Semiconductor Devices under Circuit Boundary Conditions

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Abstract. A stationary version of the standard drift-diffusion model for the flow of electrons and holes in semiconductor devices is considered. The boundary conditions are — to a certain extent — capable of describing the influence of the surrounding electrical circuit as opposed to the usual mathematical assumption of prescribed voltages. The existence of solutions and the convergence close to thermal equilibrium of a decoupled iteration method are proven.

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1. Introduction

Consider a semiconductor device situated in the domain $\Omega \subset \mathbb{R}^n$ with $n = 1$, 2 or 3. A steady state of the device can be described by the differential equations

$$\begin{aligned} \Delta\psi &= e^{\psi}u - e^{-\psi}v - C(x)\,, \\ \nabla\cdot\left(e^{\psi}\nabla u\right) &= R\,, \\ \nabla\cdot\left(e^{-\psi}\nabla v\right) &= R\,, \end{aligned} \tag{1.1}$$

for $x \in \Omega$, which are a scaled stationary version of the drift-diffusion model for flow of electrons and holes in semiconductor devices [8].

The first equation is the Poisson equation which determines the electrostatic potential ψ from the space charge density $-e^{\psi}u + e^{-\psi}v + C(x)$, where $n = e^{\psi}u$ and $p = e^{-\psi}v$ are the electron and hole densities, respectively, and $C(x)$, the doping profile, is the density of electrically active impurity ions. For the doping profile we assume

$$C \in L^{\infty}(\Omega)\,.$$

The second and third equations in (1.1) are the electron and hole continuity equations with the source term R, the recombination-generation rate, which we assume to be zero or of the form

$$R = Q(u,v,\psi)(uv-1) \qquad \text{with } Q > 0\,, \tag{1.2}$$

which corresponds to the Shockley-Read-Hall and/or Auger model (see [8]). Written in terms of the charge carrier densities the current densities $J_n = e^{\psi}\nabla u$ and $J_p = -e^{-\psi}\nabla v$ take the form

$$J_n = \nabla n - n\nabla\psi\,, \quad J_p = -\nabla p - p\nabla\psi\,,$$

which explains the term drift-diffusion equations. More general models include position (x) and field ($-\nabla\psi$) dependent mobilities multiplying the current densities as well as models for additional recombination-generation effects.

The scaling which leads to the dimensionless form (1.1) cannot be recommended in general as it does not reflect the relative sizes of different quantities. Here it was chosen for notational convenience (no parameters) because our results are not influenced by different choices of scaling.

We consider a two terminal device with Ohmic contacts for simplicity. This means that the boundary $\partial\Omega$ of Ω is the disjoint union of two closed (relative to $\partial\Omega$) contact segments C_1 and C_2 and the remaining insulating part of the boundary $\partial\Omega_N = \partial\Omega \setminus (C_1 \cup C_2)$. Assuming no electrical flux and no current flow across $\partial\Omega_N$ we pose the homogeneous Neumann boundary conditions

$$\nabla\psi\cdot\nu = \nabla u\cdot\nu = \nabla v\cdot\nu = 0 \qquad \text{at } \partial\Omega_N\,, \tag{1.3}$$

where ν denotes the unit outward normal vector along $\partial\Omega_N$. Standard assumptions for the Ohmic contacts are zero space charge:

$$e^{\psi}u - e^{-\psi}v - C = 0 \qquad \text{at } C_1 \cup C_2 \tag{1.4}$$

Figure 1.1

and thermal equilibrium:

$$uv - 1 = 0 \qquad \text{at } C_1 \cup C_2 . \tag{1.5}$$

If the whole device is in thermal equilibrium, $u \equiv v \equiv 1$ in Ω holds. The potential is then obtained by solving the problem

$$\begin{aligned} &\Delta\psi_e = 2\sinh\psi_e - C \qquad \text{in } \Omega , \\ &\nabla\psi_e \cdot \nu = 0 \quad \text{at } \partial\Omega_N , \qquad \psi_e = \psi_{bi} \quad \text{at } C_1 \cup C_2 , \end{aligned} \tag{1.6}$$

