PROCESS AND DEVICE MODELING FOR VLSI

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ABSTRACT

The appearance of Very Large Scale Integration caused a pronounced interest in concentrating on process and 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. Formulae that are applicable in a simple and easy way 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. Much emphasis is laid on the didactic potential of such a complex high order model.

KEYWORDS

Process modeling; semiconductor device modeling; very large scale integration; numerical analysis of semiconductor devices.

INTRODUCTION

It was in the early 1960's when the first integrated circuits which just contained a few devices became commercially available. Since then an evolution has taken place so that the manufacture of integrated circuits with about 500.000 transistors per single chip is possible nowadays. This upcoming 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 completely new phenomena emerged and even dominated the device behavior. 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/, /53/, /79/) has been increasing incredibly.

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 /156/ which describe all different regions of semiconductor devices in one unified manner was first suggested by Gummel /69/ for the one dimensional bipolar transistor. This approach was further developed and applied to pn-junction theory by De Mari /39/, /38/ and to IMPATT diodes by Scharfetter and Gummel /129/.

The first two dimensional numerical analysis of a semiconductor device was carried out by Kennedy and O'Brien /82/ for 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. The

first results on three dimensional device modeling have been published recently.   Transient
analysis have been performed by e.g. /90/, /107/ and models for three space dimensions have
been announced by e.g. /27/, /164/, /165/.

PROCESS MODELING

To enable the simulation of the electric behavior of a device the configuration of the
device (i.e. geometry and composition of the material it is made of) is, obviously, one of
the prerequisite pieces of input information. Optimal design of a device necessitates the
capability to predict the effect of modifying any of the various process steps involved in
device fabrication.   One principle barrier for predictive device simulation is the
uncertainty of the results of process models due to still inadequate understanding of their
underlying solid-state physics and chemistry. Particularly in the development of devices
for integrated circuits and their technology, the need for process models is growing
dramatically due to the tight coupling of two and three dimensional device effects with the
doping profile /49/.   Owing to these purposes, many computer programs capable of modeling
quite generally the various processing steps of device fabrication have been developed, and
they have proven to be extremely valuable tools, e.g. ICECREM /122/, /123/; LADIS /151/;
MEMBRE /112/; RECIPE /138/; SUPRA /29/, /84/, /85/, /102/ and the extraordinarily well
established SUPREM program /7/, /8/, /102/, /101/, /119/.

Apart from lithography which may be viewed as a fixed process that simply provides
flexibility in layout /117/, /118/, the primary fabrication processes which determine the
electrical characteristics of semiconductor devices, in particular silicon devices, are ion
implantation, diffusion and thermal oxidation.   Epitaxy, etching and deposition can
certainly play an essential role in device fabrication as well. However, as the field of
process modeling is extraordinarily wide and difficult, only the above cited process steps
will be discussed here. Furthermore, it should be noted that only a small review of the
most important models can be presented here due to the complexity of the underlying
phenomena. The aim here is just to give a flavor on what problems have to be dealt with in
providing this all-important input for device simulation. We also shall restrict ourselves
to silicon processing.

Ion Implantation

Ion implantation is the most applied doping technique in the fabrication of silicon devices,
particularly integrated devices. Implanted profiles are usually described by means of a
distribution function $f(x)$ and four characteristic quantities which are the mean value or
projected range R_p:

$$R_p = \int_{-\infty}^{\infty} x \cdot f(x) \cdot dx \tag{1}$$

the standard deviation σ_p:

$$\sigma_p = \sqrt{\int_{-\infty}^{\infty} (x-R_p)^2 \cdot f(x) \cdot dx} \tag{2}$$

the skewness γ_1:

$$\gamma_1 = \frac{\int_{-\infty}^{\infty} (x-R_p)^3 \cdot f(x) \cdot dx}{\sigma_p^3} \tag{3}$$

and the excess or kurtosis β_2:

$$\beta_2 = \frac{\int_{-\infty}^{\infty} (x-R_p)^4 \cdot f(x) \cdot dx}{\sigma_p^4} \tag{4}$$

These quantities can either be calculated /88/, /19/ or measured /122/.

At present the most universal distribution function is the Pearson type IV frequency
function which has been introduced by Hofker /74/ for process modeling. It is based on the
differential equation:

$$\frac{df}{dy}(y) = \frac{y-a}{b_0+b_1\cdot y+b_2\cdot y^2}\cdot f(y) \quad , \quad y = x - R_p \tag{5}$$

where the four constants a, b_0, b_1 and b_2 can be expressed in the four characteristic quantities (1) to (4)

$$a = -\frac{\gamma_1\cdot\sigma_p\cdot(\beta_2+3)}{10\cdot\beta_2-12\cdot\gamma_1^2-18} \tag{6}$$

$$b_0 = -\frac{\sigma_p^2\cdot(4\cdot\beta_2-3\cdot\gamma_1^2)}{10\cdot\beta_2-12\cdot\gamma_1^2-18} \tag{7}$$

$$b_1 = -\frac{\sigma_p\cdot\gamma_1\cdot(\beta_2+3)}{10\cdot\beta_2-12\cdot\gamma_1^2-18} \tag{8}$$

$$b_2 = -\frac{2\cdot\beta_2-3\cdot\gamma_1^2-6}{10\cdot\beta_2-12\cdot\gamma_1^2-18} \tag{9}$$

The shape of $f(y)$ varies considerably with b_0, b_1 and b_2. The form of solution of (5) evidently depends on the nature of the roots of the equation:

$$b_0 + b_1\cdot y + b_2\cdot y^2 = 0 \tag{10}$$

However, only the so-called Pearson type IV distribution can be used for modeling implantation profiles. In this case (10) does not have real roots which gives the restriction:

$$0 < \gamma_1^2 < 32$$

$$\beta_2 > \frac{39\cdot\gamma_1^2 + 48 + 6\cdot(\gamma_1^2+4)^{3/2}}{32 - \gamma_1^2} \tag{11}$$

Obeying this restriction the general solution of the differential equation (5) is given by:

$$f(x) = K\cdot(-(b_0+b_1\cdot(x-R_p)+b_2\cdot(x-R_p)^2))^{(\frac{1}{2\cdot b_2})}\cdot$$

$$\cdot\exp(-\frac{b_1/b_2 + 2\cdot a}{\sqrt{4\cdot b_2\cdot b_0 - b_1^2}}\cdot\text{atan}(\frac{2\cdot b_2\cdot(x-R_p) + b_1}{\sqrt{4\cdot b_2\cdot b_0 - b_1^2}})) \tag{12}$$

The constant K is the normalization constant to account for the incorporation of the total implantation dose. It can usually be determined only by numerical integration.

Diffusion

By means of diffusion processes one can obtain a desired shape of the distribution of dopants incorporated into the semiconductor by, e.g., ion implantation or which are deposited at the surface as a paste, fluid or gas of high concentration. The diffusion of dopants in semiconductors is described by the two laws of Fick, which read:

$$\overline{J}_i = -D_i\cdot(\text{grad } Ct_i - z_i\cdot\frac{q}{k\cdot T}\cdot(Ct_i - Cc_i)\cdot\text{grad }\psi) \tag{13}$$

$$\frac{\partial Ct_i}{\partial t} + \text{div } \overline{J}_i = 0 \tag{14}$$

Ct_i is the total concentration; Cc_i is the electrically inactive part of the concentration, i.e. the concentration of dopants which is not well incorporated in the silicon lattice and, thus, is not ionized (e.g. neutral clusters). $\overline{J}_i$ denotes the impurity flux; z_i is the charge state of the impurity (+1 for singly ionized acceptors, -1 for singly ionized donors). D_i represents the diffusion coefficient which depends, in general, on all sorts of quantities as we shall discuss later. ψ is the electrostatic potential. The index i of all

above cited quantities denotes the i-th impurity type as there is usually more than one kind of impurity incorporated into the silicon when a diffusion process is performed.

By substituting (13) into (14) we obtain the classical form of the diffusion equation, a continuity equation, for the i-th dopant.

$$\frac{\partial Ct_i}{\partial t} = \text{div } [D_i \cdot (\text{grad } Ct_i - z_i \cdot \frac{q}{k \cdot T} \cdot (Ct_i - Cc_i) \cdot \text{grad } \Psi)] \qquad (15)$$

The electrostatic potential Ψ is determined by the Poisson equation:

$$\text{div grad } \Psi = \frac{q}{\varepsilon} \cdot (n - p - C) \qquad (16)$$

The quantity C represents the total net concentration of all ionized impurities. For a system with k impurities we have:

$$C = - \sum_{i=1}^{k} z_i \cdot (Ct_i - Cc_i) \qquad (17)$$

Note that in (17) the influence of, e.g., charged vacancies is neglected. In all process modeling programs I am familiar with the Poisson equation is not solved as an elliptic differential equation, but rather assuming vanishing space charge and Boltzmann statistics. The electrostatic potential can then be calculated explicitly.

$$\Psi = \frac{k \cdot T}{q} \cdot \text{arsinh}(\frac{C}{2 \cdot n_i}) \qquad (18)$$

n_i denotes the intrinsic concentration at the process temperature. It may be modeled as depending on the concentration of dopants, thus, representing an effective intrinsic concentration. The assumption of vanishing space charge is very poor when considering the coupled diffusion in a structure with pn-junctions. This problem is stressed in /5/.

In the literature one can often find that field enhanced diffusion is accounted for with a so-called field enhancement factor multiplying the diffusion coefficient. It should be noted that the approach using a field enhancement factor is only correct if just one species of impurities is involved in the diffusion process.

