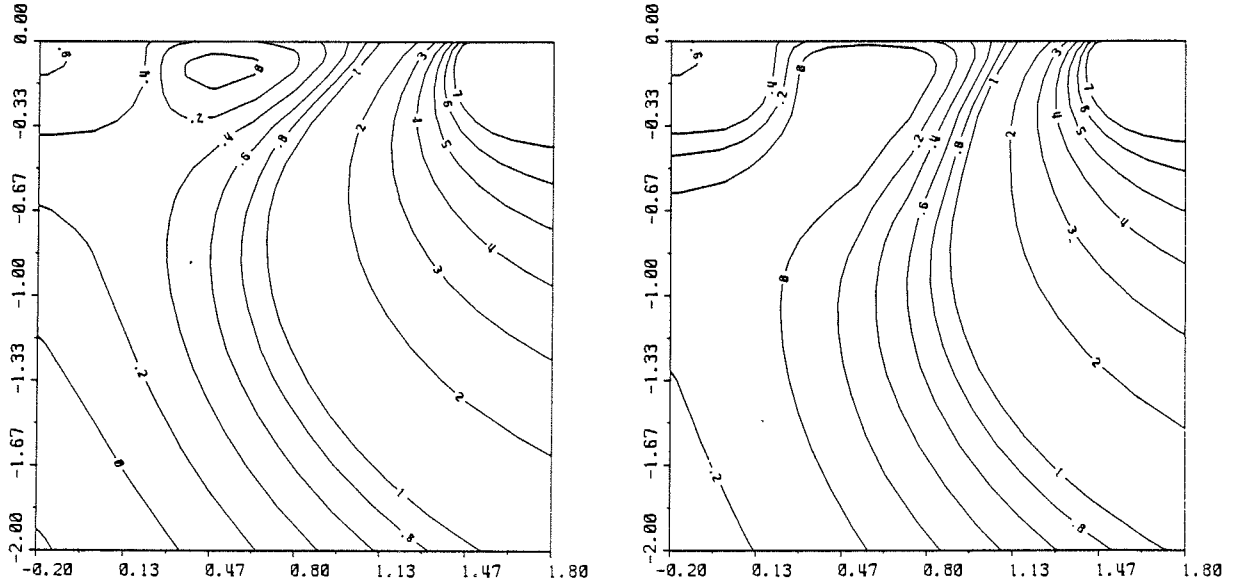


Fig. 5.2: Device 1 - Electric potential - Device 2

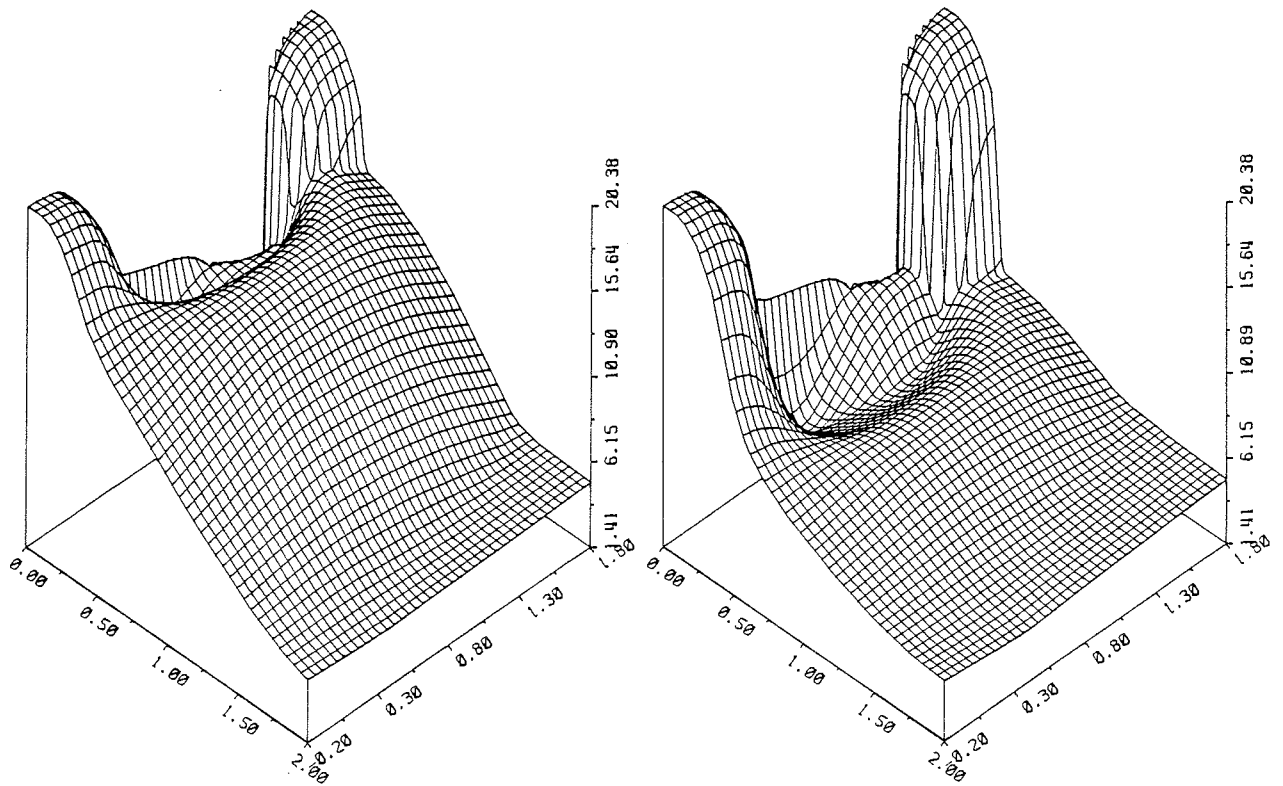


Fig. 5.3: Device 1 - Electron