STEADY STATE SEMICONDUCTOR DEVICE MODELLING
A STATE OF THE ART REPORT

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ABSTRACT

In this paper we present a state-of-the-art report on mathematical and numerical steady state semiconductor device modeling. As underlying device model we use the basic semiconductor device equations, which consist of Poisson's equation, the current relations and the continuity equations. By appropriate scaling we reformulate the device problem as singularly perturbed elliptic system with the characteristic Debye length λ as perturbation parameter. Asymptotic analysis for $\lambda \to 0+$ is used to analyse the structure of solutions. We employ the information obtained by the perturbation analysis to develop appropriate numerical simulation techniques and present simulation results for a MOS-transistor.

1. THE MATHEMATICAL MODEL

The system of partial differential equations, which describes potential distribution and current flow in an arbitrary semiconductor device, is - in the steady state case - given by (see (8),(11)):

$$\left.\begin{aligned}
&(1.1)\quad \varepsilon\Delta\psi = -q(p-n+C(x))\\
&(1.2)\quad \operatorname{div} J_n = qR\\
&(1.3)\quad \operatorname{div} J_p = -qR\\
&(1.4)\quad J_n = q(D_n \operatorname{grad} n - \mu_n n \operatorname{grad}\psi)\\
&(1.5)\quad J_p = -q(D_p \operatorname{grad} p + \mu_p p \operatorname{grad}\psi)
\end{aligned}\right\} x\in\Omega\subset\mathbb{R}^3$$

Ω denotes the semiconductor geometry. ψ denotes the electrostatic potential, $-\operatorname{grad}\psi$ the electric field, n the electron concentration, p the hole concentration, J_n the electron current density and J_p the hole current density. ε is the semiconductor permittivity constant, q the elementary charge, C the doping profile, D_n, D_p the electron and hole diffusion coefficients resp; R the recombination-generation rate. Usually Einstein's relations are assumed to hold for the mobilities μ_n, μ_p:

$$(1.6)\quad D_n = \mu_n U_T, \qquad D_p = \mu_p U_T,$$

where U_T denotes the thermal voltage. Poisson's equation (1.1) and the current continuity equations (1.2),(1.3) are directly derived from Maxwell's equations and the current relations (1.4),(1.5) are obtained from Boltzmann's transport equation by using various simplifying and partly unrealistic assumptions (see (8),(9)).
The physical parameters R, μ_n, μ_p, C have to be modeled with extreme care when accurate simulation results are desired. An assessment of commonly used models can be found in (8).
In general, the physical boundary of a device splits into insulating segments, Ohmic contacts, Schottky contacts and - for a MOS-device - a semiconductor oxide interface.
Physically appropriate boundary conditions can be found in (8).
By inserting the current relations (1.4), (1.5) into the continuity equations (1.2) and (1.3) resp. and by using Einstein's relations (1.6) we obtain

$$(1.7)\quad \operatorname{div}(\mu_n(U_T \operatorname{grad} n - n \operatorname{grad}\psi)) = R$$

$$(1.8)\quad \operatorname{div}(\mu_p(U_T \operatorname{grad} p + p \operatorname{grad}\psi)) = R$$

Poisson's equation and (1.7),(1.8) are scalar elliptic equations. Therefore the stationary semiconductor device problem constitutes a nonlinearly coupled elliptic system subject to boundary conditions.