In the following I should like to discuss models for the diffusion coefficient D_i. It is well established that the diffusion vehicles are the intrinsic point defects of the lattice, i.e. vacancies and interstitials /130/. Evidence exists that both kinds of defects are important for the diffusion of dopants in silicon. However, at this time there is a lack of mathematical models describing the diffusion by interstitials. Therefore, the following considerations are based on the vacancy mechanism. Hence, the diffusion coefficient D_i is assumed to be the sum of several diffusivities /11/, where each accounts for the impurity interactions with different charge states of lattice vacancies.

$$D_i = D_i^O + D_i^- \cdot V^- + D_i^= \cdot V^= + D_i^+ \cdot V^+ \qquad (19)$$

D_i^O is the diffusion coefficient for the dopants of the i-th species diffusing with neutral vacancies, D_i^- for those diffusing with singly negative charged vacancies, $D_i^=$ for those diffusing with doubly negative charged vacancies, and D_i^+ for those diffusing with singly positive charged vacancies. Other types of configurations are certainly also imaginable; however, the cited ones are considered to be most relevant. V^-, $V^=$ and V^+ are the concentrations of singly negative, doubly negative and singly positive charged vacancies normalized by the concentration of neutral vacancies. These concentrations can be modeled under the validity of Boltzmann statistics as:

$$V^- = \frac{n}{n_i} , \quad V^= = (\frac{n}{n_i})^2 , \quad V^+ = \frac{p}{n_i} \qquad (20)$$

n and p denote the electron and hole concentration, respectively. The individual diffusion coefficients D_i^x are usually given as expressions in Arrhenius form:

$$D_i^x = D_{oi}^x \cdot \exp(- \frac{E_{ai}^x}{k \cdot T}) \qquad (21)$$

Numerical values for the prefactors D_{oi}^x and the so-called activation energies E_{ai}^x are summarized in /54/, /55/, /119/, /134/.

Although the model (19) for the diffusion coefficient is already quite sophisticated, it has

to be applied very carefully. An additional modification, usually an enhancement, of the diffusivity takes place in oxidizing ambients as will be discussed in the next section.   If the dopant concentration becomes so high that it approaches its solubility limit in silicon - this is the case in many practical applications - the impurities are considered to precipitate or to cluster, and they will, supposingly, not diffuse. However, quantitative statements are very difficult to make at the moment. The interested reader should carefully check the, hopefully, forthcoming literature on that problem and related ones.   Currently, the most frequently used model which describes the relation between the total concentration Ct and the electrically inactive (e.g. cluster) concentration Cc is based on   the   following differential equation.

$$\frac{\partial Cc}{\partial t} = m \cdot kc \cdot (Ct - Cc)^m - kd \cdot Cc \tag{22}$$

kc and kd are the clustering and declustering rate, respectively. These are usually assumed to be temperature dependent. m is the cluster size, i.e., the number of impurity atoms which form an electrically inactive complex, the cluster. However, in /152/ it is explained, particularly for arsenic, that the allowance for electrically charged clusters seems to improve the agreement with experimental results. Different types of charged and uncharged clusters are further considered in /68/. These effects become significant when the dopant concentration reaches the solubility limit (e.g. $3 \cdot 10^{20}$ cm^{-3} for arsenic at 1000 Celsius). I should like to speculate that in essence these statements are correct, but in order to derive models which are applicable for engineering purposes much more investigatory work has still to be carried out.

Very often it is assumed that the effect of dynamic clustering and declustering is negligible. Then we obtain an algebraic, equilibrium cluster relation between the total and the electrically active concentration.

$$Ct = (Ct - Cc) + \beta c \cdot (Ct - Cc)^m \tag{23}$$

$$\beta c = m \cdot \frac{kc}{kd} \tag{24}$$

Numerical values and the temperature dependence of the equilibrium cluster coefficient βc are presented in the report /119/.

Oxidation

The thermal oxidation of silicon is one of the most important processing steps for the fabrication of modern devices. All existing models for oxide growth are based on the work of Deal and Grove in 1965 /40/. Their basic idea was the assumption of a steady state situation between three fluxes.

$$F1 = h \cdot (C^* - C^0) \tag{25}$$

$$F2 = -D \cdot \frac{\partial c}{\partial x} \doteq D \cdot \frac{C^0 - C^i}{x_{ox}} \tag{26}$$

$$F3 = k_s \cdot C^i \tag{27}$$

F1 is the flux of oxidant from the bulk of the gas to the gas-oxide interface. C^0 is the concentration of the oxidant at the oxide surface; C is the concentration of the oxidant in the oxide, which will be in equilibrium with the partial pressure in the bulk of the gas; and h is the gas phase mass transfer coefficient.

F2 denotes the flux across the oxide, which is assumed to be purely diffusive. C^i is the oxidant concentration in the oxide at the oxide-silicon interface; x_{ox} represents the oxide thickness.

F3 is the flux corresponding to the oxidation reaction at the oxide-silicon interface. k_s represents the chemical surface reaction rate /67/. In the steady state condition these three fluxes are identical and can be expressed:

$$F = \frac{k_s}{1 + \frac{k_s}{h} + \frac{k_s \cdot x_{ox}}{D}} \cdot C^* \tag{28}$$

The flux of oxidant reaching the oxide-silicon interface is described by the differential equation:

$$N_1 \cdot \frac{dx_{ox}}{dt} = F \tag{29}$$

N_1 is the number of oxidant molecules incorporated into a unit volume of oxide. The solution of (29) is:

$$x_{ox}(t) = \sqrt{(\frac{A}{2}+x_{ox}(0))^2 + B \cdot t} - \frac{A}{2} \tag{30}$$

with:

$$A = 2 \cdot D \cdot (\frac{1}{k_s} + \frac{1}{h}) \tag{31}$$

$$B = \frac{2 \cdot D \cdot C^*}{N_1} \tag{32}$$

B is refered to as the parabolic growth rate coefficient because for large t (8.9) approaches:

$$x_{ox}^2(t) = B \cdot t \ , \quad t \gg \frac{A^2}{4 \cdot B} \tag{33}$$

For small time we observe that B/A describes a linear growth rate:

$$x_{ox}(t) = \frac{B}{A} \cdot (t + \tau) \ , \quad t \ll \frac{A^2}{4 \cdot B} - \tau \tag{34}$$

By proper modeling of the growth rate coefficients, many ambient attributes can be accounted for (composition, pressure, ...). However, for very thin oxides the flux models (25) to (27) appear to be oversimplified and have to be modified /76/, /119/. An empirical formula for thin oxide thicknesses corresponding to (29) reads:

$$\frac{dx_{ox}}{dt} = \frac{B + K_1 \cdot \exp(- \frac{t}{\tau_1}) + K_2 \cdot \exp(- \frac{t}{\tau_2})}{2 \cdot x_{ox} + A} \tag{35}$$

A and B are defined in (31) and (32), respectively. The two supplementary terms compared to (29) involve functions decaying exponentially in time which dominate, as it has been confirmed by observation of an extensive collection of experimental data /119/, oxide growth in the 2nm and 20nm regime, respectively. One can expect, however, that many more modifications of this type will be introduced in order to account heuristically for effects which can be seen experimentally but have not been understood completely on a theoretical basis. As excellent reviews on the many problems of oxidation /119/, /120/ can be recommended. A more fundamental treatment of the kinetics of oxide growth, which is based on the solution of the Navier-Stokes hydrodynamic equation, has fortunately begun /28/. The most complete models for the growth rate coefficients B/A and B have been summarized in /103/, /119/.

Another effect which has to be considered in the context of oxidation is the impact on the diffusion coefficient. It has been observed by several authors, e.g. /6/, /96/, /97/, that the diffusivity is enhanced. This enhancement is, most plausibly, based on diffusion mechanisms additionally to the vacancy diffusion mechanisms which we have outlined in the last section. The additional mechanism is due to intrinsic interstitials emitted from the oxidized surface as suggested by Hu /75/ and proved experimentally by, e.g. Antoniadis and Moskowitz /9/, /10/. Some theoretical considerations on this subject can be found in /100/. It is not clear at present how the vacancy and the interstitialcy mechanism interact, or which one dominates, in the temperature range [800,1000]C /58/. Therefore, we have restricted ourselves solely to the vacancy diffusion mechanism in the last section. However, by postulating an enhancement of the interstitial concentration and their self diffusion during oxidation /6/, /11/, /12/ an increase in the diffusivity of dopants is sound. Taniguchi et al. /147/ have suggested modifying the diffusivity of boron and phosphorus, particularly, with the following empirical expression:

$$D = D_V + K \cdot (\frac{\partial x_{ox}}{\partial t})^{0,3} \cdot \exp(- \frac{x}{25 \mu m} - \frac{2,08eV}{k \cdot T}) \tag{36}$$

$$\mathbf{K} = \begin{cases} <100> & 3,08 \cdot 10^{-3} \ \dfrac{cm^{1,7}}{s^{0,7}} \\ \\ <111> & 2,67 \cdot 10^{-3} \ \dfrac{cm^{1,7}}{s^{0,7}} \end{cases} \tag{37}$$

D_v is the effective diffusion coefficient for inert ambients; x denotes the distance to the oxide-silicon interface; $\mathbf{K}$ is a constant derived from fits to experimental data. The qualitative dependence of the oxidation enhanced diffusion coefficient upon the oxide growth rate, the distance to the interface and temperature is plausible. Therefore, pragmatically, such a model can prove to be very valuable, but it clearly demonstrates how poorly the diffusion kinetics are understood. It should be noted that oxidation retarded diffusion has also been observed experimentally, e.g. /119/. This effect can be made plausible by the allowance of vacancy consumption by interstitials during oxidation. Similar models to (36) can be found in /8/, /119/, /122/, /123/.