where the Dirichlet boundary conditions follow from (1.4). The Dirichlet datum $\psi_{bi} = \sinh^{-1}(C/2)$ is called the built-in potential. The existence of a unique solution $\psi_e \in H^1(\Omega) \cap L^\infty(\Omega)$ of (1.6) and the estimate

$$\|\psi_e\|_\infty \leq \|\psi_{bi}\|_\infty$$

are standard results (see e.g. [7]). ($\|\cdot\|_p$ denotes the $L^p(\Omega)$-norm.)

An additional assumption for Ohmic contacts is that the deviation of the potential from the built-in potential is constant along the contact and equal to the contact potential

$$U_i = \psi - \psi_{bi} \qquad \text{at } C_i \quad \text{for } i = 1, 2.$$

Since a reference point for the potential can be chosen arbitrarily, we can assume $U_1 = 0$ and $U_2 = -U$ for the following where $U = U_1 - U_2$ is the applied bias. These observations together with (1.4), (1.5) imply the boundary conditions

$$\begin{aligned} &\psi = \psi_{bi} , \quad u = v = 1 \qquad \text{at } C_1 , \\ &\psi = \psi_{bi} - U , \quad u = e^U , \quad v = e^{-U} \qquad \text{at } C_2 . \end{aligned} \tag{1.7}$$

The mixed Dirichlet-Neumann boundary value problem (1.1), (1.3), (1.7) for prescribed values of U has been thoroughly investigated in the literature. We only mention the books by Markowich [7] and Mock [10]. In this — so called voltage controlled — case existence of a solution for arbitrary values of U can be shown. Moreover close to thermal equilibrium (i.e. for U close to zero) the solutions are locally unique. A decoupled iteration method (going with the name of Gummel [1] in the literature) is defined by solving the three elliptic equations in (1.1) consecutively. Gummel's method can be shown to converge close to thermal equilibrium with the assumption $R = 0$ [2].

In this paper we consider the simple circuit in figure 1.1. Thus, we have

$$U + \hat{R}I = V\,,$$

where V is the voltage provided by the power supply, $\hat{R}$ is a serial resistance and I the current through the circuit. A scaled version of this equation can be written as

$$(1-\alpha)U + \alpha I = V\,, \tag{1.8}$$

where we used the same symbols for scaled and unscaled quantities. The current through the device can be computed as the current through the contact C_2:

$$I = \int_{C_2} (J_n + J_p) \cdot \nu \, ds\,, \tag{1.9}$$

where s denotes the $(n-1)$-dimensional Lebesgue measure and ν the unit outward normal along $\partial\Omega$. Instead of U being given we prescribe α and V and include (1.8) in the problem formulation. The practically interesting cases are covered by choosing $\alpha \in [0,1]$. This includes the above mentioned voltage controlled case for $\alpha = 0$ and the current controlled case for $\alpha = 1$.

For given α and V, (1.8) is the equation of a load line in the U-I-plane. Solutions of the problem (1.1), (1.3), (1.7), (1.8) correspond to intersections of the voltage-current characteristic of the device with this load line. In this context, the condition (1.8) is also used in arc-length continuation methods for the computation of voltage-current characteristics [9]. A result on the characteristics is contained in the following lemma. It asserts that the current and the contact voltage have the same signs. Although physically obvious, this result is not trivial for the mathematical model. It has been shown in [6] that for certain models of avalanche generation it is not necessarily true. However, it holds for the class of recombination-generation models considered here.

Lemma 1.1. *Let the recombination-generation term be of the form (1.2) or $R = 0$. Then*

$$\operatorname{sign}(U) = \operatorname{sign}(I)$$

holds for any solution of (1.1), (1.3), (1.7).

