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A SINGULAR PERTURBATION ANALYSIS OF THE FUNDAMENTAL SEMICONDUCTOR DEVICE EQUATIONS - ANALYSIS AND NUMERICAL EXPERIMENTS*

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ABSTRACT

We present a singular perturbation analysis of the fundamental semiconductor device equations. These describe potential and carrier distributions in semiconductor devices and are a system of three second order eliptic equations – Poisson's and the continuity equations – subject to Neumann-Dirichlet conditions. The minimal Debye-length of the device under consideration is taken as the perturbation parameter. Using matched asymptotic expansions we demonstrate the occurence of internal layers at surfaces across the impurity distribution (which appears as an inhomogeneity of Poisson's equation) has a jump-discontinuity (these surfaces are called 'junctions') and also the occurence of boundary layers at semi-conductor-oxide interfaces. We derive the layer-equations and the reduced problem (charge-neutral-approximation). The layer solutions which characterize the solution of the singularly perturbed problem close to junctions and interfaces, respectively decay exponentially away from the junctions and interfaces, respectively. Numerical results obtained with the aid of the singular perturbation analysis are presented.

RESUMO

Apresenta-se neste trabalho uma análise das equações fundamentais de semicondutores. Estas equações diferenciais, que descrevem as distribuições de potencial e 'carriers', formam um sistema elítico de segunda ordem (as equações de Poisson e continuidade) sujeito a condições de contorno mistas (Dirichlet e Neumann). Utiliza-se para a análise o método de perturbações singulares, tomando como parâmetro o menor comprimento de Debye. Com o emprego de expansões acopladas, demonstra-se a ocorrência de camadas internas em torno das junções (superfícies através das quais a distribuição de impurezas, que aparece como uma não-homogeneidade na equação de Poisson, tem um salto) como também a ocorrência de camada limite na interface semicondutor-óxido. Apresentam-se resultados numéricos obtidos mediante o emprego de perturbações singulares.

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1. INTRODUCTION

A singular perturbation analysis of the two-dimensional, static equations which describe potential distribution and current flow in a semiconductor device is presented.

The basic semiconductor device equations are (see Van Roosbroeck [14], Selberherr [11]):

$$\left.\begin{aligned} \operatorname{div}(\varepsilon_s \nabla\psi) &= q(n-p-C(x,y)) \\ \operatorname{div}(D_n\nabla n-\mu_n n\nabla\psi) &= R \\ \operatorname{div}(D_p\nabla p+\mu_p p\nabla\psi) &= R \end{aligned}\right] \quad (x,y)\in\Omega$$

Poisson's equation (1.a)

electron continuity equation (1.b)

hole continuity equation (1.c)

where the dependent variables are

ψ : electrostatic potential,
n : electron density,
p : hole density.

Ω is a bounded domain in $\mathbb{R}^2$ representing the device geometry; ε_s is the semiconductor permittivity (which will be assumed to be constant in the sequel); μ_n, μ_p are the electron and hole mobilities, respectively; D_n, D_p are the electron and hole diffusion coefficients, respectively, and q is the elementary charge. $C(x,y)$ is the doping profile, which means that it is the difference between the electrically active concentration of donors and the electrically active concentration of acceptors. R is the recombination-generation rate. In the sequel we will neglect recombination-generation effects, that means we set $R=0$. Of course only solutions with $n>0$, $p>0$ are admitted.

The electron and hole current densities J_n and J_p are given by

$$J_n = q(D_n\nabla_n - \mu_n n\nabla\psi) \tag{2.a}$$

$$J_p = -q(D_p\nabla_p + \mu_p p\nabla\psi). \tag{2.b}$$

Numerical values for the parameters (for silicon at room temperature) are given in Table 1. A detailed discussion of the physical parameters and of their modelling is given in Selberherr [11].

The elliptic system of differential equations (1) has to be supplemented by appropriate boundary conditions for ψ,n,p. We assume that $\partial\Omega$ splits up into disjoint parts, namely, $\partial\Omega_C$, $\partial\Omega_{is}$ and $\partial\Omega_{os}$. $\partial\Omega_{is}$ and $\partial\Omega_{os}$ are open, $\partial\Omega_{os}$ is connected and $\partial\Omega_C = \bigcup_{k=0}^{r} C_k$, $r \geq 0$ where the C_k are closed and connected arcs with positive (one-dimensional) Lebesgue measure, $C_i \cap C_j = \emptyset$ for $i \neq j$.

Dirichlet boundary conditions for ψ,n,p are given on $\partial\Omega$ (the C_k are Ohmic contacts) and zero Neumann boundary conditions are prescribed on $\partial\Omega_{is}$ (insulating segments). $\partial\Omega_{os}$ represents a semiconductor-oxide interface occuring in MOS-tecnology (see [13] for a survey on MOS-devices). The oxide is located in a bounded domain Φ satisfying $\overline{\Phi} \cap \overline{\Omega} = \overline{\partial\Omega_{os}}$ and

$$\Delta\psi = 0, \qquad (x,y) \in \Phi \tag{3}$$

holds. The carrier densities n,p only exists in $\overline{\Omega}$. Usually $\partial\Phi$ splits into three parts, namely $\partial\Phi_C$ (oxide-contact) where a Dirichlet condition for ψ is prescribed, $\partial\Phi_{is}$ (insulating segment) where a zero Neumann condition for ψ holds, and the interface $\partial\Omega_{os}$. ψ has to be continuous across $\partial\Omega_{os}$ and

$$[\varepsilon\nabla\psi\cdot\vec{n}]_{\partial\Omega_{os}} = 0, \qquad \varepsilon(x,y) = \begin{cases} \varepsilon_o, & (x,y)\in\Phi \\ \varepsilon_s, & (x,y)\in\Omega \end{cases} \tag{4}$$

holds where ε_o is the oxide permittivity ($\frac{\varepsilon_o}{\varepsilon_s} \approx \frac{1}{3}$) ($[f]_\Gamma$ denotes the jump of the function f across the curve Γ) and $\vec{n}$ is the exterior unit normal vector of $\partial\Omega$. The condition (4) represents the continuity of the electrical displacement across the semiconductor oxide interface.

The electron and hole current density components $J_n\cdot\vec{n}$ and $J_p\cdot\vec{n}$ (perpendicular to $\partial\Omega_{os}$) vanish on $\partial\Omega_{os}$. This gives boundary conditions for n and p (by using (3)) at the interface. The Dirichlet boundary conditions for n and p at the Ohmic contacts are given by the vanishing-space-charge condition

$$(n-p-C(x,y))|_{\partial\Omega_C} = 0 \tag{5}$$

and the thermal equilibrium condition

$$np|_{\partial\Omega_C} = n_i^2 \tag{6}$$

where n_i is the intrinsic number of the semiconductor.

In the following we assume that Ω splits up into N+1 connected subdomains Ω_i, ($\overline{\Omega} = \bigcup_{i=0}^{N} \overline{\Omega}_i$), such that C does not change sign in each of the Ω_i and C has jump-discontinuities across the curves $\overline{\Gamma}_i = \overline{\Omega}_{i-1} \cap \overline{\Omega}_i$ (abrupt doping), $\overline{\Gamma}_i \cap \overline{\Gamma}_j = \emptyset$ holds for i=j. Ω_i is called an n-region if $C|_{\overline{\Omega}_i} > 0$ and it is called a p-region if $C|_{\overline{\Omega}} < 0$. Γ_i is a pn junction if it is the joint boundary of a p and an n-region and it is an nn (pp) junction if it is the joint boundary of two n (p) regions.

The boundary conditions for the potential (at the Ohmic contacts) are

$$\psi|_{C_k} = U_T \; \ell n \frac{n}{n_i} \Big|_{C_k} + U_k \tag{7.a}$$

where U_k represents the potential applied to the Ohmic contact C_k. We remark that for some devices not every n or p region "has" an Ohmic contact (the thyristors, for example, see [13]).

An externally applied potential U_G is given at the oxide (gate) contact $\partial\Phi_C$:

$$\psi|_{\partial\Phi_C} = U_G - U_F \tag{7.b}$$

where (the flat band voltage) U_F is a constant which depends on the semiconductor, on the oxide contact and on the doping. The applied potentials U_K, U_G are constants, too.

We also assume that the Ohmic contacts C_k have positive distance from the junctions Γ_i.