DEVICE MODELING

The most familiar model of carrier transport in a semiconductor device has been proposed by Van Roosbroeck /156/. It consists of Poisson's equation (38), the current continuity equations for electrons (39) and holes (40) and the current relations for electrons (41) and holes (42)

$$\text{div } \mathbf{\mathcal{E}} \text{ grad } \mathbf{\Psi} = -q \cdot (p - n + C) \tag{38}$$

$$\text{div } \vec{J}_n = -q \cdot (G - R) + q \cdot \partial n / \partial t \tag{39}$$

$$\text{div } \vec{J}_p = q \cdot (G - R) - q \cdot \partial p / \partial t \tag{40}$$

$$\vec{J}_n = -q \cdot (\mu_n \cdot n \cdot \text{grad } \mathbf{\Psi} - D_n \cdot \text{grad } n) \tag{41}$$

$$\vec{J}_p = -q \cdot (\mu_p \cdot p \cdot \text{grad } \mathbf{\Psi} + D_p \cdot \text{grad } p) \tag{42}$$

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 /156/ and its secondary literature or text books on semiconductor physics e.g. /21/, /73/, /131/, /139/.

However, it is of prime importance to note that the equations (41) and (42) do not characterize effects which are caused by degenerate semiconductors (e.g. heavy doping). /91/, /154/, /158/ 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 /113/, /157/. 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 (41) and (42) do not describe velocity overshoot phenomena which become apparent at feature lengths of 0.1μm for silicon and 1μm for gallium-arsenide /61/; and certainly no effects which are due to ballistic transport, the existence of which is still questionable /72/, are included. The latter start to become important for feature sizes below 0.01μm for silicon and 0.1μm for gallium-arsenide /60/. 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 /61/, /109/, /108/.

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 savely 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 /49/ 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 /49/, /151/. Some glimpses of modeling doping profiles with handy analytical expressions are given in e.g. /133/. One assumption which is usually made with satisfactory success (at room temperature) is the total ionization of all dopants (43).

$$C = N_D - N_A = N_D^+ - N_A^-$$ (43)

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 (44).

$$n = n_i \cdot e^{(\Psi - \Psi_n)/U_T} \qquad p = n_i \cdot e^{(\Psi_p - \Psi)/U_T}$$ (44)

This assumption principally neglects degeneracy; but moderate degeneracy can be included /52/ by introducing an effective, doping dependent intrinsic number (45).

$$n_i = n_i(T,N)$$ (45)

$$n_i(T,N) = n_i(T) \cdot e^{52.7K \cdot (\ln(N/10^{17}cm^{-3}) + \sqrt{(\ln(N/10^{17}cm^{-3}))^2 + 0.5})/T}$$

$$n_i(T) = 3.88 \cdot 10^{16} cm^{-3} \cdot (T/K)^{1.5} \cdot e^{-7000K/T}$$

$$N = N_D + N_A$$

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 /62/. The formula for bandgap narrowing in (45) was first suggested by Slotboom /136/. For a doping concentration of $1.3 \cdot 10^{17}$ 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 thouroghly enough to be modeled satisfactorily /77/.

Another assumption which is unfortunately not at all free of doubts is the validity of the Einstein-Nernst relations (46).

$$D_n = \mu_n \cdot U_T \qquad D_p = \mu_p \cdot U_T$$ (46)

Some guidelines on how to extend these relations for degenerate material are given in e.g. /14/. It is important to remember that the current relations (41) and (42) 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 (39) and (40). 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.

<u>Additional Assumptions for MOS-Models</u>

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. (39)-(40) may be rewritten as

$$\text{div } \vec{J}_n = 0 \qquad\qquad\qquad (47)$$

$$\vec{J}_p = 0 \qquad\qquad\qquad (48)$$

for the n-channel device and

$$\text{div } \vec{J}_p = 0 \qquad\qquad\qquad (49)$$

$$\vec{J}_n = 0 \qquad\qquad\qquad (50)$$

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 neglection 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 (47)-(50) 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. 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 /127/.
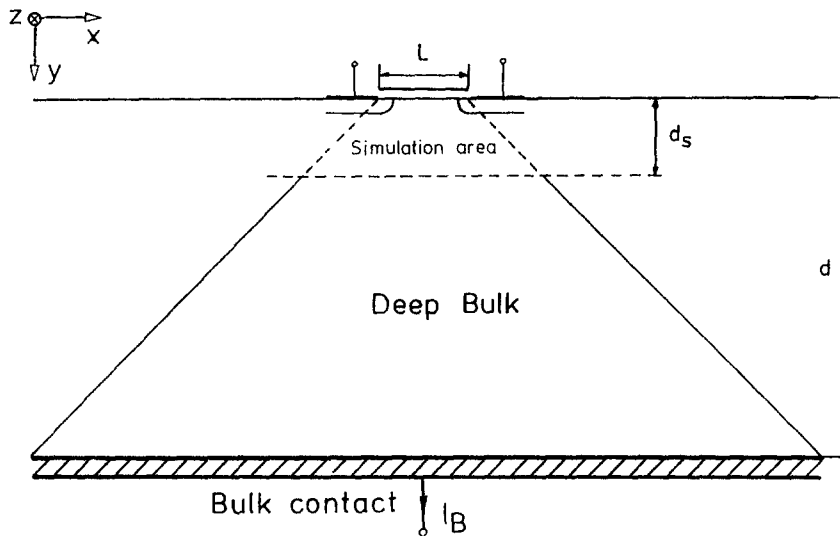
Fig. 1: Current flow in deep bulk

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 /18/ into both directions perpendicular to its flow (x- and z- direction in Fig. 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.

$$\frac{d\psi}{dy} = \frac{I_B}{KA} = \frac{I_B}{K(L+2y)(W+2y)}$$ (51)

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

$$R_{Bulk} = \frac{\int_{d_s}^{d} \frac{d\psi}{dy}\,dy}{I_B} = \frac{1}{2K(W-L)} \left(\ln(\frac{L+2d}{L+2d_s}) - \ln(\frac{W+2d}{W+2d_s}) \right) .$$ (52)

For L=W this equation simplifies to

$$R_{Bulk} = \frac{d-d_s}{K(L+2d)(L+2d_s)} .$$ (53)

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 quali-tatively.

MODELS OF PHYSICAL PARAMETERS

Modeling Mobility

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 /77/, /131/ in dependence of temperature (54).

$$\mu_L(T) = A \cdot (T/K)^{-g} \tag{54}$$

$$A_n = 7.12 \cdot 10^8 \ cm^2/Vs \qquad\qquad A_p = 1.35 \cdot 10^8 \ cm^2/Vs$$
$$g_n = 2.3 \qquad\qquad\qquad\qquad\qquad g_p = 2.2$$

The pure lattice mobility is reduced through the scattering processes at ionized impurities. (55) is a well established formula which models temperature dependent ionized impurity scattering /26/ and electron-hole scattering /52/. The latter is extremely important in low doped regions where high injection takes place.

$$\mu_{LI}(N,T) = \mu_L(T) \cdot a + \mu_{min} \cdot (1 - a) \tag{55}$$

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

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

$$\mu_{minn} = 55.24 \ cm^2/Vs \qquad\qquad \mu_{minp} = 49.7 \ cm^2/Vs$$
$$b_n = -3.8 \qquad\qquad\qquad\qquad b_p = -3.7$$
$$c_n = 0.73 \qquad\qquad\qquad\qquad c_p = 0.7$$
$$N_{0n} = 1.072 \cdot 10^{17} \ cm^{-3} \qquad\qquad N_{0p} = 1.606 \cdot 10^{17} \ cm^{-3}$$

Similar expressions which have been partly deduced from measurement and/or theory have been presented in /13/, /41/, /45/, /87/, /129/.

To properly simulate the mobility in MOS transistors, one has to deal with surface roughness and field dependent surface scattering. /33/, /124/, /143/ presented interesting measured results on inversion layer mobility; /150/, /149/ gave some excellent ideas on how to treat theoretically these and other scattering mechanisms; /163/ suggested a heuristic formula for field dependent surface scattering which is applicable for two-dimensional simulations, but whose adequacy is questioned in /150/. However, we have developed (56) which models phenomenologically with best fit to measurement surface roughness as well as field dependent surface scattering /132/.

$$\mu_{LIS}(y,E_p,E_t,N,T) = \mu_{LI}(N,T) \cdot \frac{y+y_r}{y+b \cdot y_r} \tag{56}$$

$$y_r = y_0/(1+E_p/E_{p0})$$
$$b = 2+E_t/E_{t0}$$
$$E_p = \max(0,(E_x \cdot J_x + E_y \cdot J_y)/(J_x^2+J_y^2)^{1/2})$$
$$E_t = \max(0,(E_x \cdot J_y - E_y \cdot J_x) \cdot J_x/(J_x^2+J_y^2))$$

$$y_{0n} = 5 \cdot 10^{-7} \ cm \qquad\qquad\qquad y_{0p} = 4 \cdot 10^{-7} \ cm$$
$$E_{p0n} = 10^4 \ V/cm \qquad\qquad\qquad E_{p0p} = 8 \cdot 10^3 \ V/cm$$
$$E_{t0n} = 1.8 \cdot 10^5 \ V/cm \qquad\qquad E_{t0p} = 3.8 \cdot 10^5 \ V/cm$$