Proof. Multiplication of (1.9) by $e^U - 1$ gives

$$(e^U - 1)I = \int_{C_2} \left((u-1)e^{\psi}\nabla u - (v^{-1}-1)e^{-\psi}\nabla v\right) \cdot \nu \, ds\,.$$

Since the integrand in the above integral vanishes along C_1 and $\partial\Omega_N$ we can replace C_2 by $\partial\Omega$. Integration by parts implies

$$\begin{aligned}(e^U - 1)I &= \int_\Omega \left((u-1)R - (v^{-1}-1)R + e^{\psi}|\nabla u|^2 + e^{-\psi}\frac{|\nabla v|^2}{v^2}\right) dx \\ &= \int_\Omega \left(Q(u,v,\psi)\frac{(uv-1)^2}{v} + e^{\psi}|\nabla u|^2 + e^{-\psi}\frac{|\nabla v|^2}{v^2}\right) dx\,.\end{aligned} \tag{1.10}$$

A priori estimates (see [7]) show that u and v are strictly positive.

For $U = 0$ (1.10) implies that u and v are constant and, thus, $I = 0$. On the other hand, u and v cannot be constant for $U \neq 0$ by the boundary conditions (1.7). In this case the term on the right hand side above is positive which completes the proof.#

A consequence of lemma 1.1 is a global uniqueness result for the equilibrium problem:

Corollary 1.1. *The solution of the equilibrium problem ($V = 0$ in (1.8)) is unique and given by $\psi = \psi_e$, $u = v = 1$, $U = I = 0$.*

In sections 2 and 3 of this paper the problem with vanishing recombination-generation rate is considered. We introduce a decoupled fixed point iteration which, for $\alpha = 0$, reduces to Gummel's method for the voltage controlled case and, for one-dimensional problems and $\alpha = 1$, to a method introduced by Kerkhoven [3] for the current controlled case.

A result in [7] states that for $R = 0$ the voltage-current characteristic contains a continuous branch through the origin which is unbounded in the voltage direction. This implies solvability of (1.1), (1.3), (1.7), (1.8) for arbitrary V if $\alpha < 1$ and in the absence of recombination-generation. An alternative proof of this existence result using the above mentioned fixed point iteration is contained in section 3.

For the current controlled case $\alpha = 1$, existence is shown close to thermal equilibrium only. Theorem 3.2 below is a generalization to the multi-dimensional case of a result in [3]. The question of existence of solutions of the current controlled problem for arbitrary currents is still an open problem in both the one-dimensional and multi-dimensional cases.

We also prove that close to thermal equilibrium the fixed point iteration is a contraction. This result contains as special cases convergence theorems for the voltage as well as current controlled cases [2], [3].

Finally we lift the assumption of vanishing recombination-generation rate in section 4 and prove an existence result close to thermal equilibrium by an application of the implicit function theorem. It should be mentioned that the proof of this result requires very stringent assumptions on the device geometry, in particular on the behaviour of the boundary close to the points where contacts and insulating segments meet.

2. The fixed point iteration

In this and the following section we restrict ourselves to the case $R = 0$. The important effect of this assumption is that for given potential ψ the continuity equations are decoupled.

The electron current

$$I_n = \int_{C_2} e^{\psi} \nabla u \cdot \nu \, ds$$

can be computed from the Dirichlet integral

$$Q_\psi(u) := \int_\Omega e^{\psi} |\nabla u|^2 \, dx$$

by integration by parts:

$$\begin{aligned} Q_\psi(u) &= -\int_\Omega (u-1)\nabla \cdot (e^{\psi}\nabla u)\, dx + \int_{\partial\Omega} (u-1) e^{\psi} \nabla u \cdot \nu \, ds \\ &= (e^U - 1) I_n \end{aligned}$$