The performance by the device under consideration is mainly determined by the location of the subdomains of the oxide (for MOS-devices) and by the location of the Ohmic contacts.

As illustration for the notation of the device geometry we show a typical MOS-transistor in Figure 1. There are two n-regions and one p-region (n-channel-transistor), three Ohmic contacts (C_1: source-contact, C_2: drain contact, C_0: bulk contact) and one oxide contact ($\partial\Phi_C$: gate contact). The vertical boundaries of Ω and Φ are insulating ($\partial\Omega_{is}$ and $\partial\Phi_{is}$ respectively). We remark that

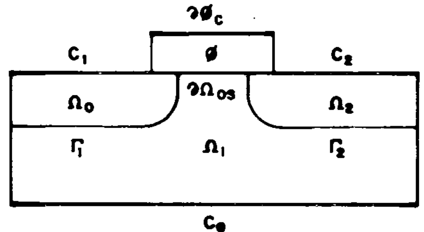

Fig. 1. MOS-transistor $C \begin{cases} >0 \text{ in } \overline{\Omega}_0, \overline{\Omega}_2 \\ <0 \text{ in } \overline{\Omega}_1 \end{cases}$

the rectangular shape of Ω and Φ as shown in Figure 1 is a simplification commonly used for numerical simulation (see [12]). The following theory however is not restricted to particular shapes of domains.

There have heen many analytical and numerical investigations of (1) (with R=0). Mock in [6] showed the existence of a solution subject to the mixed set of boundary conditions and proved that this solution is unique if the applied potentials U_k are sufficiently small. He only assumed $C \in L^{\infty}(\Omega)$. Continuous dependence of the solutions on the boundary data was also shown in this paper. A very similar existence proof was given recently by Bank, Jerome and Rose in [1].

The parabolic semiconductor problem (with homogeneous Neumann boundary conditions on $\partial\Omega$) was investigated by Mock in [8], who also discussed finite difference methods in [7] and [9].

In this paper we scale the problem (1) appropriately and obtain a singular perturbation problem. The singular perturbation parameter λ is the minimal normed Debye length of the device under consideration. Using matched asymptotic expansions (as $\lambda \to 0+$) we demonstrate the occurence of a boundary layer in ψ,n and p at oxide-semiconductor interfaces and the occurence of internal layers (in ψ) at pn, nn and pp junctions.

We derive the reduced problem (zero space charge approximation) which is obtained by setting the singular perturbation parameter to zero, and the (boundary and internal) layer equations.This facilitates an asymptotic analysis,*i.e.* a qualitative description of solutions for small λ (which is the usual case in practice. The singular perturbation approach was applied to the one dimensional semiconductor problem by Vasileva and Stelmakh in [16], Markowich and Ringhofer in [2] and Markowich, Ringhofer, Selberherr and Langer in [3].

The main advantage of the singular perturbation approach is that it gives qualitative information on the behavior of the solutions. The *a priori* information can be used to construct appropriate discretisation methods for the numerical solution of the semiconductor device equations. In particular efficient mesh-strategies employing only a reasonable number of grid points (but still giving accurate numerical approximations even in layer regions) can be obtained (see [5]).

We present numerical results obtained by using a computer program by A. Franz *et al.* fully based on the singular perturbation approach.

Parameter	Physical Meaning	Numerical Value
q	elementary charge	10^{-19}As
ε_s	semiconductor permittivity constant	10^{-12}As/Vcm
ε_o	oxide permittivity constant	$\frac{1}{3} \cdot 10^{-12}$As/Vcm
μ_n	electron mobility	10^3cm^2/Vs
μ_p	hole mobility	10^3cm^2/Vs
D_n	electron diffusion constant	25 cm^2/s
D_p	hole diffusion constant	25 cm^2/s
n_i	intrinsic number	10^{10}/cm^3
U_T	thermal voltage	0.025 V

Table 1. Numerical values of the parameters for Silicon and Silicon Oxide at room temperature $T \approx 300$ K. (The numerical values given for μ_n, μ_p, D_n, D_p must be understood as averages, since these quantities are generally modelled by functions of x and y.)

2. THE SINGULARLY PERTURBED PROBLEM

We assume the validity of Einstein's relation

$$\frac{D_n}{\mu_n} = \frac{D_p}{\mu_p} = U_T \quad (= \text{const}) \tag{8.a}$$

where U_T is the thermal voltage. Then the problem (1) can be put into a simpler form by the transformation (called Boltzmann Statistics),

$$n = n_i e^{\psi/U_T} u, \qquad p = n_i\, e^{-\psi/U_T} v. \tag{8.b}$$

Here $u = \exp(-\phi_n/U_T)$, $v = \exp(\phi_p/U_T)$ where ϕ_n, ϕ_p are the electron and hole quasifermilevels respectively ($u>0$, $v>0$ must hold). Then (1) takes the form (by using (8), assuming R=0 and ε_s to be constant)

$$\left.\begin{aligned} &\varepsilon_s \Delta\psi = q(n_i e^{\psi/U_T} u - n_i^{\psi/U_T} v - C(x,y)) && (9.a)\\ &\operatorname{div}(\mu_n\, e^{-\psi/U_T}\, \nabla u) = 0 && (9.b)\\ &\operatorname{div}(\mu_p\, e^{-\psi/U_T}\, \nabla v) = 0 && \end{aligned}\right] (x,y)\in\Omega.$$

The continuity equations (9.b)-(9.c) are in self-adjoint form. We assume that C is bounded in Ω and set

$$\bar{C} = \sup_{\Omega}|C(x,y)|, \quad D = C/\bar{C} \tag{10.a}$$

and

$$\ell = \mathrm{diam}(\Omega) = 1. \tag{10.b}$$

The dependent variables are scaled as follows

$$\psi_s = \psi/U_T, \quad n_s = n/\bar{C}, \quad p_s = p/\bar{C}, \quad u_s = u, \quad v_s = v \tag{10.c}$$

while the independent variables are scaled as

$$x_s = x/\ell, \quad y_s = y/\ell, \quad (x_s,y_s)\in\bar{\Omega}_s \cup \bar{\Phi}_s . \tag{10.d}$$

Then, after dropping the subscript s, (9) is transformed into

$$\lambda^2\Delta\psi = \delta^2 e^{\psi}u - \delta^2 e^{-\psi}v - D \tag{11.a}$$

$$\mathrm{div}(e^{\psi}\nabla u) = 0 \qquad (x,y)\in\Omega \tag{11.b}$$

$$\mathrm{div}(e^{-\psi}\nabla v) = 0 \tag{11.c}$$

and (3) remains unchanged:

$$\Delta\psi = 0, \quad (x,y)\in\Phi \tag{12}$$

where

$$\lambda^2 = (\lambda_D/\ell)^2 = \frac{\varepsilon_s U_T}{\ell^2 q\bar{C}}, \tag{13.a}$$

$$\delta^2 = n_i/\bar{C} \tag{13.b}$$

holds. λ_D is the minimal Debye length of the device.

For (11) we assumed that the mobilities μ_n,μ_p are constant throughout the device (for numerical values see Table 1). The following theory however carries over to the case that μ_n,μ_p are smooth and positive functions of x and y.

The (scaled) boundary conditions are

$$\nabla\psi\cdot\vec{n}|_{\partial\Omega_{is}} = \nabla u\cdot\vec{n}|_{\partial\Omega_{is}} = \nabla v\cdot\vec{n}|_{\partial\Omega_{is}} = 0 \tag{14.a}$$

(the (unit) vector $\vec{n}$ is perpendicular to $\partial\Omega$ and is assumed to exist almost everywhere) and

$$u|_{C_k} = e^{-U_k/U_T}, \quad v|_{C_k} = e^{U_k/U_T} \tag{14.b}$$

$$\psi|_{C_k} = \ln\left[\frac{D+\sqrt{D^2+4\delta^4}}{2\delta^2}\right]\Bigg|_{C_k} + U_k/U_T \tag{14.c}$$

for $k=0,\ldots,r$.

Equations (14) are derived from (5), (6), (7) by using (8.b).