In regions with a high electric field component parallel to current flow, drift velocity saturation has to be taken into account. (57) combines, also phenomenologically, this physical effect and the lattice-impurity-surface mobility using a Mathiessen-type rule with a weakly temperature dependent saturation velocity /25/, /77/, /78/.

$$\mu_{tot}(y,E_p,E_t,N,T) = (\mu_{LIS}(...)^\beta + (v_s/E_p)^\beta)^{1/\beta} \tag{57}$$

$$v_{sn} = 1.53 \cdot 10^9 \cdot T^{-0.87} \ cm/s \qquad\qquad v_{sp} = 1.62 \cdot 10^8 \cdot T^{-0.52} \ cm/s$$
$$\beta_n = -2 \qquad\qquad\qquad\qquad\qquad \beta_p = -1$$

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. (58) represents the well known Shockley-Read-Hall term for modeling thermal generation/recombination. The carrier lifetimes can be simulated as being doping dependent /36/, /104/.

$$(G - R)_{th} = \frac{n_i^2 - p \cdot n}{\tau_n(p+p_1)+\tau_p(n+n_1)} \tag{58}$$

$$\tau_n = 3.95 \cdot 10^{-5} s/(1+N/7.1 \cdot 10^{15} cm^{-3}) \qquad \tau_p = 3.52 \cdot 10^{-5} s/(1+N/7.1 \cdot 10^{15} cm^{-3})$$

Surface generation/recombination /70/ can be treated in a fairly similar manner by (59).

$$(G - R)_s = \frac{n_i^2 - p \cdot n}{(p+p_1)/s_n+(n+n_1)/s_p} \cdot \delta(y) \tag{59}$$

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

$$s_n = 100 \text{ cm/s} \qquad\qquad s_p = 100 \text{ cm/s}$$

Impact ionization can be modeled by an exponentially field dependent generation term /31/, /32/. The constants in (60) are essentially taken from /155/.

$$G_a = \frac{\bar{J}_n}{q} \cdot A_n \cdot exp \left(- \frac{B_n \cdot \bar{J}_n}{\bar{E} \cdot \bar{J}_n} \right) +$$

$$+ \frac{\bar{J}_p}{q} \cdot A_p \cdot exp \left(- \frac{B_p \cdot \bar{J}_p}{\bar{E} \cdot \bar{J}_p} \right) \tag{60}$$

$$A_n = 7 \cdot 10^5 \text{ cm}^{-1} \qquad\qquad A_p = 1.588 \cdot 10^6 \text{ cm}^{-1}$$
$$B_n = 1.23 \cdot 10^6 \text{ V/cm} \qquad\qquad B_p = 2.036 \cdot 10^6 \text{ V/cm}$$

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 /98/, /99/, Miller /105/, Chynoweth /31/, /32/, Lee /83/, Moll /110/, /111/, Ogawa /114/, Van Overstraeten /155/, Grant /63/, Dalal /37/. Their results are summarized in Fig. 2 for electrons and in Fig. 3 for holes. Additionally, the measured results are compared to theoretical results of Baraff /17/ (material constants from Sze /144/, /145/). Also drawn in Fig. 2 and Fig. 3 are theoretical limits published by Okuto /115/, /116/, 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 /71/). A more concise treatment of the ionization probabilities has been undertaken theoretically by /4/, /30/, /86/, /135/, /146/, /148/, /150/, /153/, /162/ and experimentally by /125/, /140/.

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 (61) in general gives satisfactory results /34/, /36/, /50/, /52/.

$$(G - R)_{Aug} = (n_i^2 - p \cdot n)(C_n \cdot n + C_p \cdot p) \tag{61}$$

$$C_n = 2.8 \cdot 10^{-31} \text{ cm}^6/s \qquad\qquad C_p = 9.9 \cdot 10^{-32} \text{ cm}^6/s$$

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 (62). However, that means that no interaction of the different phenomena does exist.

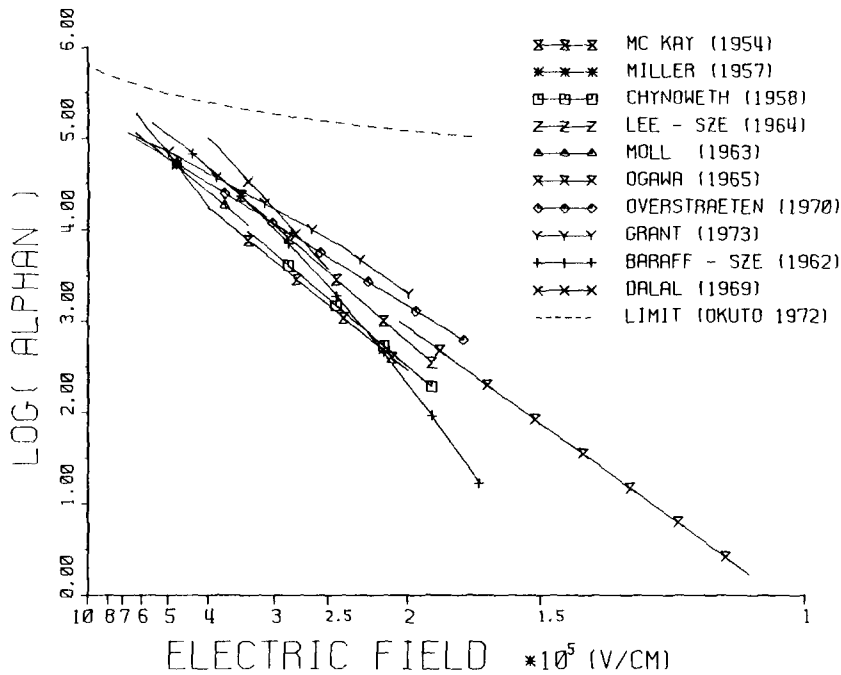$$(G-R)_{tot} = (G-R)_{th} + (G-R)_s + (G-R)_{Aug} + G_a \tag{62}$$

MC KAY (1954)
MILLER (1957)
CHYNOWETH (1958)
LEE - SZE (1964)
MOLL (1963)
OGAWA (1965)
OVERSTRAETEN (1970)
GRANT (1973)
BARAFF - SZE (1962)
DALAL (1969)
LIMIT (OKUTO 1972)

Fig. 2: Ionization probabilities for electrons

MILLER (1957)
CHYNOWETH (1958)
LEE - SZE (1964)
MOLL (1963)
OGAWA (1965)
OVERSTRAETEN (1970)
GRANT (1973)
BARAFF - SZE (1962)
LIMIT (OKUTO 1972)
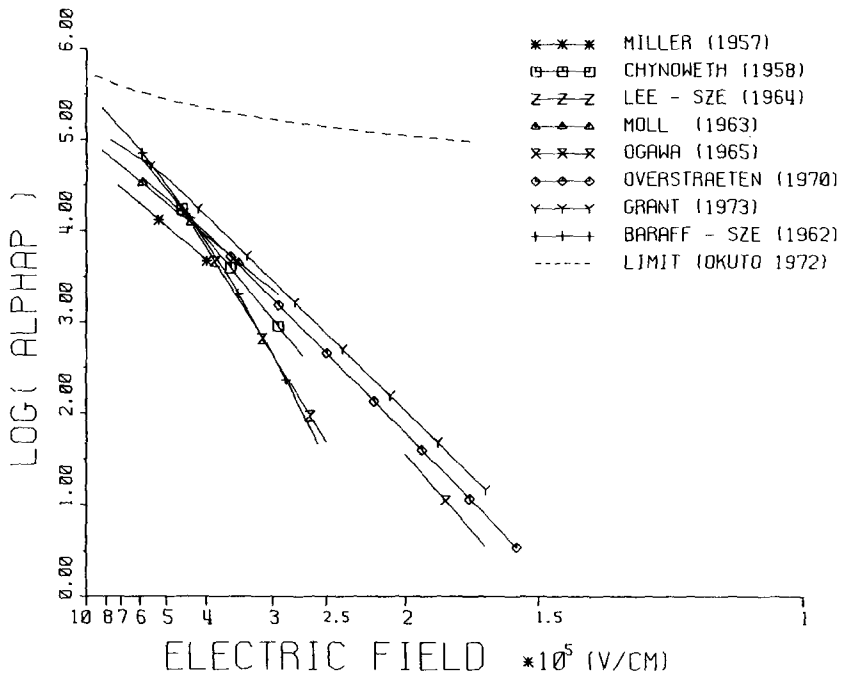
Fig. 3: Ionization probabilities for holes

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 essential indeed for the development of a numerical solution method.

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 (38)-(42) are posed in a domain D of R^n (n=1,2,3) with a piecewise smooth boundary ∂D. Equations (38)-(42) 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:

$$\partial \psi / \partial n|_{\perp} = \partial n / \partial n|_{\perp} = \partial p / \partial n|_{\perp} = 0 \tag{63}$$

Here $n_{\perp}$ 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:

$$\psi = \psi_D + \psi_{\text{built-in}}, \quad n \cdot p = n_i^2, \quad n - p - C = 0 \tag{64}$$

The last two conditions in (64) can be rewritten as:

$$n = (\sqrt{C^2 + 4 \cdot n_i^2} + C)/2$$
$$\tag{65}$$
$$p = (\sqrt{C^2 + 4 \cdot n_i^2} - C)/2$$

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:

$$\vec{J}_n \cdot n_{\perp} = \vec{J}_p \cdot n_{\perp} = 0$$
$$\tag{66}$$
$$\varepsilon_{\text{sem}} \cdot \partial \psi / \partial n_{\perp}|_{\text{sem}} = \varepsilon_{\text{ins}} \cdot \partial \psi / \partial n_{\perp}|_{\text{ins}}$$

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

Dependent Variables

For analytical purposes it is often useful to use other variables than n and p to describe the system (38)-(42). 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:

$$n = n_i \cdot e^{(\psi - \varphi_n)/U_t}, \quad p = n_i \cdot e^{(\varphi_p - \psi)/U_t} \tag{67}$$

$$n = n_i \cdot e^{\psi/U_t} \cdot u, \quad p = n_i \cdot e^{-\psi/U_t} \cdot v \tag{68}$$

(67) can be physically interpreted as the application of Boltzmann statistics. However (67) 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 (38)-(42) 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 (39), (40) and current relations (41), (42) 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 prefered for actual computations. We personally favour the set (ψ, n, p).