density - Device 2

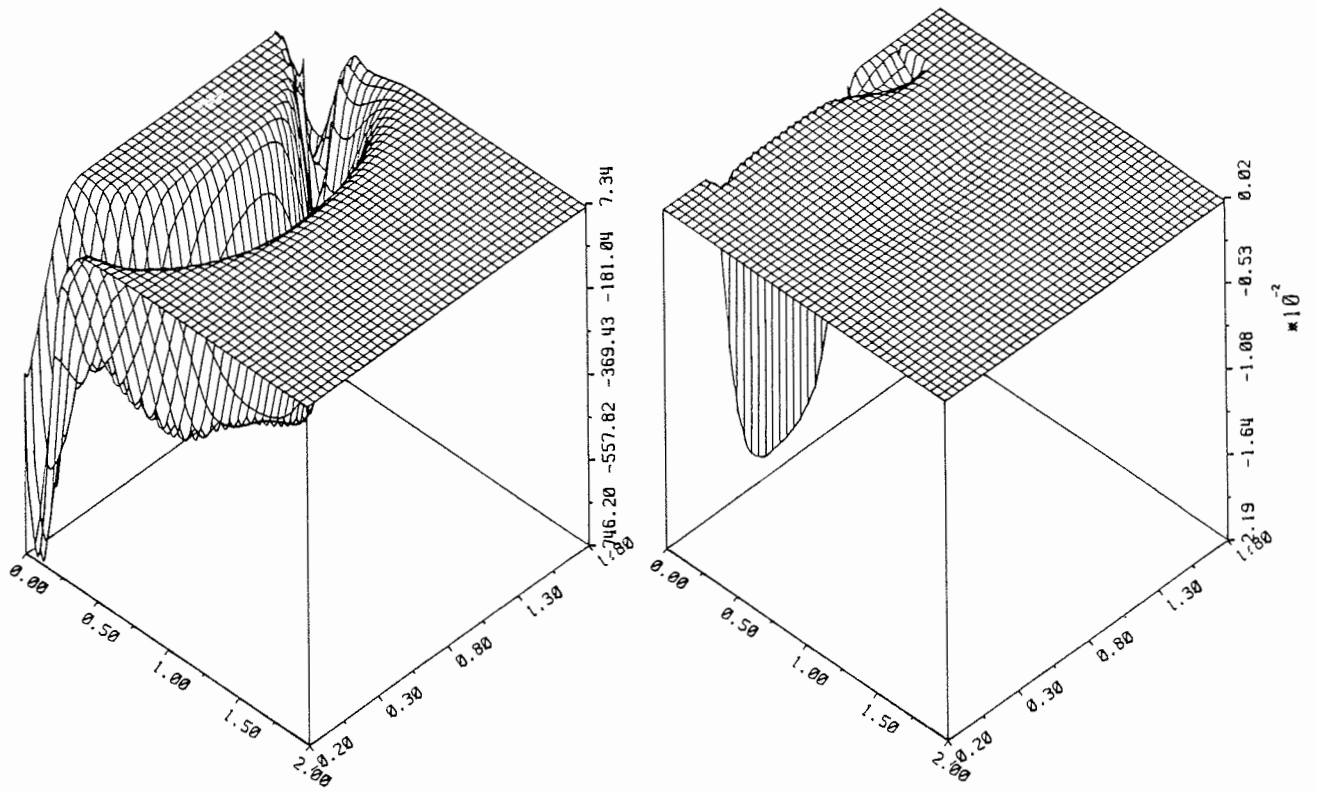


Fig. 5.4: Device 1 - Electron current density - Device 2

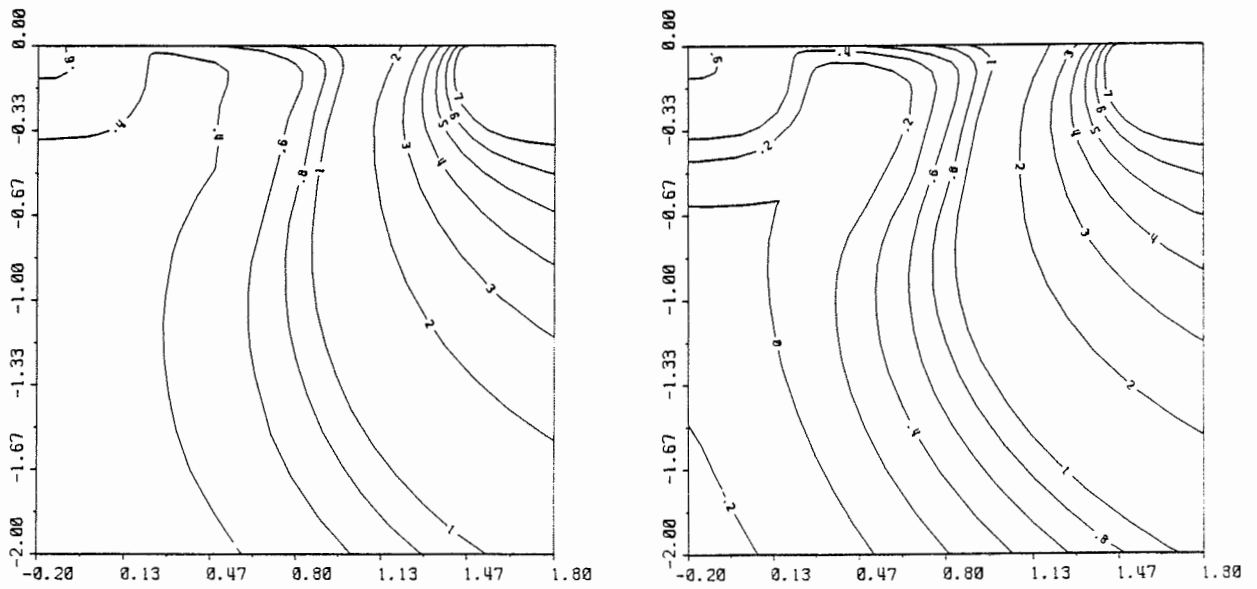