Boundary conditions on $\partial\Phi$ are

$$\nabla\psi\cdot\vec{\zeta}|_{\partial\Phi_{is}} = 0 \tag{15.a}$$

($\vec{\zeta}$ denotes the exterior unit normal vector of $\partial\Phi$)

$$\psi|_{\partial\Phi_C} = U_G/U_T - U_F/U_T =: \psi_G \tag{15.b}$$

and

$$[\psi]_{\partial\Omega_{os}} = 0 \tag{15.c}$$

$$[\varepsilon^*\nabla\psi\cdot\vec{n}]_{\partial\Omega_{os}} = 0, \qquad \varepsilon^* = \begin{cases} 1, & (x,y)\in\Omega \\ \varepsilon_o/\varepsilon_s, & (x,y)\in\Phi \end{cases} \tag{15.d}$$

$$\nabla u\cdot\vec{n}|_{\partial\Omega_{os}} = \nabla v\cdot\vec{n}|_{\partial\Omega_{os}} = 0 \tag{15.e}$$

u and v are only defined in $\bar{\Omega}$.

For modern devices $\bar{C}\geq 10^{17}\text{cm}^{-3}$. With the realistic value $\ell=5\times10^{-3}$cm and the numerical values for q,ε_s,U_T given in Table 1 we get $\lambda^2\leq 10^{-7} \ll 1$. Therefore the problem (11), (12), (14), (15) constitutes a singularly perturbed quasilinear elliptic system of differential equations (subject to mixed Neumann-Dirichlet boundary and interface conditions).

The parameter $\delta^2 \ll 1$, too (normally $\delta^2 < 10^{-7}$ holds). This however gets compensated by the Dirichlet boundary conditions (14.d), (14.e) which imply that $\delta^2(e^{\psi}u - e^{-\psi}v) = O(1)$ at Ohmic contacts as $\delta^2 \to 0$. Note that the potential difference between an Ohmic contact in a n-region and an Ohmic contact in a p-region behaves asymptotically (as $\delta^2 \to 0$) like $\ell n\, \delta^{-4}$ for constant applied potentials.

The scaling factors for the current densities J_n, J_p are $q\mu_n \bar{C} U_T$ and $q\mu_p \bar{C} U_T$ respectively. Then the scaled current densities are given by

$$J_n = \delta^2 e^{\psi} \nabla u, \tag{16.a}$$

$$J_p = -\delta^2 e^{-\psi} \nabla v. \tag{16.b}$$

The scaled carrier densities follow from (9)

$$n = \delta^2 e^{\psi} u, \tag{16.c}$$

$$p = \delta^2 e^{-\psi} v. \tag{16.d}$$

3. ASYMPTOTIC EXPANSIONS

We are now concerned with the asymptotic behavior of the solutions of (11), (12), (14),(15) as $\lambda \to 0+$.

When we set $\lambda=0$ in (11.a) we see that $\psi(\lambda=0)$ has to be discontinuous at pn, nn and pp junctions(since D is discontinuous at these junctions)assuming that $u(\lambda=0)$ and $v(\lambda=0)$ are continuous in Ω (note that (11.b), (11.c) only admit weak solutions in $C(\Omega)$ if $\psi \in L^{\infty}(\Omega)$). Therefore, standard singular perturbation theory implies that we have to expect an internal layer in ψ (that is, a region of fast variation of ψ) at these junctions. Also, boundary layers occur at $\partial\Omega$ if the reduced solutions (*i.e.* the solutions of (11) with $\lambda=0$) do not fulfill the boundary conditions.

For the following analysis we assume the profile D is discontinuous across only one (open) C^{∞} curve Γ which splits Ω into two connected subdomains Ω_+ and Ω_-. Also we assume that $D|_{\overline{\Omega}_+} \in C^{0,\alpha}(\overline{\Omega}_+)$, $D|_{\overline{\Omega}_+} \in C^{0,\alpha}(\overline{\Omega}_-)$ for some $\alpha>0$ and $[D]_{\Gamma} \neq 0$ and that $\overline{\Gamma} \cap \partial\Omega_C = \emptyset$. D does not change sign in $\overline{\Omega}_+$ and in $\overline{\Omega}_-$.

We denote by $t(x,y)$ the oriented distance of (x,y) from Γ, that means $t>0$ in Ω_+ and $t<0$ in Ω_-, $s(x,y) = (s_1(x,y), s_2(s,y))$ is the point on Γ which is closest to (x,y) (s is unique in a sufficiently small strip about Γ).Similarly

$r(x,y)\geq 0$ denotes the distance of (x,y) to $\partial\Omega$. $q(x,y)=(q_1(x,y),q_2(x,y))$ denotes the point on $\partial\Omega$ closest to (x,y). Note that $\nabla r|_{\partial\Omega} = -\vec{n}$ and $\nabla t|_{\Gamma}$ is the unit-normal vector of Γ pointing into Ω_+. The local coordinates (t,s) and (r,q) are illustrated by Figure 2.

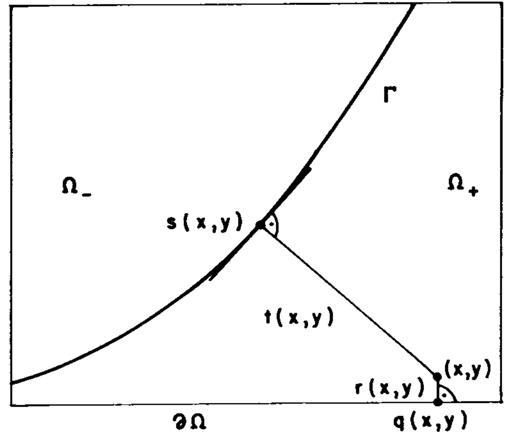

Fig. 2. Local coordinates.

For a function f defined in Ω (or $\bar{\Omega}$) we set

$$f^{\Gamma}(t,s) \equiv f(x,y)$$

and

$$f^{\partial}(r,q) \equiv f(x,y)$$

in neighbourhoods of Γ and $\partial\Omega$ where s and q respectively are unique.

We define for some $s\in\Gamma$

$$f^{\Gamma}(0+,s) := \lim_{\substack{(a,b)\to s \\ (a,b)\in\Omega_+}} f(a,b)$$

$$f^{\Gamma}(0-,s) := \lim_{\substack{(a,b)\to s \\ (a,b)\in\Omega_-}} f(a,b)$$

(assuming that the limits exist).

We also set

$$\frac{\partial s}{\partial(x,y)} = \begin{pmatrix} \frac{\partial s_1}{\partial x} & \frac{\partial s_2}{\partial x} \\ \frac{\partial y_1}{\partial y} & \frac{\partial y_2}{\partial y} \end{pmatrix}, \quad \frac{\partial q}{\partial(x,y)} = \begin{pmatrix} \frac{\partial q_1}{\partial x} & \frac{\partial q_2}{\partial x} \\ \frac{\partial q_1}{\partial y} & \frac{\partial q_2}{\partial y} \end{pmatrix},$$

$$\nabla_s f^{\Gamma} = \begin{pmatrix} \frac{\partial f^{\Gamma}}{\partial s_1} \\ \frac{\partial f^{\Gamma}}{\partial s_2} \end{pmatrix}, \qquad \nabla_q f^{\partial} = \begin{pmatrix} \frac{\partial f^{\partial}}{\partial q_1} \\ \frac{\partial f^{\partial}}{\partial q_2} \end{pmatrix}$$

and remark that

$$\left(\frac{\partial s}{\partial(x,y)}\right)^T \nabla t|_\Gamma = \left(\frac{\partial q}{\partial(x,y)}\right)^T \nabla r|_{\partial\Omega} = 0$$

holds (the superscript T denotes transposition).

Following standard singular perturbation theory we make the 'ansatz':

$$\begin{pmatrix} \psi(x,y,\lambda) \\ u(x,y,\lambda) \\ v(x,y,\lambda) \end{pmatrix} \sim \sum_{i=0}^{\infty} \lambda_i \left[\begin{pmatrix} \bar{\psi}_i(x,y) \\ \bar{u}_i(x,y) \\ \bar{v}_i(x,y) \end{pmatrix} + \begin{pmatrix} \hat{\psi}_i((t(x,y)/\lambda),s(x,y)) \\ \hat{u}_i((t(x,y)/\lambda),s(x,y)) \\ \hat{v}_i((t(x,y)/\lambda),s(x,y)) \end{pmatrix} + \right.$$

$$\left. + \begin{pmatrix} \tilde{\psi}_i((r(x,y)/\lambda),q(x,y)) \\ \tilde{u}_i((r(x,y)/\lambda),q(x,y)) \\ \tilde{v}_i((r(x,y)/\lambda),q(x,y)) \end{pmatrix} \right] \tag{17}$$

where the functions marked with '-' are independent of λ, the functions marked with '^' are defined on $(-\infty,\infty) \times \Gamma$ and decay to zero as $\tau = t/\lambda \to \pm\infty$ (internal layer terms), the functions marked with '~' are defined on $[0,\infty] \times \partial\Omega$ and decay to zero as $\rho = r/\lambda \to \infty$ (boundary layer terms).