Scaling

Since the dependent variables in the system (38)-(42) are of different order of magnitude and show a strongly different behavior in regions with small and large space charge the first step towards a structural analysis of (38)-(42) has to be an appropriate scaling. A standard way of scaling (38)-(42) has been given by De Mari /39/. There ψ is scaled by the thermal voltage U_t, n and p are scaled by n_i (similar to Mock /106/) and the independent variables are scaled such that all multipying 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 /160/. This approach makes the system (38)-(42) accessible to an asymptotic analysis which is given together with applications in /92/, /95/ and /94/. 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	$k{\cdot}T/q$
n,p	α	$\max\|C\|$

(69)

After scaling the equations become:

$$\lambda^2{\cdot}\text{div grad }\psi = n - p - C \tag{70}$$

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

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

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 grad ψ e.g./133/ is assumed. Since the independent variable x has been scaled, equations (70) are now posed on a domain D^s with maximal diameter equal to one. The small constant λ^2 multiplying the Laplacian in (70) is the minimal Debye length of the device:

$$\lambda^2 = \frac{\epsilon{\cdot}U_t}{1^2{\cdot}q{\cdot}\alpha} \tag{71}$$

1 and α are defined in (69). Thus for high doping ($\alpha{>}{>}1$) λ^2 will be small. For instance for a silicon device with characteristic length 25μm and $\alpha=10^{20}\text{cm}^{-3}$ we compute for λ^2 at approximate room temperature T=300K: $\lambda^2=4.10^{-10}$.

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

The Singular Perturbation Approach

(70) 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 (70) by using asymptotic expansions: In the subdomains of D^s where the solutions behave smoothly we expand them into power series of the form:

$$w(x,\lambda) = \sum_{i=0}^{\infty} w_i^-(\vec{x}){\cdot}\lambda^i, \quad w=(\psi,n,p)^T \tag{72}$$

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 behavior is represented by a discontinuity across an n-1 dimensional manifold Γ:$(\vec{x}=\vec{x}(s)$, s 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:

$$C = C^\sim + C^\wedge \tag{73}$$

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 (72) is not valid and has to be supplemented by a "layer" term according to the singular perturbation analysis:

$$w(\vec{x},\lambda) = \sum_{i=0}^{\infty} [w_i^\sim(\vec{x}) + w_i^\wedge(s,t/\lambda)] \cdot \lambda^i, \quad w=(\psi,n,p)^T \tag{74}$$

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 (74) 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 $\sum w_i^\wedge \cdot \lambda^i$. $w_o^\sim$ has to satisfy the reduced equations:

$$0 = n_o^\sim - p_o^\sim - C^\sim \tag{75}$$

$$\text{div} (\text{grad } n_o^\sim - n_o^\sim \cdot \text{grad} \psi_o) = -R^\sim \tag{76}$$

$$\text{div} (\text{grad } p_o^\sim + p_o^\sim \cdot \text{grad} \psi_o) = -R^\sim \tag{77}$$

For the sake of simplicity but without loss of generality the mobilities μ_n and μ_p have been assumed to be constant. (75)-(77) is subject to the boundary conditions (63)-(66). Of course the condition of vanishing space charge is redundant with (75). Since $C^\sim$ is discontinuous at Γ and (75)-(77) represents a second order system of two equations four "interface conditions" have to be imposed at Γ. They are of the form:

$$n_o^\sim \cdot e^{-\psi_o}|_{\vec{x}=\vec{x}-} = n_o^\sim \cdot e^{-\psi_o}|_{\vec{x}=\vec{x}+} \tag{78}$$

$$p_o^\sim \cdot e^{\psi_o}|_{\vec{x}=\vec{x}-} = p_o^\sim \cdot e^{\psi_o}|_{\vec{x}=\vec{x}+} \tag{79}$$

$$\vec{J}_{n_o}^\sim \cdot n\llcorner|_{\vec{x}=\vec{x}-} = \vec{J}_{n_o}^\sim \cdot n\llcorner|_{\vec{x}=\vec{x}+} \tag{80}$$

$$\vec{J}_{p_o}^\sim \cdot n\llcorner|_{\vec{x}=\vec{x}-} = \vec{J}_{p_o}^\sim \cdot n\llcorner|_{\vec{x}=\vec{x}+} \tag{81}$$

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

$$\vec{J}_{n_o}^\sim = \text{grad } n_o^\sim - n_o^\sim \cdot \text{grad } \psi_o$$

$$\tag{82}$$

$$\vec{J}_{p_o}^\sim = \text{grad } p_o^\sim + p_o^\sim \cdot \text{grad } \psi_o$$

(75)-(77) together with (78)-(81) and the boundary conditions (63)-(66) 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 (78)-(81)) has to be solved implicitly by any discretisation method which requires a reasonable number of grid points.

The equations for the rapidly varying parts $w_i^\wedge$ 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 $w_i^\wedge$ 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.

NUMERICAL SOLUTION OF THE SEMICONDUCTOR EQUATIONS

In this chapter we discuss some of the problems occuring 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 (38)-(42). As outlined in the previous chapter the solution exhibits a smooth behavior 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 R^2 and $\vec{x} = (x,y)^T$ denotes the independent variable.

Discretization Schemes

Using Finite Elements or Finite Differences one has to take into account that Poisson's equation (38) is of a different type than the continuity equations. Poisson's equation - in the scaling of Markowich /92/ using the variables (ψ,u,v)

$$\lambda^2 \cdot \text{div grad } \psi = e^\psi \cdot u - e^{-\psi} \cdot v - C \tag{83}$$

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. /56/) except for the discontinous 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 equation (83) is discretized by:

$$\lambda^2 \cdot (\text{div grad}_h \psi)_{ij} = n_{ij} - p_{ij} - C(x_i,y_j) \tag{84}$$

$$E^x_{i+1/2,j} = (\psi_{i+1,j} - \psi_{i,j})/h_i$$

$$E^y_{i,j+1/2} = (\psi_{i,j+1} - \psi_{i,j})/k_j \tag{85}$$

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

$$(\text{div grad } \psi)_{i,j} = 2 \cdot (E^x_{i+1/2,j} - E^x_{i-1/2,j})/(h_i + h_{i-1}) +$$

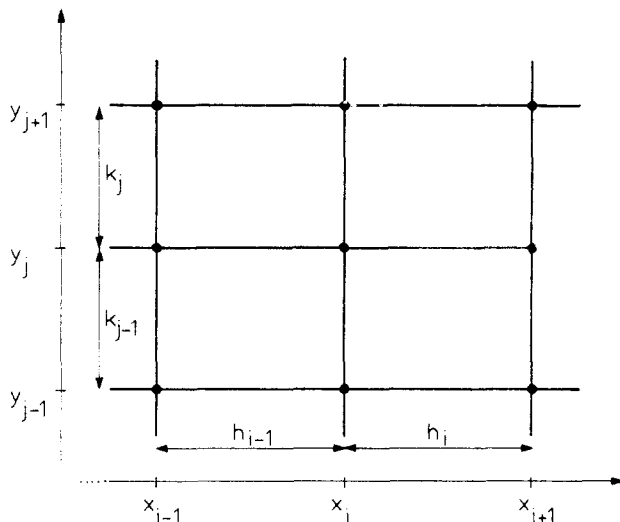$$+ 2 \cdot (E^y_{i,j+1/2} - E^y_{i,j-1/2})/(k_j + k_{j-1}) \tag{86}$$

Fig. 4: 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 /59/ - (86) 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:

$$\max |w_h - w| <= c \cdot H \tag{87}$$

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 /95/ shows that derivatives of ψ, $n^{\wedge}$ and $p^{\wedge}$ in (74) are of magnitude $O(\lambda^{-3}) - O(\lambda^{-4})$ locally near the junction (λ is defined in (71)). /95/ shows also that, even if a nonuniform mesh is used, the amount of gridpoints required to equidistribute the error term in (87) can be proportional to λ^{-2} which is of course prohibitive. Therefore a discretisation scheme is needed where the constant c in (87) does not depend on the higher derivatives of the rapidly varying terms ψ, $n^{\wedge}$ and $p^{\wedge}$. For the case of Finite Differences such a scheme was given by Scharfetter and Gummel /129/. They approximate:

$$\vec{J}_n = \text{grad } n - n \cdot \text{grad } \psi \tag{88}$$

$$\text{div } \vec{J}_n = \partial J_n^x/\partial x + \partial J_n^y/\partial y = R \tag{89}$$

by:

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

$$J_{n_{i,j+1/2}}^y = \Upsilon((\psi_{i,j+1} - \psi_{i,j})/2) \cdot (n_{i,j+1} - n_{i,j})/k_j - \tag{90}$$
$$- (n_{i,j} + n_{i,j+1})/2 \cdot (\psi_{i,j+1} - \psi_{i,j})/k_j$$

$$\Upsilon(s) = s \cdot \coth(s)$$

$$2 \cdot (J_{n_{i+1/2,j}}^x - J_{n_{i-1/2,j}}^x)/(h_i + h_{i-1}) +$$

$$+ 2 \cdot (J^y_{n_{i,j+1/2}} - J^y_{n_{i,j-1/2}})/(k_j + k_{j-1}) = R_{i,j} \tag{91}$$

The continuity equation for holes is discretized analogously. Scharfetter and Gummel gave a physical reasoning for the derivation of their scheme. Markowich et al. /95/ proved that in one dimension the Scharfetter-Gummel scheme is uniformly convergent. That means that the error constant c in (87) does not depend on the derivatives of Ψ, $n^{\char`\^}$ and $p^{\char`\^}$ in (74) and therefore not on λ. For two dimensions /95/ shows that the choice $\Upsilon(s) = s \cdot \coth(s)$ is necessary for uniform convergence. Exponentially fitted schemes like the Scharfetter-Gummel scheme have been analyzed by Kellog /81/, /80/ and Doolan /44/ (for different classes of problems). The reason for the uniform convergence of these schemes is that inside the pn-junction layers the interface conditions (78)-(81) 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 /51/ 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 /22/, /23/, /35/. 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. /121/. Macheck /89/ 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

$$\alpha_1(x,y) = [1 - \Psi_1(x,y)] \cdot [1 - \Psi_2(x,y)]$$
$$\alpha_2(x,y) = \Psi_1(x,y) \cdot [1 - \Psi_2(x,y)]$$
$$\alpha_3(x,y) = \Psi_1(x,y) \cdot \Psi_2(x,y)$$
$$\alpha_4(x,y) = [1 - \Psi_1(x,y)] \cdot \Psi_2(x,y) \tag{92}$$

for u, and

$$\beta_1(x,y) = [1 - \sigma_1(x,y)] \cdot [1 - \sigma_2(x,y)]$$
$$\beta_2(x,y) = \sigma_1(x,y) \cdot [1 - \sigma_2(x,y)]$$
$$\beta_3(x,y) = \sigma_1(x,y) \cdot \sigma_2(x,y)$$
$$\beta_4(x,y) = [1 - \sigma_1(x,y)] \cdot \sigma_2(x,y) \tag{93}$$

for v, where

$$\Psi_1(x,y) = f(x, \frac{\partial \Psi}{\partial x})$$
$$\Psi_2(x,y) = f(y, \frac{\partial \Psi}{\partial y})$$
$$\sigma_1(x,y) = f(x, -\frac{\partial \Psi}{\partial x})$$
$$\sigma_2(x,y) = f(y, -\frac{\partial \Psi}{\partial y}) \tag{94}$$

with: $f(x,a) = (\exp(ax)-1)/(\exp(a)-1)$ \tag{95}

The advantage of these shape functions is that they accomodate nicely the layer behavior 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 /89/. However, no theoretical investigations have been carried out so far to analyse the uniform convergence properties of this method.

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 /24/. 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. First 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 /95/ 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 (75)-(77) 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.

Linearization 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 /69/ and uses the fact that the current relations are linear in the variables u and v (as defined in (68)). In these variables the equations become (again we use the scaling of /89/):

$$\lambda^2 \cdot \text{div grad } \psi = e^{\psi} \cdot u - e^{-\psi} \cdot v - C \tag{96}$$

$$\text{div } \vec{J}_n = R, \quad \vec{J}_n = e^{\psi} \cdot \text{grad } u \tag{97}$$

$$\text{div } \vec{J}_p = -R, \quad \vec{J}_p = -e^{-\psi} \cdot \text{grad } v \tag{98}$$

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

$$\lambda^2 \cdot \text{div grad } \psi^{k+1} = e^{\psi^{k+1}} \cdot u^k - e^{-\psi^{k+1}} \cdot v^k - C \tag{99}$$

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

$$\tag{100}$$

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

$$\tag{101}$$

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

together with the boundary conditions for u and v. (100) and (101) are two decoupled linear equations for u^{k+1} and v^{k+1}. Poissons's equation (99) 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 (99)-(101) it may not be necessary to let this inner iteration "fully converge" /64/.

The advantage of Gummels's method is obvious. (99)-(101) 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 (99)-(101) 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 (99). 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 /93/.

The second approach to the solution of the nonlinear equations (38)-(42) is a damped

modified Newton method. To solve the general equation $F(x)=0$ one computes the sequence $\langle x^k \rangle$ by:

$$M^k \cdot d^k = -F(x^k), \quad x^{k+1} = x^k + t^k \cdot d^k \tag{102}$$

For the usual Newton method $M^k = F'(x^k)$ and $t^k = 1$ holds. Bank and Rose /16/ 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:

$$|M^k \cdot d^k + F(x^k)| = O(|F(x^k)|^p) \tag{103}$$

holds asymptotically for $k \to \infty$.

Alternatively Bank and Rose /15/ suggested $M^k = \lambda^k I + F'(x^k)$ where λ^k is proportional to $|F(x^k)|$. Franz /59/ tested this method with good success. However, he additionally chooses damping parameters t^k according to Deuflhard /42/, /43/.

Solution of Linear Systems

For any of the linearization procedures which have been outlined in the last chapter a large sparse linear equation system (104) has to be solved repeatedly.

$$A \cdot x = b \tag{104}$$

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 /46/. Classical Gaussian elimination is not feasible for our systems of equations because the rank of A in (104) 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. /47/) 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 usually has 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 be emphasized. 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 (104) into three matrices D, E, F (105).

$$A = D - E - F \tag{105}$$

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 (104) can be rewritten to (106):

$$B \cdot x + (A-B) \cdot x = b \tag{106}$$

One obtains an iterative scheme by setting:

$$B \cdot x^{k+1} = b - (A-B) \cdot x^k \tag{107}$$

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

$$x^{k+1} = (I-B^{-1} \cdot A) \cdot x^k + B^{-1} \cdot b \tag{108}$$

The scheme (108) will converge if condition (109) holds:

$$\rho(I-B^{-1} \cdot A) < 1 \tag{109}$$

(109) is a necessary and sufficient condition where ρ denotes the spectral radius /159/. Any relaxation method can be derived by differently choosing the matrix B from the splitting of A (105). The simplest scheme, the point-Jacobi method, uses D for B. Matrix D is a diagonal matrix and, therefore, it 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 w within the range $]0,2[$. The iteration matrix B is defined:

$$B = D/w - E \tag{110}$$

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 (109) holds. However, this is generally difficult to prove. A sufficient condition for convergence is that A is positive definite (111) which is the normal case for five-point-star discretized PDEs.

$$x^T \cdot A \cdot x > 0 \quad \text{for all } x \neq 0 \tag{111}$$

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 (47), (48)). However, the transformation:

$$n = e^{\psi} \cdot u, \quad p = e^{-\psi} \cdot v \tag{112}$$

results in a similarity transformation of the iteration matrix in (109).
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 by accelerated quite remarkably with the conjugate gradient method or the Chebyshev method. An excellent survey on these topics can be found in /65/, /66/.

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 /142/. 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:

$$(A+N) \cdot x = (A+N) \cdot x + (b-A \cdot x) \tag{113}$$

which suggests the iterative procedure:

$$(A+N) \cdot x^{k+1} = (A+N) \cdot x^k + (b-A \cdot x^k) \tag{114}$$

When the right hand side is known and if (A+N) can be factorized easily, (114) 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. /57/, /137/, /142/. 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 /59/ 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. /48/, the "alternating direction implicit" methods e.g. /20/, /57/, /161/ and the Fourier methods /141/, /159/. 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 (115) is applied with a properly chosen relative accuracy ε:

$$|x^{k+1}-x^k| < \varepsilon \cdot |x^{k+1}| \tag{115}$$

Since increments still accumulate when (115) is already satisfied we suggest to use (116) instead of (5.12):

$$|x^{k+1}-x^k| < \varepsilon \cdot |x^{k+1}| \cdot (1-\rho(G)) \tag{116}$$

ρ (G) can be estimated as $\lim\limits_{k\to\infty} |x^{k+1}-x^k|/|x^k-x^{k-1}|$.

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 /46/.