2. SINGULAR PERTURBATION ANALYSIS

An important step towards the structural analysis of a mathematical model is an appropriate scaling, which introduces dimensionless quantities and isolates the relevant dimensionless parameter on which the model depends.
We define $\tilde{C}$ as a characteristic doping concentration, $\tilde{l}$ as a characteristic length and $\tilde{\mu}$ as a characteristic mobility of the device under consideration and introduce the scaled quantities:

$$(2.1)\quad n_s = \frac{n}{\tilde{C}},\ p_s = \frac{p}{\tilde{C}},\ \psi_s = \frac{\psi}{U_T},\ x_s = \frac{x}{\tilde{l}},\ C_s = \frac{C}{\tilde{C}},$$
$$\mu_{n_s} = \frac{\mu_n}{\tilde{\mu}},\ \mu_{p_s} = \frac{\mu_p}{\tilde{\mu}}$$

The scaled semiconductor device equations are obtained by expressing ψ,n and p in terms of ψ_s,n_s and p_s resp., observing

$$div_x = \frac{1}{l} div_{x_s}, \quad grad_x = \frac{1}{l} grad_{x_s},$$

$$\Delta_x = \frac{1}{l^2}\Delta_{x_s}$$ and by multiplying the current relations and the continuity equations by $\frac{1}{q\tilde{\mu}U_T\tilde{C}}$. They read after dropping the subscript s:

$$\left.\begin{aligned}
&(2.2)\quad \lambda^2\Delta\psi = n-p-C(x)\\
&(2.3)\quad div\, J_n = R\\
&(2.4)\quad div\, J_p = -R\\
&(2.5)\quad J_n = \mu_n(gradn - ngrad\psi)\\
&(2.6)\quad J_p = -\mu_p(gradp + pgrad\psi)
\end{aligned}\right\} x\varepsilon\Omega.$$

Ω now stands for the scaled semiconductor domain, J_n,J_p and R for the scaled current densities and recombination-generation rate resp.
λ is a characteristic normed Debye length of the device:

$$(2.7)\quad \lambda^2 = \frac{U_T\varepsilon}{l^2 q\tilde{C}}$$

For a typical Silicon device (at room temperature) of length $l \approx 5\times10^{-3}$ cm and characteristic doping concentration $\tilde{C} \approx 10^{17}cm^{-3}$ we calculate $\lambda^2 \approx 10^{-7}$. In practice λ is a small constant. It appears as multiplier of the Laplacian of the potential in Poisson's equation and is therefore expected to influence directly the variation of solutions. In the mathematical terminology a problem, in which a small parameter multiplies a derivative of highest order, is called a singular perturbation problem (see (1),(2)). The appropriate mathematical tool for the analysis of the structure of solutions of singular perturbation problems is asymptotic analysis for the singular perturbation parameter $\lambda\to0+$. At the first glance it looks intriguing to set $\lambda=0$ in (2.2) and to accept the so obtained zero-space-charge-approximation as 'neighbouring problem'. Since, in doing so, we lose one degree of freedom in imposing boundary conditions, we have to drop the conditions imposed for ψ and retain the conditions for the carrier concentrations n and p.
The performance of a semiconductor device is mainly determined by the number and location of pn-junctions, which are surfaces, at which the doping profile changes sign (boundaries between n and p-domains). Usually the doping profile varies rapidly across junctions (see (10)), and therefore we assume for simplicity that junctions are abrupt, i.e. the doping profile has jump-discontinuities across device junctions. Since the solutions of the zero-space-charge-approximation (also called reduced problem in the context of singular perturbation theory) satisfy

$$(2.8)\quad 0 = \bar{n}-\bar{p}-C \quad in\ \Omega$$

we conclude that either the 'reduced' electron concentration $\bar{n}$ or the reduced hole concentration $\bar{p}$ or both quantities are discontinuous at abrupt junctions. However, the solutions of the 'full' singularly perturbed device problem are continuous in Ω and therefore they cannot be approximated uniformly in Ω by the reduced solutions for small λ. By employing the methods of singular perturbation theory it can be shown that the reduced solutions only approximate the 'full' solutions outside thin 'layer' strips of width $0(\lambda|\ln\lambda|)$ about junctions, semiconductor oxide interfaces and Schottky contacts and that the potential and the carrier concentrations vary fast (exponentially) within the layer strips:

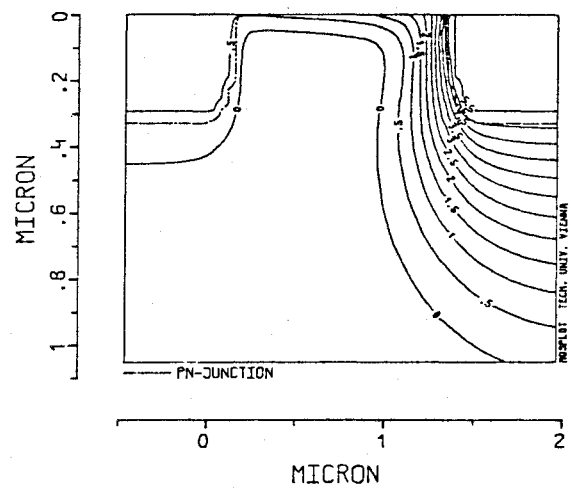
$$(2.9)\quad \begin{aligned}
|\psi-\bar{\psi}| &\le C_1\exp(-\frac{C_2 r}{\lambda}),\\
|n-\bar{n}| &\le C_1\exp(-\frac{C_2 r}{\lambda}),\\
|p-\bar{p}| &\le C_1\exp(-\frac{C_2 r}{\lambda}),
\end{aligned}$$

where r(x) denotes the normal distance of $x\varepsilon\Omega$ to the critical surface ($\bar{\psi}$,$\bar{n}$,$\bar{p}$ denote the reduced solutions). The potential and the carrier concentrations are moderately varying functions away from junctions, Schottky contacts and semiconductor-oxide interfaces. They only vary fast close to these critical surfaces.
A detailed mathematical analysis can be found in the references (4),(5) and (6).

3. NUMERICAL SIMULATION OF SEMICONDUCTOR DEVICES

For the numerical solution of the semiconductor device problem the scaled current relations (2.5),(2.6) are inserted into the scaled continuity equations (2.3),(2.4) resp. and the so obtained elliptic system is approximated by a discrete system of nonlinear equations originating from an appropriate finite difference or finite element method (see (8)). A mayor problem is the construction of appropriate meshes on which the discretisation is performed. Usually, this is done by equidistributing the local discretisation error (see (3)), which corresponds to balancing large derivatives of solutions by small meshsizes. Obviously, the solution structure obtained by the singular perturbation analysis yields large meshsizes in outer regions (away from layer strips) and small meshsizes within layer strips. Asymptotic a-priori grids can be constructed using the asymptotic behaviour of solutions (see (3)) and the convergence properties of discretisation methods can be

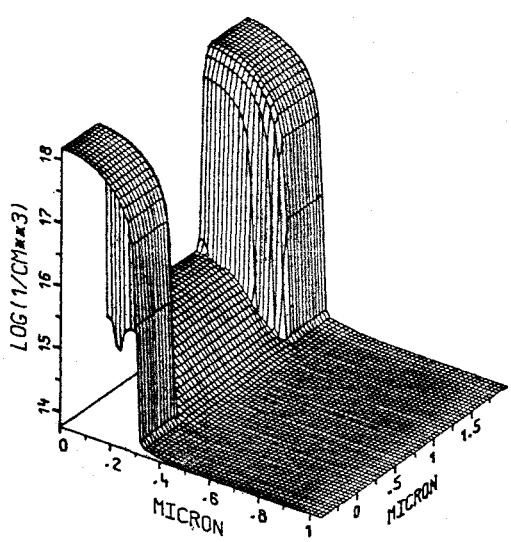
assessed.
In order to illustrate the theory we present numerical results for a MOS-transistor. The simulation was performed with the code MINIMOS (7), which uses a specialized exponentially fitted finite difference method (Scharfetter-Gummel method).
The steeply graded doping profile of the n-channel MOS-transistor is depicted in Figure 1. The channel length is 1.5 μm, the channel width 1 μm and the junction depth is approximately 0.3 μm. The applied gate-source voltage was chosen to be 2V, the drain-source voltage 5V and the source-bulk voltage is 0V. The computed drain current is 1.65×10^{-5}A and the bulk current -2.74×10^{-6}A. The device operates in the saturation regime close to breakdown since the bulk current is - due to impact ionisation - already about one sixth of the drain current.
In Figure 2 we show a level-curve plot of the potential. The electron and the hole concentrations are shown in the Figures 3 and 4. The layer strips about the two pn-junctions and at the semiconductor oxide interface - as explained by the singular perturbation analysis - are clearly visible. n,p and ψ vary moderately away from these critical surfaces. The impact ionisation rate is depicted in Figure 5.