We insert (17) into (11), (12), (14), (15) and obtain equations for the i-th term in the series (17) by comparing coefficients of λ. We start with

THE REDUCED PROBLEM. Evaluation of (11) away from Γ and $\partial\Omega$ and comparison of $O(1)$ terms gives (after dropping the index 0) the zeroth order reduced problem

$$0 = \delta^2 e^{-\bar{\psi}}\bar{u} - \delta^2 e^{-\bar{\psi}}\bar{v} - D(x,y) \tag{18.a}$$

$$\operatorname{div}(e^{\bar{\psi}}\nabla\bar{u}) = 0 \qquad (x,y)\in\Omega \setminus \Gamma. \tag{18.b}$$

$$\operatorname{div}(e^{-\bar{\psi}}\nabla\bar{v}) = 0 \tag{18.c}$$

In the context of semiconductor device physics this problem is referred to as 'zero-space charge approximation'. By investigating the internal and boundary layer problems we will supplement (18) by interface and boundary conditions.

THE INTERNAL LAYER PROBLEM. We evaluate (11.b) close to Γ but away from $\partial\Omega$ and compare $O(\lambda^{-2})$ terms (after carrying out the differentiations). This yields:

$$\hat{u}_{o\tau\tau} + \hat{u}_{o\tau}\hat{\psi}_{o\tau} = 0$$

(subscripts τ denote differentiation with respect to τ) and therefore $\hat{u}_{0\tau} = \alpha(s)e^{-\hat{\psi}_{0\tau}}$. From $\hat{u}_0(\tau,s)\to 0$ as $\tau \to \pm\infty$ we get $\hat{u}_0\equiv 0$. Similarly $\hat{v}_0\equiv 0$ follows. u and v do not have zeroth order internal layers.

For the following we set $\hat{u}=\hat{u}_1$, $\hat{v}=\hat{v}_1$ and $\hat{\psi}=\hat{\psi}_0$. Comparing $O(\lambda^{-1})$ terms in (11.b) (again after differentiation) and evaluation close to Γ but in Ω_+ gives

$$\hat{u}_{\tau\tau} + \hat{\psi}_\tau(\bar{u}_t^\Gamma(0+,s)+\hat{u}_\tau) = 0, \qquad \tau>0$$

and evaluation close to Γ but in Ω_-:

$$\hat{u}_{\tau\tau} + \hat{\psi}_\tau(\bar{u}_t^\Gamma(0-,s)+\hat{u}_\tau) = 0, \qquad \tau<0.$$

Integration yields

$$\hat{u}_\tau(\tau,s) = \begin{cases} \bar{u}_t^\Gamma(0+,s)(e^{-\hat{\psi}(\tau,s)}-1), & \tau>0 \\ \bar{u}_t^\Gamma(0-,s)(e^{-\hat{\psi}(\tau,s)}-1), & \tau<0 \end{cases} \tag{19}$$

Proceeding analogously to (11.e) leads to

$$\hat{v}_\tau(\tau,s) = \begin{cases} \bar{v}_t^\Gamma(0+,s)(e^{\hat{\psi}(\tau,s)}-1), & \tau>0 \\ \bar{v}_t^\Gamma(0-,s)(e^{\hat{\psi}(\tau,s)}-1), & \tau<0 \end{cases} \tag{20}$$

We used that $\hat{\psi},\hat{u},\hat{v}$ and their τ-derivatives vanish at $\tau = \pm\infty$ for all $s\in\Gamma$.

The internal-layer problem for $\hat{\psi}$ is obtained by evaluating (11.a) close to Γ (but away from $\partial\Omega$) and by comparing $O(1)$ coefficients:

$$\hat{\psi}_{\tau\tau} = \delta^2 e^{\bar{\psi}^\Gamma(0+,s)+\hat{\psi}-\bar{u}^\Gamma(0,s)} - \delta^2 e^{-\bar{\psi}^\Gamma(0+,s)-\hat{\psi}-\bar{v}^\Gamma(0-,s)} - D^\Gamma(0+,s), \quad \tau>0 \tag{21.a}$$

$$\hat{\psi}_{\tau\tau} = \delta^2 e^{\bar{\psi}^\Gamma(0-,s)+\hat{\psi}-\bar{u}^\Gamma(0-,s)} - \delta^2 e^{-\bar{\psi}^\Gamma(0-,s)-\hat{\psi}-\bar{v}^\Gamma(0-,s)} - D^\Gamma(0-,s), \quad \tau<0. \tag{21.b}$$

Interface condition for (21.a)-(21.b) are derived by using that $\psi\in C^1(\Omega)$ which implies $\psi^\Gamma(0+,s)=\psi^\Gamma(0-,s)$ and $\psi_t^\Gamma(0+,s)=\psi_t^\Gamma(0-,s)$. Inserting (17) into these relations and comparing $O(1)$ and $O(\lambda^{-1})$ coefficients yields

$$\hat{\psi}(0+,s) - \hat{\psi}(0+,s) = \bar{\psi}^\Gamma(0+,s)-\bar{\psi}^\Gamma(0+,s) \tag{21.c}$$

$$\hat{\psi}_\tau(0+,s) = \hat{\psi}_\tau(0-,s) \tag{21.d}$$

$$\hat{\psi}(+\infty,s) = \hat{\psi}(-\infty,s) = 0 \tag{21.e}$$

(19)-(21) are supposed to hold for all $s\in\Gamma$. $\hat{\psi}$ is discontinuous at $\tau=0$ for all $s\in\Gamma$ since $[\bar{\psi}]_\Gamma = 0$.

The continuity of u,v across Γ and the expansions

$$u(x,y,\lambda) \sim \bar{u}(x,y) + \lambda\hat{u}((t/\lambda),s) + \ldots \tag{22.a}$$

$$v(x,y,\lambda) \sim \bar{v}(x,y) + \lambda\hat{v}((t/\lambda),s) + \ldots \tag{22.b}$$

(the dots denote a power series in λ starting with the $O(\lambda^2)$ term) imply by comparing $O(1)$-terms:

$$[\bar{u}]_\Gamma = 0, \qquad [\bar{v}]_\Gamma = 0 \tag{23.a}$$

and using (19), (20)

$$\bar{u}_t^\Gamma(0+,s)e^{-\hat{\psi}(0+,s)} = \bar{u}_t^\Gamma(0-,s)e^{-\hat{\psi}(0-,s)}$$

$$\bar{v}_t^\Gamma(0+,s)e^{\hat{\psi}(0+,s)} = \bar{v}_t^\Gamma(0-,s)e^{\hat{\psi}(0-,s)}.$$

(21.c) implies

$$u_t^\Gamma(0+,s)e^{\bar{\psi}^\Gamma(0+,s)} = \bar{u}_t^\Gamma(0-,s)e^{\bar{\psi}^\Gamma(0-,s)}$$

$$\bar{v}_t^\Gamma(0+,s)e^{-\bar{\psi}^\Gamma(0+,s)} = \bar{v}_t^\Gamma(0-,s)e^{-\bar{\psi}^\Gamma(0-,s)}.$$

So we obtain the interface conditions for the reduced problem

$$[e^{\bar{\psi}}\nabla\bar{u}\cdot\nabla t]_\Gamma = 0, \qquad [e^{-\bar{\psi}}\nabla\bar{v}\cdot\nabla t]_\Gamma = 0 \tag{23.b}$$

since $f_t^\Gamma(0,s) = \nabla f(x,y)\cdot\nabla t(x,y)|_{(x,y)=s\in\Gamma}$ holds.