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 shows the doping profiles of two devices the geometrical channel length of which is 1.6μm. The oxide thickness is 30nm; the junction depth is about .44μ and the lateral subdiffusion is about 0.23μm. The profile on the right hand side has just an additional channel implantation in order to suppress the punch through effect. We shall now discuss 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. 6, Fig. 7 and Fig. 8) corresponds to the doping profile on the right hand side of Fig. 5.
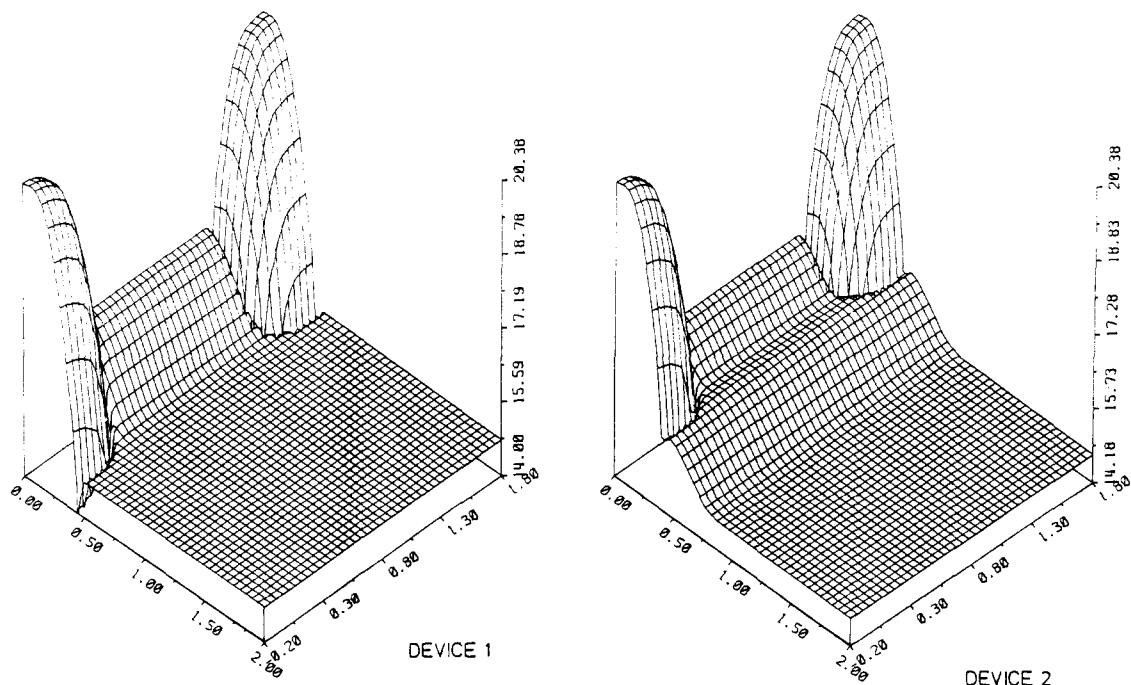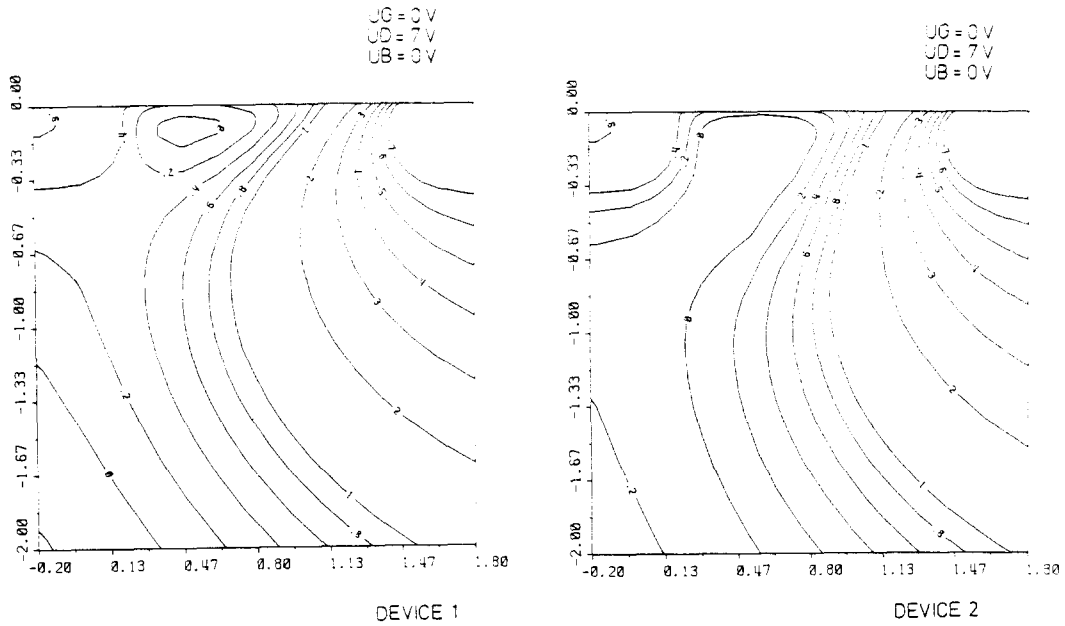

Fig. 5: Device 1 - Doping profile - Device 2

Fig. 6: Device 1 — Electric potential — Device 2

Fig. 6 shows the contour lines of the electric potential for both devices. We can nicely 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 multi 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 behavior.

Fig. 7 shows the electron distribution in a logarithmic scale. The punch through channel is fully suppressed by the deep channel implant. It also seems wortwhile to note that the qualitative behavior of the electron density at the surface is identical for both devices.
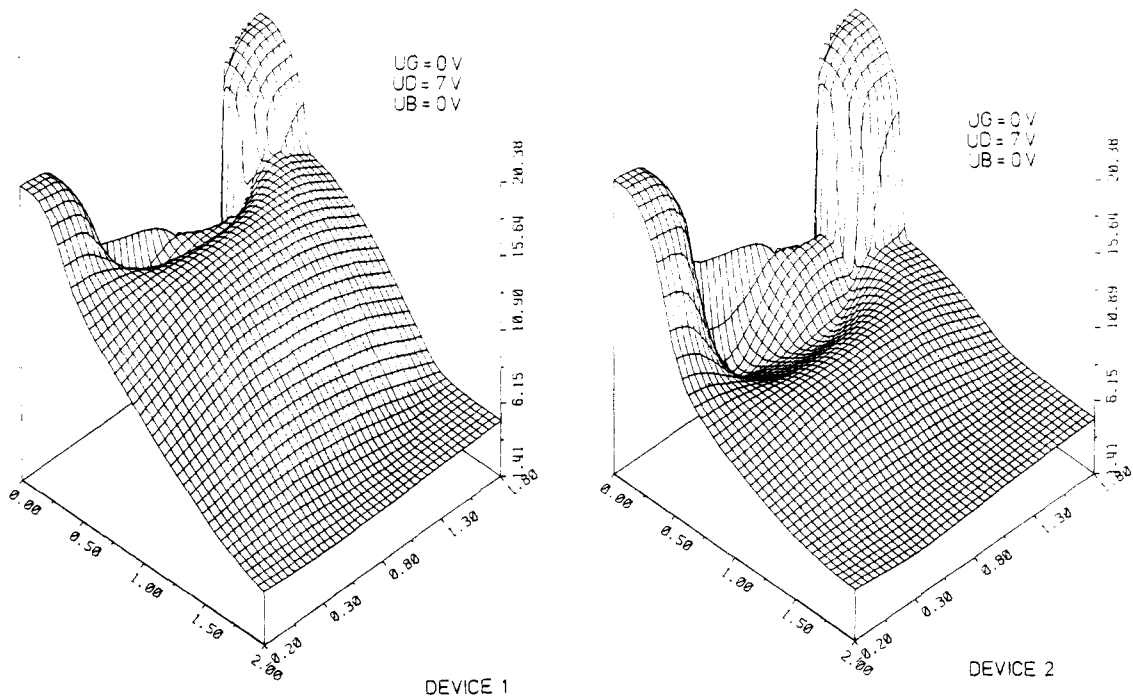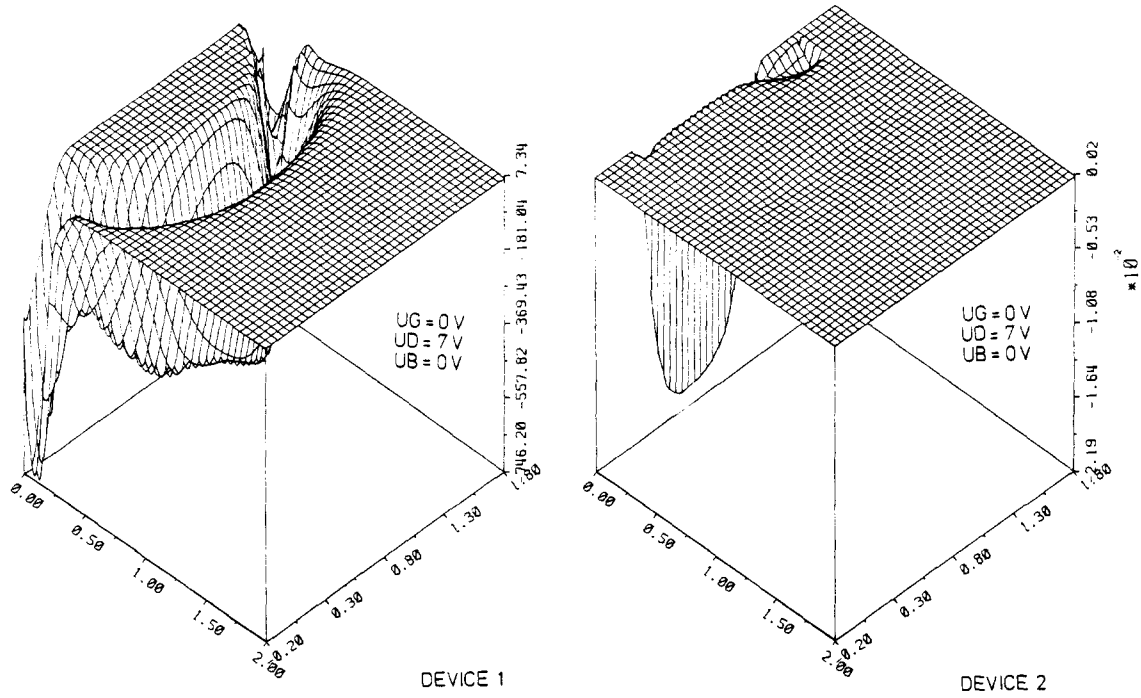