Note that u is the minimizer for the Dirichlet integral among all $H^1(\Omega)$-functions which satisfy the boundary conditions for u. Introducing the function ϕ_ψ by

$$Q_\psi(\phi_\psi) = \min_{\phi \in \mathcal{H}} Q_\psi(\phi) \qquad \text{with} \quad \mathcal{H} = \{\phi \in H^1(\Omega) \mid \phi|_{C_1} = 0,\ \phi|_{C_2} = 1\}$$

we obtain u from

$$u = (e^U - 1)\phi_\psi + 1\,. \tag{2.1a}$$

Since the relation $Q_\psi(u) = (e^U - 1)^2\kappa(\psi)$ holds for the Dirichlet integral $\kappa(\psi) := Q_\psi(\phi_\psi)$ of ϕ_ψ the electron current can be computed from

$$I_n = (e^U - 1)\kappa(\psi)\,.$$

Analogously we obtain

$$I_p = -(e^{-U} - 1)\kappa(-\psi)$$

for the hole current $I_p = -\int_{C_2} e^{-\psi}\nabla v \cdot \nu\, ds$ and the formula

$$v = (e^{-U} - 1)\phi_{-\psi} + 1 \tag{2.1b}$$

for v. The circuit condition (1.8) can be written as

$$(1-\alpha)U + \alpha(e^U - 1)\kappa(\psi) - \alpha(e^{-U} - 1)\kappa(-\psi) = V\,. \tag{2.2}$$

Now we are in the position to define the fixed point operator $T(\psi) = \hat{\psi}$ by

Step 1: For given ψ compute ϕ_ψ and $\phi_{-\psi}$ by solving the boundary value problems

$$\begin{aligned} &\nabla \cdot (e^{\pm\psi}\nabla\phi_{\pm\psi}) = 0 \qquad \text{in } \Omega\,, \\ &\phi_{\pm\psi}|_{C_1} = 0\,, \quad \phi_{\pm\psi}|_{C_2} = 1\,, \quad \nabla\phi_{\pm\psi}\cdot\nu|_{\partial\Omega_N} = 0 \end{aligned} \tag{2.3}$$

and $\kappa(\pm\psi)$ by evaluating the respective Dirichlet integrals.

Step 2: Solve the equation (2.2) for U.

Step 3: Compute u and v from (2.1).

Step 4: Compute $\hat{\psi}$ by solving the problem

$$\begin{aligned} &\Delta\hat{\psi} = e^{\hat{\psi}}u - e^{-\hat{\psi}}v - C(x) \qquad \text{in } \Omega\,, \\ &\hat{\psi} = \psi_{bi} \quad \text{at } C_1\,, \qquad \hat{\psi} = \psi_{bi} - U \quad \text{at } C_2\,, \\ &\nabla\hat{\psi}\cdot\nu = 0 \qquad \text{at } \partial\Omega_N\,. \end{aligned} \tag{2.4}$$

Obviously fixed points of T correspond to solutions of (1.1), (1.3), (1.7), (2.2). We point out that for a numerical realization of an iteration step $\psi_{k+1} = T(\psi_k)$ the main computational effort goes into the solution of the boundary value problems for ϕ_ψ, $\phi_{-\psi}$ and $\hat{\psi}$. Thus, the cost of one iteration step is equivalent to that for Gummel's method for the voltage driven problem.

For the operator T to be well defined we certainly need that ψ is bounded. Thus, we introduce the sets

$$\mathcal{S}_K := \{\psi \in L^\infty(\Omega) \mid \|\psi\|_\infty \le K\}$$

and prove

Lemma 2.1. *The operator $T: \ \mathcal{S}_K \to H^1(\Omega)\cap L^\infty(\Omega)$ is well defined by the steps 1–4 above.*

Proof. The boundedness of ψ is sufficient for unique solvability in $H^1(\Omega)$ of the problems (2.3). The maximum principle provides the estimates

$$0 \le \phi_{\pm\psi} \le 1 \,.$$

The membership of $\phi_{\pm\psi}$ in $H^1(\Omega)$ implies that $\kappa(\pm\psi)$ takes finite values. In the following we shall need two properties of these Dirichlet integrals:

$$\kappa(\psi) = e^{\psi}\kappa(0) \qquad \text{for } \psi \equiv \text{const} \tag{2.5}$$