OHMIC CONTACTS. A straight-forward calculation shows that the Dirichlet boundary conditions on $\partial\Omega_C$ for ψ, u and v fulfill (18.a). Therefore we do not expect boundary layers at $\partial\Omega_C$. That means

$$\tilde{\psi}_0(\rho,q) \equiv \tilde{u}_0(\rho,q) \equiv \tilde{v}_0(\rho,q) \equiv 0 \quad \text{for } \rho>0 \text{ and } q\in\partial\Omega_C. \tag{24}$$

To prove (24) one has to proceed as Markowich, Ringhofer, Selberherr and Langer [3] did for the one-dimensional semiconductor problem.

(24) implies that we have to impose the same Dirichlet boundary conditions for the reduced problem (18) as for the full singularly perturbed problem:

$$\bar{\psi}|_{\partial\Omega_C} = \psi|_{\partial\Omega_C}, \quad \bar{u}|_{\partial\Omega_C} = u|_{\partial\Omega_C}, \bar{v}|_{\partial\Omega_C} = v|_{\partial\Omega_C} \tag{25}$$

where ψ,u,v on $\partial\Omega_C$ are given by (14).

INSULATING SEGMENTS. We assume that D is differentiable in a neighbourhood of $\partial\Omega$ and that

$$\nabla D\cdot\vec{n}|_{\partial\Omega_{is}} \equiv 0 \tag{26}$$

holds. Differentiating (18.a) gives

$$0 = \delta^2(e^{\bar{\psi}}\bar{u}+e^{-\bar{\psi}}\bar{v})\nabla\bar{\psi} + \delta^2(e^{\bar{\psi}}\nabla\bar{u}-e^{-\bar{\psi}}\nabla\bar{v}) - \nabla D. \tag{27}$$

Since $e^{\bar{\psi}}\bar{u}+e^{-\bar{\psi}}\bar{v}>0$ in $\bar{\Omega}$ we get

$$\nabla\bar{\psi}\cdot\vec{n}|_{\partial\Omega_{is}} \equiv 0 \tag{28.a}$$

if

$$\nabla\bar{u}\cdot\vec{n}|_{\partial\Omega_{is}} \equiv \nabla\bar{v}\cdot\vec{n}|_{\partial\Omega_{is}} \equiv 0 \tag{28.b}$$

holds. (18.a) is compatible with the zero Neumann conditions for ψ,u,v on $\partial\Omega_{is}$ and we get

$$\tilde{\psi}_0(\rho,q) \equiv \tilde{u}_0(\rho,q) \equiv \tilde{v}_0(\rho,q) \equiv 0 \quad \text{for } \rho>0,\ q\in\partial\Omega_{is} \tag{29}$$

as well as

$$\tilde{\psi}_1(\rho,q) \equiv \tilde{u}_1(\rho,q) \equiv \tilde{v}_1(\rho,q) \equiv 0 \quad \text{for } \rho>0,\ q\in\partial\Omega_{is}. \tag{30}$$

No zeroth and first order layers occur at $\partial\Omega_{is}$. If we had not assumed (26) then (30) and (28.a) would not hold (of course (29) would still be valid).

(28.a,b) define homogeneous Neumann boundary conditions for (18) on $\partial\Omega_{is}$.

OXIDE-SEMICONDUCTOR INTERFACE. As for junctions we get $\tilde{u}_0 \equiv \tilde{v}_0 \equiv 0$ and setting $\tilde{u} \equiv \tilde{u}_1$, $\tilde{v} \equiv \tilde{v}_1$, $\tilde{\psi} \equiv \tilde{\psi}_0$ we obtain

$$\tilde{u}_\rho(\rho,q) = \bar{u}_r^\partial(0,q)(e^{-\tilde{\psi}(\rho,q)}-1), \qquad \rho>0,\ q\in\partial\Omega_{os} \tag{31.a}$$

$$\tilde{v}_\rho(\rho,q) = \bar{v}_r^\partial(0,q)(e^{\tilde{\psi}(\rho,q)}-1), \qquad \rho>0,\ q\in\partial\Omega_{os}. \tag{31.b}$$

Since we set

$$u(x,y,\lambda) \sim \bar{u}(x,y) - \lambda\hat{u}((t/\lambda),s) + \lambda\tilde{u}((r/\lambda),q) + \ldots \tag{32.a}$$

$$v(x,y,\lambda) \sim \bar{v}(s,y) - \lambda\hat{v}((t/\lambda),s) + \lambda\tilde{v}((r/\lambda),q) + \ldots \tag{32.b}$$

we get by inserting (32) into (15.e) and by comparing $O(1)$ coefficients

$$0 = (\nabla\bar{u}\cdot\vec{n})(q) + \bar{u}_r^\partial(0,q)(e^{-\tilde{\psi}(0,q)}-1), \quad q\in\partial\Omega_{os}$$

$$0 = (\nabla\bar{v}\cdot\vec{n})(q) + \bar{v}_r^\partial(0,q)(e^{\tilde{\psi}(0,q)}-1), \quad q\in\partial\Omega_{os}.$$

Therefore

$$0 = \bar{u}_r^\partial(0,q) = \bar{v}_r^\partial(0,q), \quad q\in\partial\Omega_{os}$$

and $\tilde{u}(\rho,q) \equiv \tilde{v}(\rho,q) \equiv 0$ for $\rho>0$, $q\in\partial\Omega_{os}$. Boundary conditions for $\bar{u},\bar{v}$ on $\partial\Omega_{os}$ are

$$\nabla\bar{u}\cdot\vec{n}|_{\partial\Omega_{os}} = \nabla\bar{v}\cdot\vec{n}|_{\partial\Omega_{os}} = 0. \tag{33}$$

If

$$\nabla D\cdot\vec{n}|_{\partial\Omega_{os}} = 0 \tag{34}$$

holds then (33) implies (as for insulating segments)

$$\nabla\bar{\psi}\cdot\vec{n}|_{\partial\Omega_{os}} = 0. \tag{35}$$

By evaluating close to $\partial\Omega_{os}$ but away from Γ we obtain the boundary layer equation for $\psi|_{\partial\Omega_{os}}$ which is analogous to the interface problem (21):

$$\tilde{\psi}_{\rho\rho} = \delta^2 e^{\overline{\psi}^{\partial}(0,q)+\tilde{\psi}}\overline{u}^{\partial}(0,q) - \delta^2 e^{-\overline{\psi}^{\partial}(0,q)-\tilde{\psi}}\overline{v}^{\partial}(0,q) - D^{\partial}(0,q),\ \rho>0,\ q\in\partial\Omega_{os} \tag{36.a}$$

$$\tilde{\psi}(\infty,q) = 0, \qquad q\in\partial\Omega_{os}. \tag{36.b}$$

To obtain the boundary condition for (36) at $\rho=0$ we solve Laplace's equation in the oxide.

Let $G(x,y,\xi,\eta)$ denote the Green's function (see [10], Chapter 2, Section 7) of the problem

$$\Delta\phi = f \text{ in } \Phi$$

$$\phi|_{\partial\Phi_C} = g,\quad \nabla\phi\cdot\vec{\zeta}|_{\partial\Phi_{is}} = h,\quad \nabla\phi\cdot\vec{\zeta}|_{\partial\Omega_{os}} = k$$

(note that $\vec{\zeta}|_{\partial\Omega_{os}} = -\vec{n}|_{\partial\Omega_{os}}$). Then, since $\psi=\psi_G+\phi$ fulfills

$$\Delta\phi = 0 \text{ in}$$

$$\phi|_{\partial\Phi_C} = 0,\quad \nabla\phi\cdot\vec{\zeta}|_{\partial\Phi_{is}} = 0,\ \nabla\phi\cdot\vec{\zeta}|_{\partial\Omega_{os}} = \frac{\varepsilon_s}{\varepsilon_o}\nabla\psi\cdot\vec{n}|_{\partial\Omega_{os}}$$

we get

$$\psi = \psi_G - \frac{\varepsilon_s}{\varepsilon_o}\int_{\partial\Omega_{os}} G(x,y,\xi,\eta)\nabla\psi(\xi,\eta)\cdot\vec{n}(\xi,\eta)d(\xi,\eta)\ .$$