ELECTROSTATIC POTENTIAL

Figure 2

L = 1.5 MICRON N-CHANNEL
W = 1 MICRON
UGS = 2 V
ID = 1.68E-5 A UDS = 5 V
IB = -2.74E-6 A USB = 0 V



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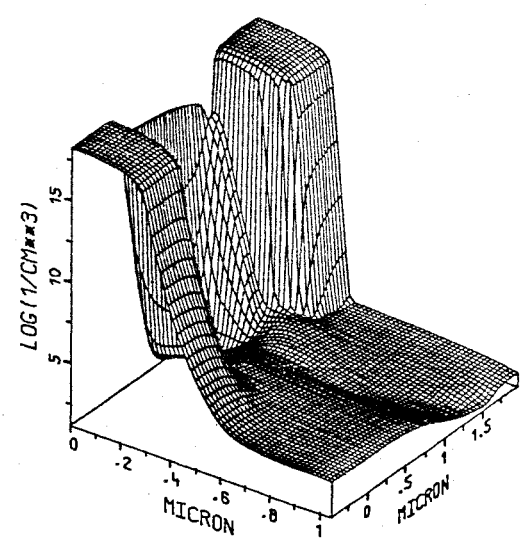
DOPING CONCENTRATION

Figure 1



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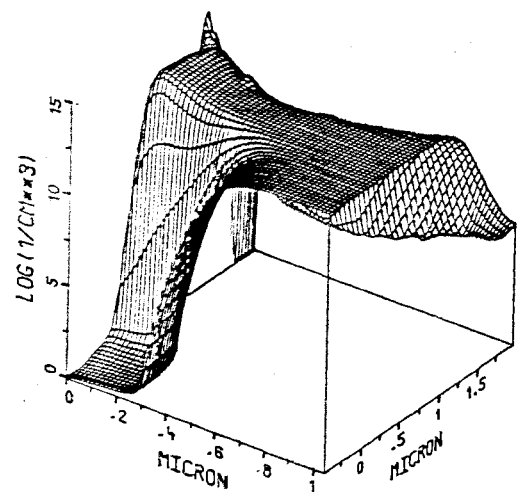
ELECTRON CONCENTRATION

Figure 3



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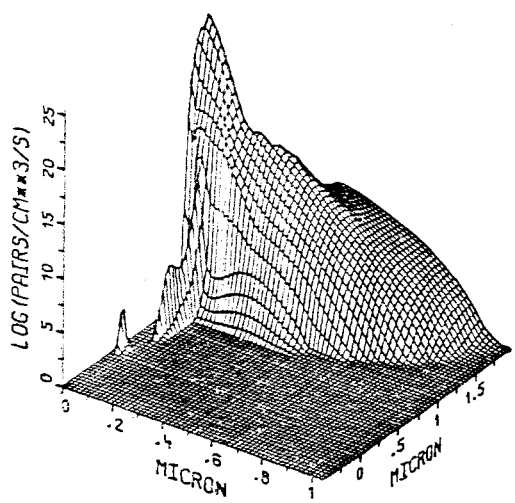
HOLE CONCENTRATION

Figure 4



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IMPACT IONIZATION RATE

Figure 5

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