Fig. 7: Device 1 — Electron density — Device 2

Fig. 8: Device 1 – Electron current density – Device 2

In Fig. 8 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 /126/, /128/. 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 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.
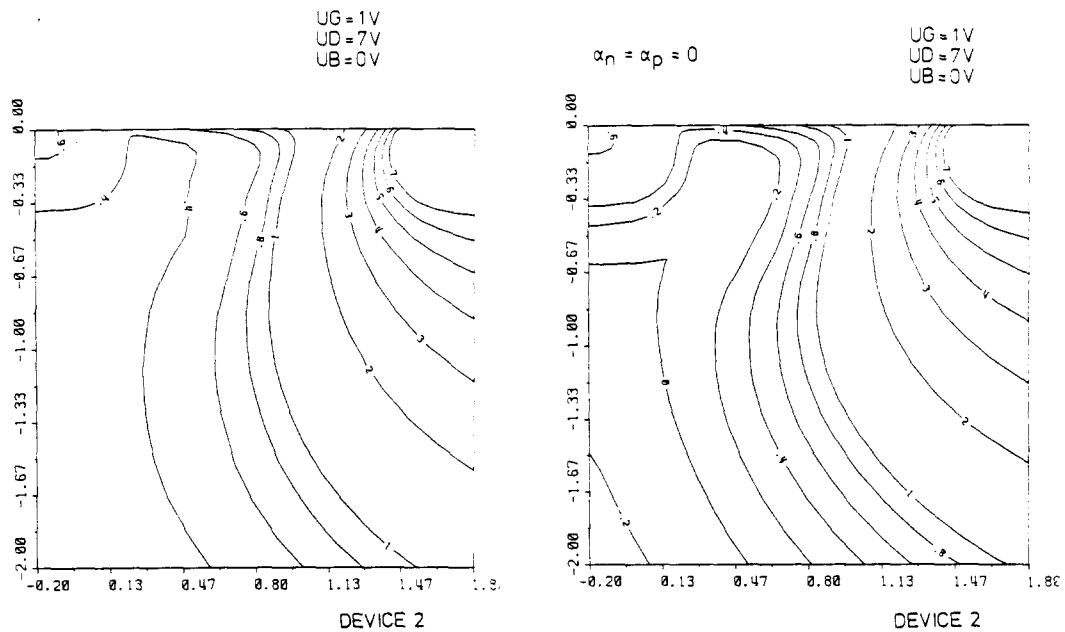

Fig. 9: with aval. – Electric potential – without aval.

Fig. 9 shows the electric potential. Almost no barrier exists between source and channel, whereas an acceptable barrier is still simulated when neglecting impact ionization.
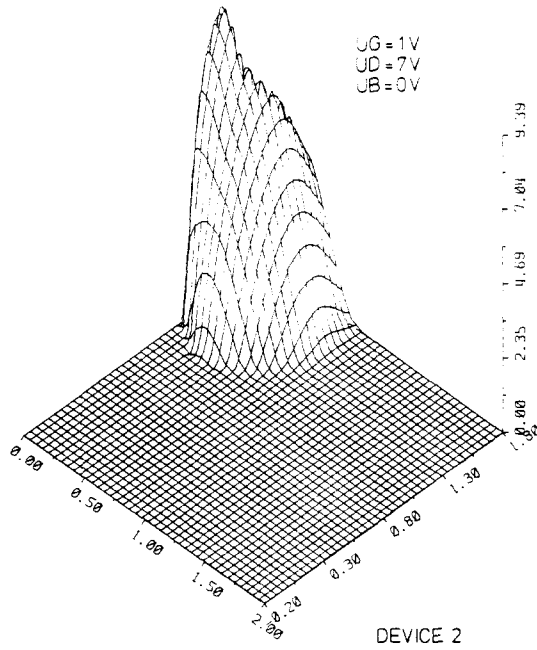

Fig. 10: with aval. - Generation rate - without aval.

In Fig. 10 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. 11 and Fig. 12. A large increase of the carrier densities due to avalanche generation can be seen from these figures. This inrease results not only from carrier generation but also from the rigid source-substrate barrier lowering (cf. Fig. 9).
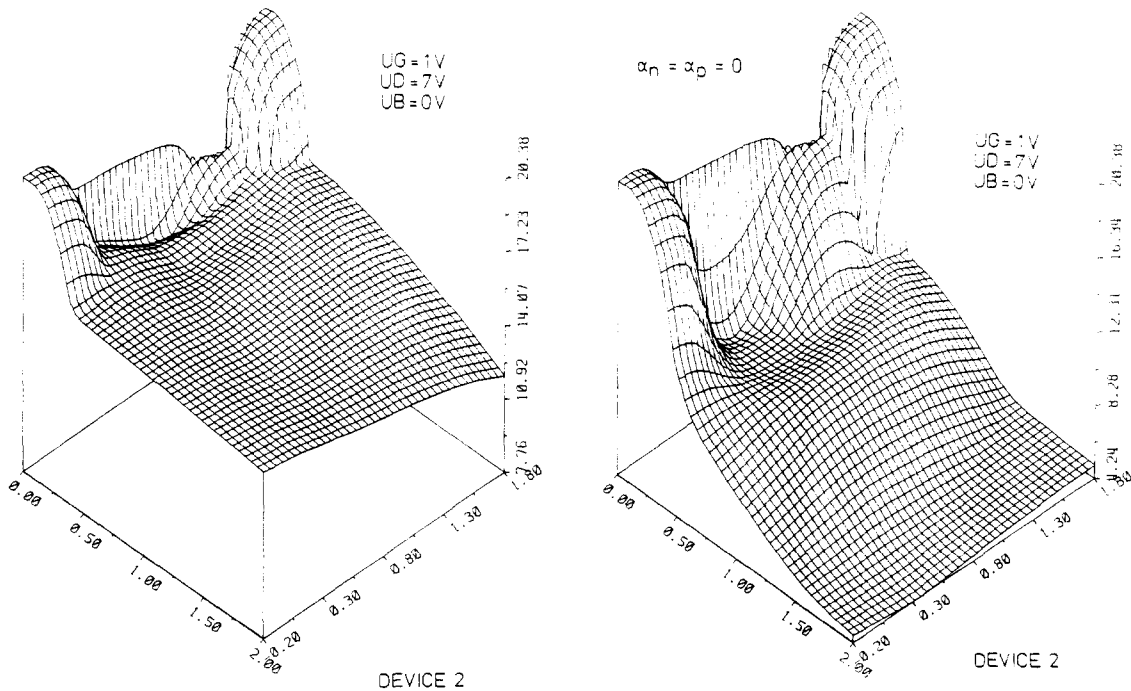

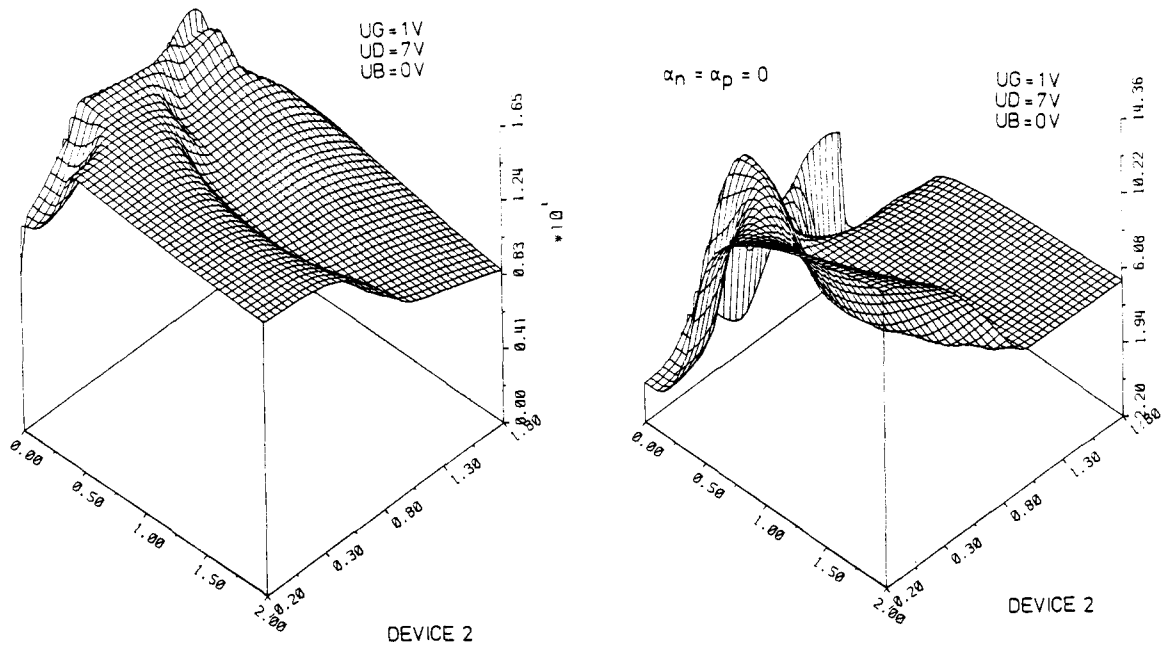Fig. 11: with aval. - Electron density - without aval.

UG = 1V
UD = 7V
UB = 0V

$\alpha_n = \alpha_p = 0$

UG = 1V
UD = 7V
UB = 0V

DEVICE 2

DEVICE 2

Fig. 12: with aval. - Hole density - without aval.

CONCLUSION

The state of the art in modeling processes and the electrical behavior of semiconductor devices has been sketched. The underlying physics has been discussed and the importance of increasingly sophisticated numerical methods has briefly been outlined. It has become evident that only progress in basic physics will lead to the development of models which are capable of simulating device behavior 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. The power of a numerical model to predict device behavior has been demonstrated using our MOS-transistor simulation program MINIMOS.

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