This gives the boundary condition (for the singularly perturbed problem in Ω):

$$\psi|_{\partial\Omega_{os}} + \frac{\varepsilon_s}{\varepsilon_o}\int_{\partial\Omega_{os}} G(x,y,\xi,\eta)|_{(x,y)\in\partial\Omega_{os}}\nabla\psi(\xi,\eta)\cdot\vec{n}(\xi,\eta)d(\xi,\eta) = \psi_G. \tag{37}$$

In the sequel we assume that if $\overline{\Gamma}$ hits $\overline{\partial\Omega}_{os}$ (which in fact happens in MOS-technology) then $\overline{\Gamma}$ is perpendicular to $\overline{\partial\Omega}_{os}$, that means

$$\nabla t(S)\cdot\nabla r(S) = 0 \quad \text{for} \quad \{S\} = \overline{\Gamma} \cap \overline{\partial\Omega}_{os}. \tag{38}$$

We insert expansion

$$\psi(x,y,\lambda) \sim \bar{\psi}(x,y) + \hat{\psi}((t/\lambda),s) + \tilde{\psi}((r/\lambda),q) + \dots \tag{39}$$

(the dots now denote a power series starting with the $O(\lambda)$ term whose coefficients have the same form as the $O(1)$ terms) into (37). Assuming that

$$C_1 \leq |\psi_G|\lambda \leq C_2 \tag{40}$$

where C_1,C_2 are independent of λ, we obtain by comparing $O(\lambda^{-1})$ terms and by using (38):

$$\int_{\partial\Omega_{os}} G(x,y,\xi,\eta)|_{(x,y)\in\partial\Omega_{os}} \cdot\psi_\rho(0,q(\xi,\eta))d(\xi,\eta) = \lambda \frac{\varepsilon_o}{\varepsilon_s}\psi_G. \tag{41}$$

This integral equation is uniquely soluble (for $\tilde{\psi}_\rho(0,q)$) since $\tilde{\psi}_\rho(0,q)=(\nabla w\cdot\vec{\zeta})(q)$ where w is the (unique) solution of

$$\Delta w = 0 \text{ in } \Phi$$

$$w|_{\partial\Phi_C} = \nabla w\cdot\vec{\zeta}|_{\partial\Phi_{is}} = 0, \qquad w|_{\partial\Omega_{os}} = \lambda\frac{\varepsilon_o}{\varepsilon_s}\psi_G.$$

Obviously $w\in C^\infty(\bar{\Phi}-CR(\partial\Phi))$ holds.

If Φ is a rectangle as in Figure 1 (which is a common assumption in MOS-modelling) with $d=\text{dist}(\partial\Omega_{os},\partial\Phi_C)$ then w is a linear function and $\nabla w\cdot\vec{\zeta}|_{\partial\Omega_{os}} = -\lambda\frac{\varepsilon_o}{\varepsilon_s}\psi_G$. In this case

$$\tilde{\psi}_\rho(0,q) = -\lambda\frac{\varepsilon_o}{d\varepsilon_s}\psi_G. \tag{42}$$

No zeroth order layer occurs at the oxide-semiconductor interface if the right hand side of (42) is not $O(1)$ as $\lambda\to 0_+$. (41) (or equivalently (42) if Φ is a rectangle) provides the missing boundary condition for the interface layer problem (36). Equations for the higher order terms of the expansion (17) can be derived in an analogous way.

When the asymptotics of ψ,u,v are known then expansions of n,p and of J_n, J_p as given by (16) can easily be derived. We get from (17)

$$n(x,y,\lambda) = \bar{n}(x,y) + \hat{n}((t/\lambda),s) + \tilde{n}((r/\lambda),q) + \dots \quad (43)$$

$$p(x,y,\lambda) = \bar{p}(x,y) + \hat{p}((t/\lambda),s) + \tilde{p}((r/\lambda),q) + \dots \quad (44)$$

(32) and (39) imply

$$\bar{n} = \delta^2 e^{\bar{\psi}}\bar{u}, \quad \hat{n}(\tau,s) = \begin{cases} \delta^2 e^{\bar{\psi}^\Gamma(0+,s)}(e^{\hat{\psi}(\tau,s)}-1)\bar{u}^\Gamma(0,s), & \tau>0 \\ \delta^2 e^{\bar{\psi}^\Gamma(0-,s)}(e^{\hat{\psi}(\tau,s)}-1)\bar{u}^\Gamma(0,s), & \tau<0 \end{cases} \quad (45.a)$$

$$\tilde{n}(\rho,q) \equiv 0 \quad \text{for } \rho>0,\ q\in\partial\Omega_C \cup \partial\Omega_{is} \quad (45.b)$$

$$\tilde{n}(\rho,q) = \delta^2 e^{\bar{\psi}^\partial(0,q)}(e^{\tilde{\psi}(\rho,q)}-1)\bar{u}^\partial(0,q), \quad \rho>0,\ q\in\partial\Omega_{os} \quad (45.c)$$

$$\bar{p} = \delta^2 e^{-\bar{\psi}}\bar{v} \quad (45.d)$$

and similar expressions for $\hat{p}$ and $\tilde{p}$.

Differentiation of (32) and use of (19), (20) gives

$$J_n(x,y,\lambda) = \bar{J}_n(x,y) + \hat{J}_n(x,y) + \hat{J}_n((t/\lambda),s) + \tilde{J}_n((r/\lambda),q) + \dots \quad (46.a)$$

$$J_p(x,y,\lambda) = \bar{J}_p(x,y) + \hat{J}_p(x,y) + \hat{J}_p((t/\lambda),s) + \tilde{J}_n((r/\lambda),q) + \dots \quad (46.b)$$

with

$$\bar{J}_n = \delta^2 e^{\bar{\psi}}\nabla\bar{u} \quad (47.a)$$

$$\bar{J}_p = -\,\delta^2 e^{\bar{\psi}}\nabla\bar{v} \quad (47.b)$$

$$\hat{J}_n(\tau,s) = \begin{cases} \delta^2 e^{\bar{\psi}^\Gamma(0+,s)}(e^{\hat{\psi}(\tau,s)}-1)\left.\dfrac{\partial s(x,y)}{\partial(x,y)}\right|_{(x,y)=s}\cdot\nabla_s\bar{u}^\Gamma(0+,s), & \tau>0 \\ \delta^2 e^{\bar{\psi}^\Gamma(0-,s)}(e^{\hat{\psi}(\tau,s)}-1)\left.\dfrac{\partial s(x,y)}{\partial(x,y)}\right|_{(x,y)=s}\cdot\nabla_s\bar{u}^\Gamma(0-,s), & \tau<0 \end{cases} \quad (48.a)$$

$$\tilde{J}_n(\rho,q) \equiv 0 \quad \text{for } \rho>0,\ q\in\partial\Omega_C \cup \partial\Omega_{is} \quad (48.b)$$

$$\tilde{J}_n(\rho,q) = \delta^2 e^{\bar{\psi}^\partial(0,q)}(e^{\tilde{\psi}(\rho,q)}-1)\left.\frac{\partial q(x,y)}{\partial(x,y)}\right|_{(x,y)=q}\cdot\nabla_q\bar{u}^\partial(0,q),\ q\in\partial\Omega_{os}. \quad (48.c)$$

Analogous expressions hold for $\hat{J}_p$ and $\tilde{J}_p$. Since $\left(\frac{\partial s}{\partial(x,y)} \right)^T \nabla t|_\Gamma \equiv$ $\equiv \left(\frac{\partial q}{\partial(x,y)} \right)^T \nabla r|_{\partial\Omega} \equiv 0$ holds we get

$$\hat{J}_n \cdot \nabla t|_\Gamma \equiv \tilde{J}_n \cdot \nabla r|_{\partial\Omega_{os}} \equiv \hat{J}_p \cdot \nabla t|_\Gamma \equiv \tilde{J}_p \cdot \nabla r|_{\partial\Omega_{os}} \equiv 0 \ . \tag{49}$$

Therefore, the current density components perpendicular to the junctions (to the semiconductor oxide interface) have no zeroth order layers while the current density components parallel to the junctions (to the semiconductor-oxide interface) may very well have zeroth order layers. This phenomenon is illustrated by the MOS-transistor simulation performed by Selberherr in [12].

So far we only considered one curve of discontinuity of D. Generally, an internal layer in ψ occurs at each junction Γ_i and each layer-term $\hat{\psi}_i$ fulfills the corresponding layer problem (21) (with Γ_i-local coordinates (s_i,t_i)).