Fig. 5.5: with aval. - Electric potential - without aval.

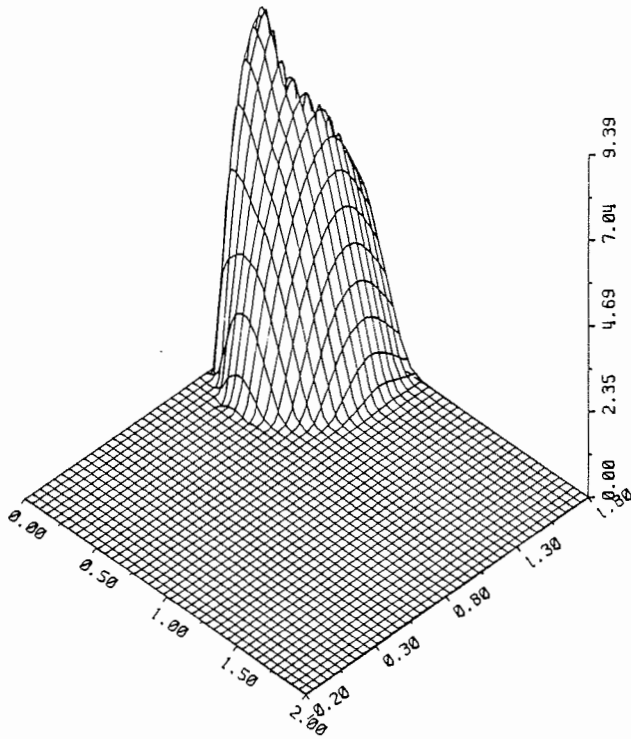


Fig. 5.6: with aval. - Generation rate - without aval.