4. INTERPRETATION OF RESULTS AND CONCLUSIONS

At first we discuss the reduced problem.

Markowich in [4] showed (assuming a zero generation-recombination rate) that the reduced problem always has (at least one) solution $(\bar{u},\bar{v})$ fullfilling:

$$\min_{\partial\Omega_D} \bar{u} \leq \bar{u} \leq \max_{\partial\Omega_D} \bar{u} \tag{50}$$

$$\min_{\partial\Omega_D} \bar{v} \leq \bar{v} \leq \max_{\partial\Omega_D} \bar{v} \tag{51}$$

where $\partial\Omega_D$ is the union of Ohmic contacts (the estimates (50), (51) also hold for the full solutions u,v under the vanishing-generation-recombination assumption).

The reduced carrier densities $\bar{n},\bar{p}$ can be computed from (18.a) and (45.a):

$$\bar{n} = \frac{D+\sqrt{D^2+4\delta^4\bar{u}\,\bar{v}}}{2}, \qquad \bar{p} = \frac{-D+\sqrt{D^2+4\delta^4\bar{u}\,\bar{v}}}{2} \ . \tag{52}$$

(51), (52) imply

$$\bar{u}\cdot\bar{v} \leq \exp\left(\frac{|V_{max}|}{U_T} \right)$$

where $|V_{max}|$ is the largest voltage (in absolute value) applied to two contacts.

Therefore

$$\bar{n} = \begin{cases} D+O(\delta^4 \exp(\frac{|V_{max}|}{U_T})), & D>0 \\ O(\delta^4 \exp(\frac{|V_{max}|}{U_T})), & D<0 \end{cases} \tag{53.a}$$

$$\bar{p} = \begin{cases} O(\delta^4 \exp(\frac{|V_{max}|}{U_T})), & D>0 \\ -D+O(\delta^4 \exp(\frac{|V_{max}|}{U_T})), & D<0 \end{cases} \tag{53.b}$$

The low-injection condition

$$\delta^4 \exp(\frac{|V_{max}|}{U_T}) \text{ is small} \tag{54}$$

implies that the reduced electron density $\bar{n}$ is close to the doping profile in n-regions (D>0), close to zero in p-regions (D<0) and that the reduced hole density $\bar{p}$ is close to zero in n-regions and close to the negative doping profile in p-regions. Assuming the validity of the asymptotic expansions (17) it follows that the full solutions n and p also have these features away from junctions and oxide-semiconductor interfaces.

Now we turn to the discussion of the layer terms. Markowich in [4] proved that the internal layer problem (21) has a unique solution, which decays exponentially as $\tau \to \pm\infty$ and which is monotone on $(-\infty,0]$ and on $[0,\infty)$. The width of the internal layer at $s \in \Gamma$ is $O(\lambda(|\ln\lambda| + \sqrt{|\bar{\psi}^{\Gamma}(0+,s)-\bar{\psi}^{\Gamma}(0-,s)|}))$, which means that it depends linearly on the square root of the potential drop across the junction.

A unique monotone, exponentially decaying (as $\rho \to \infty$) solution of the oxide-semiconductor interface problem (36), (37) exists. For this problem the width of the layer is $O(\lambda(|\ln\lambda| + \sqrt{|\bar{\psi}(0,q)|}))$ at $q \in \partial\Omega_{os}$ again depending linearly on the square root of the potential drop at the interface.

The internal/boundary layer terms decay exponentially away from the junctions and boundary respectively. The layer regions are strips about the junctions and boundary pieces respectively (see Figure 3 for an illustration) and outside these layer-strips the layer terms are less than $O(\lambda)$ which means that

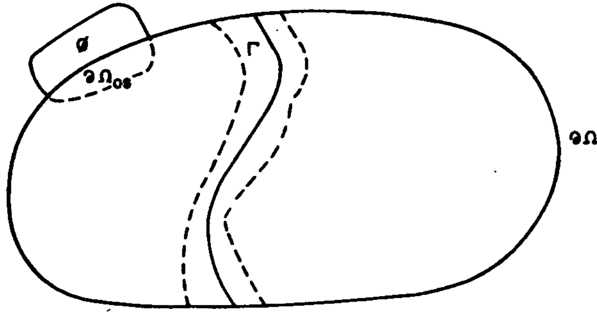

Fig. 3. Layer strips.

the solution is qualitatively and quantitatively described by the reduced solution there (assuming that the asymptotic expansion represents a solution of the singularly perturbed problem).

Markowich, Ringhofer, Selberherr and Langer in [3] showed the validity of the asymptotic expansion for a one-dimensional device close to thermal equilibrium and Markowich in [4] proved the analogous result for two and three-dimensional devices. No general estimate for the error in approximating the full solutions by the zeroth order terms of the expansions (21) is known yet. Numerical results indicate that the approximation quality decays as the applied maximal voltage increases and these numerical results suggest (at least for the one-dimensional problem) an error (in the max-norm) of $\mathcal{O}(\lambda(|\ell n\delta|+(|V_{max}|/U_T)))$ in approximating the potential ψ by the sum of the reduced solution $\bar{\psi}$ and the layer terms $\tilde{\psi}$ and $\hat{\psi}$. For silicon devices δ and λ are of the same order of magnitude.

Therefore, if $\lambda \frac{|V_{max}|}{U_T} \ll 1$, the reduced solutions $\bar{\psi},\bar{n},\bar{p}$ are close to the full solutions ψ,n,p away from layer regions and only in these thin strips about junctions and oxide-semi-conductor interfaces the layer terms $\hat{\psi}$ and $\tilde{\psi}$, $\hat{n}$ and $\tilde{n}$, $\hat{p}$ and $\tilde{p}$ have to be added to the reduced solutions to get an accurate approximation.

A thorough numerical test of the validity of the singular perturbation approach was performed by Markowich, Ringhofer, Selberherr and Langer in [3] for the one-dimensional problem. Two-dimensional tests are on the way and will be published soon. Qualitative agreement is assumed for even high biasing conditions and then large errors are only expected to occur within the layer strips.

The layer-type behavior of solutions is apparent in the following numerical examples.

Beside the understanding of the qualitative behavior of the solutions the singular perturbation approach also provides a tool for the construction of efficient meshes for the numerical solution of the problem (1)-(3) by finite difference methods. The main tool for mesh-construction is equidistribution of the local discretization errors of Poisson's equation. The error introduced by discretizing the continuity equations does not have to be taken into account when using a Scharfetter-Gummel type discretization since this method is (at least for n=1,2) uniformly convergent in λ (that means the global error is asymptotically independent of λ, see [5]).

The local discretization error of the five-point scheme for Poisson's equation (for n=2) at $\vec{x}_{ij} = (x_i, y_i)$ can be estimated by

$$|\ell_{ij}| \leq \text{const } \lambda^2 (h_i |\psi_{xxx}(\vec{x}_{ij})| + k_j |\psi_{yyy}(\vec{x}_{ij})|) \tag{55}$$

where *e.g.* h_i denotes the i-th x-mesh size, that is, $x_{i+1} = x_i + h_i$, $y_{j+1} = y_j + k_j$. The derived asymptotic expansions show that the third derivatives of ψ are $O(1)$ outside layer strips and they are $O(\lambda^{-3})$ within layers. Given an error tolerance κ, (55) implies $O(\lambda\kappa)$ mesh sizes in the layers and $O(\kappa)$ mesh sizes outside the layers will be obtained by equidistribution. More information is given in [5].

This strategy was implemented in a two-dimensional device finite difference simulation code by A. Franz, G. Franz, S. Selberherr, C. Ringhofer and P. Markowich in 1982.

5. NUMERICAL EXPERIMENTS

To demonstrate the power of the singular perturbation approach we present simulations of two devices, namely a two dimensional diode and an MOS-transistor. The codes used for the simulation are fully based on the singular perturbation approach as discussed in the last section. To obtain realistic results we used exponentially graded doping profiles (instead of piecewise constant ones) and non zero recombination generation. Also non-constant mobility models are used (see [11] for details).

Figure 4 shows the doping profile of the diode on a logarithmic scale (that is $\log|C/cm^3|$ is depicted). The unit of the x and y axes is cm^{-3}. The highly doped region is an n-region and the low-doped is a p-region. For this device

$\lambda^2 \approx 10^{-6}$ holds.