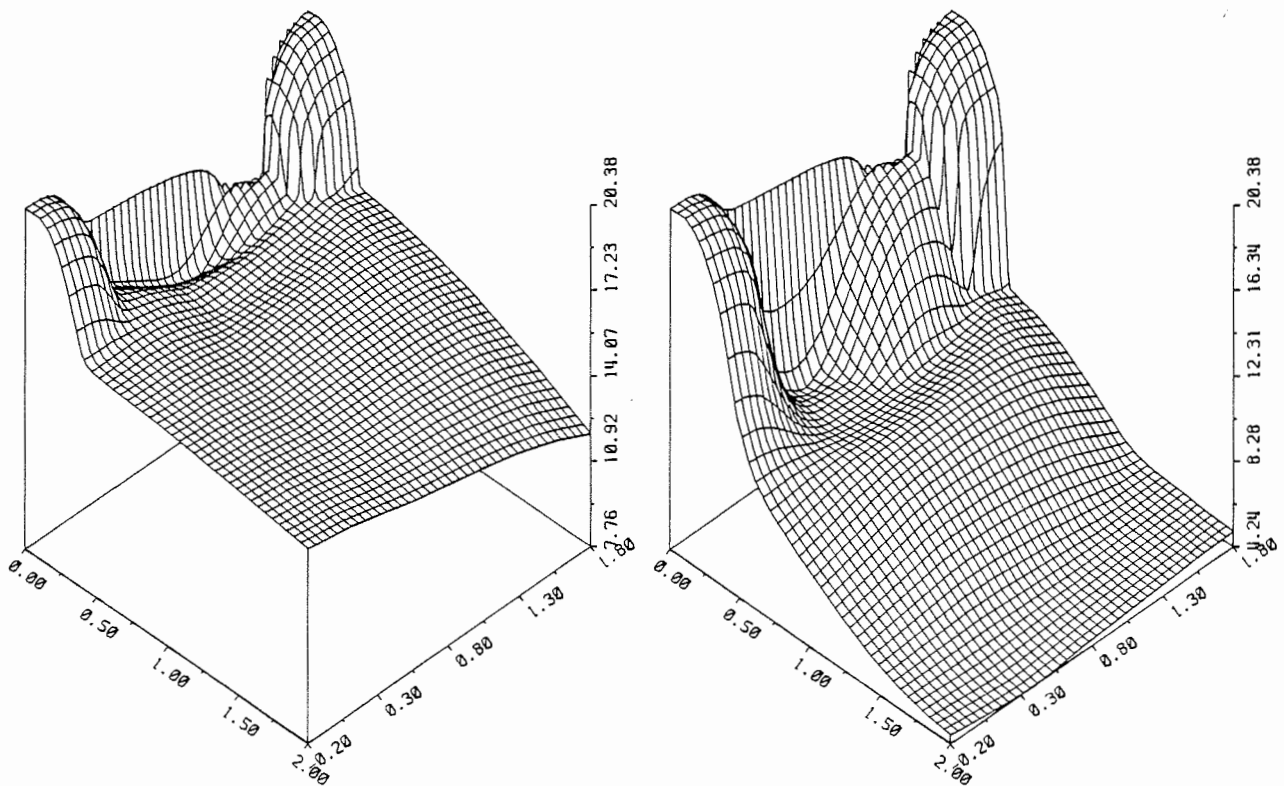


Fig. 5.7: with aval. - Electron density - without aval.