Figure 5 shows the grid used for the computation of the discrete solution for V_{max} = 0.7 Volts forward bias (the cathode and anode contacts are symbolized by the thick lines). The accumulation of grid point about the pn-junction is clearly visible. Figure 6 depicts the potential (in Volts). The ρn-layer is apparent. The electron concentration is shown in Figure 7 (also on a logarithmic scale). Because of the (rather) high injection the p-region is flooded with electrons and therefore the ρn-layer is 'washed out'. The layer-like behavior at the anode contact arises because the boundary condition forces the electron concentration to assume a very small value. We remark that this is not a boundary layer which is due to the small value of λ, it actually comes from the large applied bias.

Figure 8 depicts the electron current density. The peak at the edge of the cathode contact is due to the fact that weak singularities in the gradients of ψ, n and p occur at those boundary points where Neumann and Dirichlet boundary pieces meet.

Figure 9 shows the electron concentration for V_{max} = -20 Volts (reverse bias). Now the ρn-layer is highly pronounced, the electron concentration is small (compared to the maximal doping) in the p-region and it is large (of the same order of magnitude as the doping) in the n-region. The electron current is small in the whole device (since the diode is 'closed' in reverse bias) but the singularity at the edge of the cathode is again clearly visible (see Figure 10).

The geometry of an MOS-transistor was already shown in Figure 1. Figure 11 depicts the doping profile (again $\log|C/cm^3|$ is plotted). Figure 12 shows a contour plot of the potential for 1 Volt gate bias, 7 Volts drain-bias and 0 Volts bulk bias. The internal layers at the two pn-junctions and the layer at the semiconductor-oxide interface are visible. These layers are even more apparent in the electron concentration (Figure 13).

We finally remark that a comparison of the results obtained by solving the model equations and measurements is given by Selberherr [11], [12]. Excellent agreement (of the current-voltage characteristics) was established for most physically relevant biasing situations.

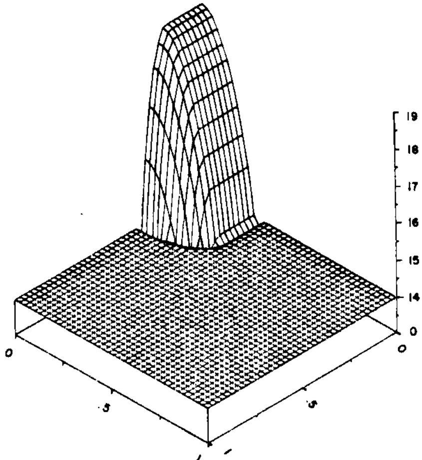

Fig. 4. Doping profile $[cm^{-3}]$ (log).

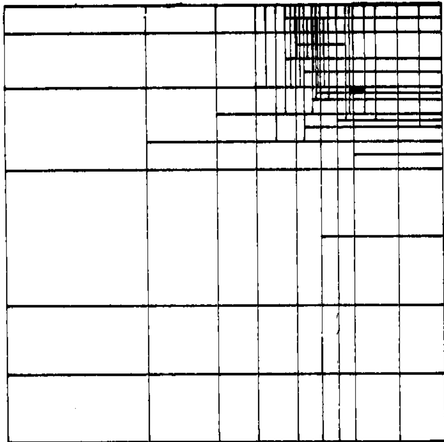

Fig. 5. Mesh for 0.7V forward bias.

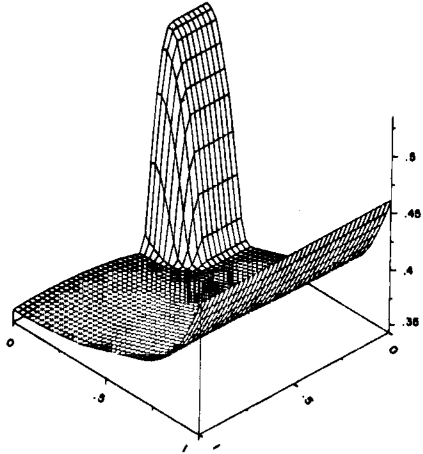

Fig. 6. Potential distribution (0.7V) [V] (lin).

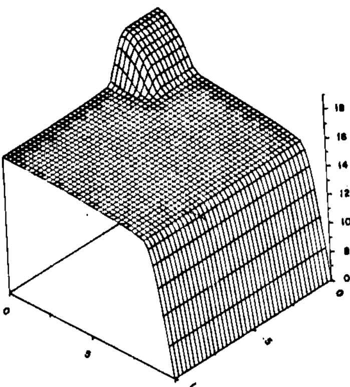

Fig. 7. Electron concentration (0.7V) $[cm^{-3}]$ (log).

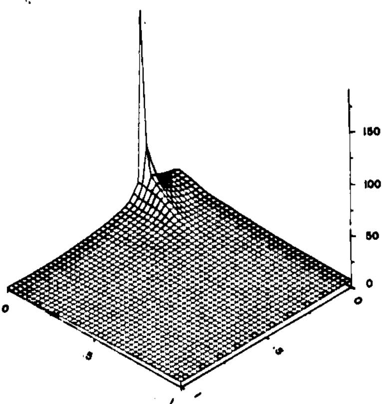

Fig. 8. Electron current density (0.7V) $[A/cm^2]$ (lin).

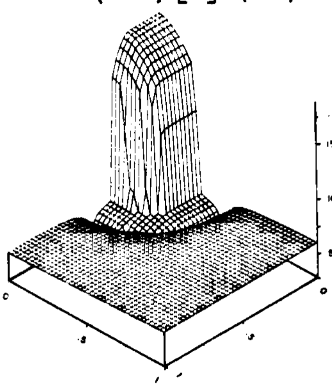

Fig. 9. Electron concentration (-20V) $[cm^{-3}]$ (log).

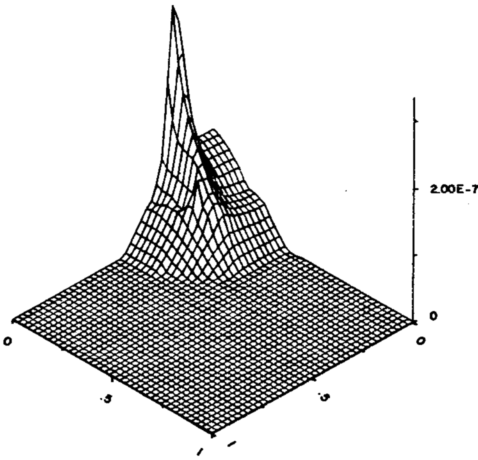

Fig. 10. Electron current density (-20V) [A/cm^2] (lin).

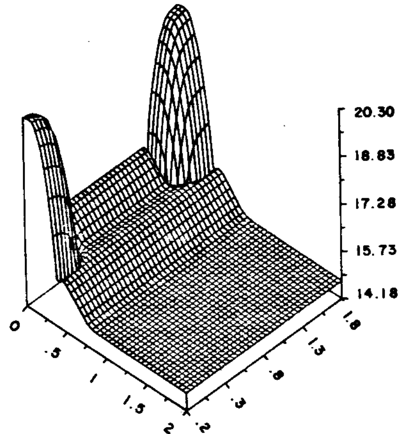

Fig. 11. Doping concentration.

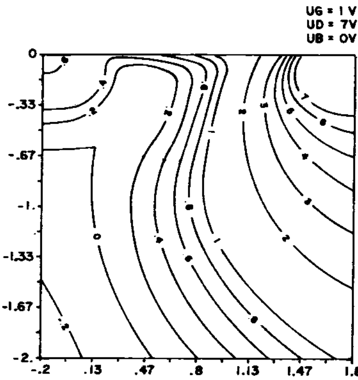

Fig. 12. Electrical potential.

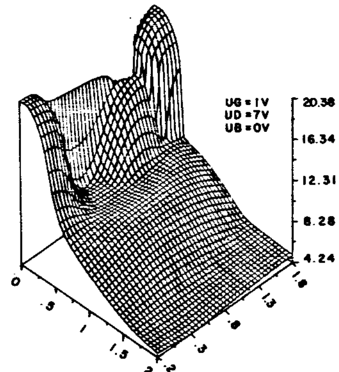

Fig. 13. Electron distribution.

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