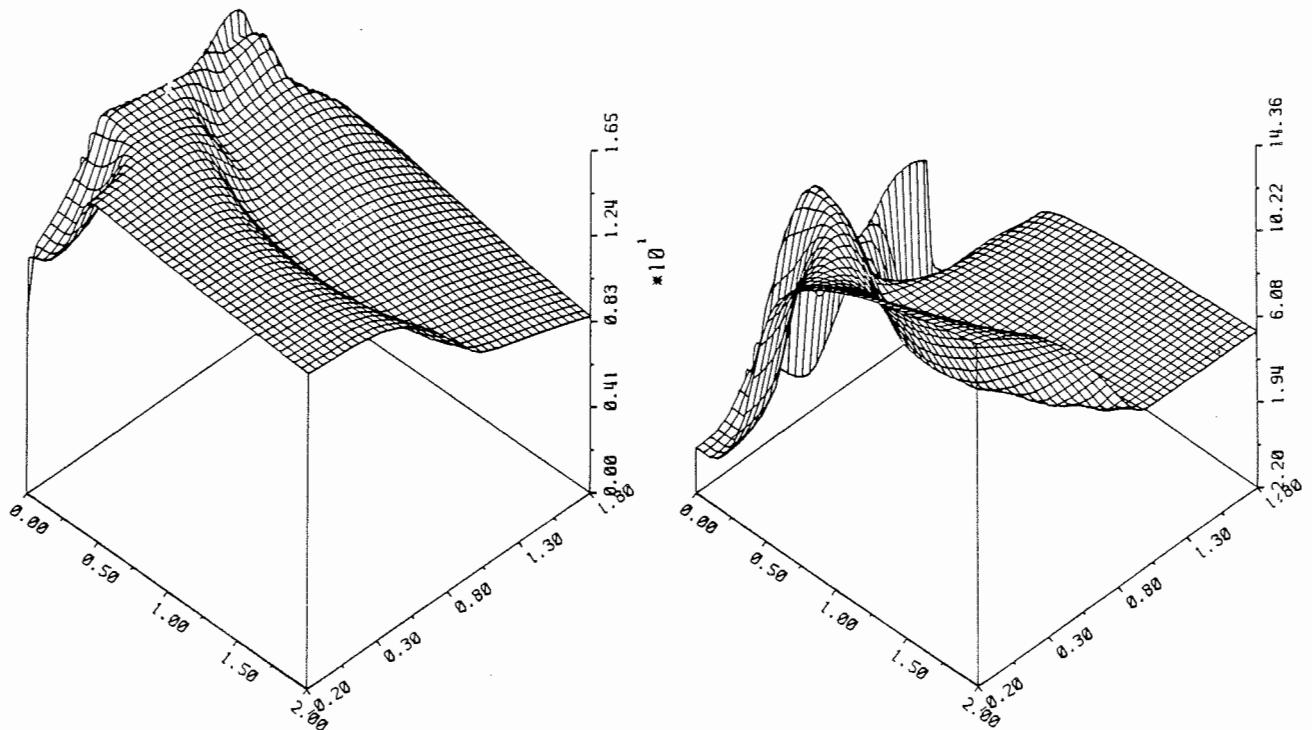


Fig. 5.8: with aval. - Hole density - without aval.

7. CONCLUSION

In this paper we tried to sketch the state of the art in modeling semiconductor devices, particularly MOS transistors, with numerical methods. The underlying physics has been discussed and the importance of increasingly sophisticated numerical methods has been briefly outlined. It has become evident that only progress in basic semiconductor physics will lead to the development of models which are capable of simulating device behaviour more reliably and which will match the technological advances of the recent device miniaturisation. One highly important objective of a model, its ability to predict the performance of a new device prior to having built the actual device, can only be reached if the physical parameters of the basic equations are analyzed even more thoroughly. This possibly implies a complete re-evaluation of some commonly accepted assumptions and approximations and it also seems to be the only way to get rid of the enormous amount of fitting parameters and the heuristic formulae which just simulate more or less precisely some complex physical phenomena.

The power of a numerical model to predict device behaviour has been demonstrated using our MOS-transistor simulation program MINIMOS. However, still much effort in analysis and simulation will have to be spent to make device miniaturisation and integration keep pace with the speed of recent days.

ACKNOWLEDGMENT

This work has been supported by the "Fond zur Förderung der wissenschaftlichen Forschung" (Projekt Nr. S22/11). Essential help of Siemens AG, Munich, in providing MOS devices is gratefully acknowledged. Many helpfull discussions with Dr. P. Markowich and Dr. C. Ringhofer are very appreciated. The authors wish to thank Dipl.Ing. D. Schornböck and the whole staff of the computer center for the excellent computer access.

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