Since $\phi_\psi = \phi_0$ in this case, this property obviously holds. The second property reads

$$\psi_1 \le \psi_2 \text{ in } \Omega \quad \Rightarrow \quad \kappa(\psi_1) \le \kappa(\psi_2)\,. \tag{2.6}$$

This holds because of

$$\kappa(\psi_1) = \min_{\phi\in\mathcal{H}} Q_{\psi_1}(\phi) \le Q_{\psi_1}(\phi_{\psi_2}) \le Q_{\psi_2}(\phi_{\psi_2}) = \kappa(\psi_2)\,.$$

A combination of (2.5) and (2.6) yields

$$e^{-K}\kappa(0) \le \kappa(\pm\psi) \le e^{K}\kappa(0) \qquad \text{for } \psi \in \mathcal{S}_K\,. \tag{2.7}$$

In particular, we have $\kappa(\pm\psi) > 0$ which implies that (2.2) has a unique solution U for any $\alpha \in [0,1]$ because the right hand side of (2.2) considered as a function from $\mathbb{R}$ to $\mathbb{R}$ is strictly monotonically increasing and onto.

Carrying out step 3 is trivial. From the estimates for $\phi_{\pm\psi}$ we get

$$e^{-|U|} \le u, v \le e^{|U|}\,. \tag{2.8}$$

An application of lemma 3.2.1 in [7] implies the existence of a unique solution $\hat\psi \in H^1(\Omega)\cap L^\infty(\Omega)$ of (2.4) and the estimates

$$\|\hat\psi\|_\infty \le \|\psi_{bi}\|_\infty + |U|\,.\# \tag{2.9}$$

3. Existence results

In this section the fixed point operator T is used for proving two existence theorems. The first one is a global theorem with assumptions excluding the purely current driven problem.

Theorem 3.1. *Let $\alpha \in [0,1)$ hold. Then problem (1.1), (1.3), (1.7), (2.2) has a solution $(\psi, u, v) \in \left(H^1(\Omega) \cap L^\infty(\Omega)\right)^3$ with a contact voltage U satisfying*

$$|U| \le \frac{|V|}{1-\alpha} . \tag{3.1}$$

Proof. We set

$$K = \frac{|V|}{1-\alpha} + \|\psi_{bi}\|_\infty .$$

Then $\mathcal{S}_K$ is a closed, bounded, convex subset of $L^2(\Omega)$. The momotonicity of the left hand side of (2.2) implies the estimate (3.1) independently of ψ. Considering (2.9), it is clear that T maps $\mathcal{S}_K$ into itself.

The continuous dependence of solutions of elliptic equations on the coefficients (see [5]) implies that the mappings $\psi \mapsto \phi_{\pm\psi}$ from $L^2(\Omega)$ to $H^1(\Omega)$ and $\psi \mapsto \kappa(\pm\psi)$ from $L^2(\Omega)$ to $\mathbb{R}$ are continuous. This obviously implies the continuous dependence of $U \in \mathbb{R}$ and $u, v \in H^1(\Omega)$ (obtained by carrying out steps 2 and 3 above) on $\psi \in L^2(\Omega)$. Finally, another application of well posedness results for elliptic equations gives the continuity of the operator T.

From the a priori estimates (2.8) and (3.1) we also obtain a uniform bound for the $H^1(\Omega)$-norm of $T(\psi)$ which — by the Rellich-Kondrachov theorem — implies complete continuity of T. An application of Schauder's fixed point theorem completes the proof.#

The second result deals with the purely current driven situation. We can only prove a local result close to thermal equilibrium. Note that for the equilibrium problem ($V = 0$) an iteration based on the operator T converges in one step. This is due to the fact that $U = 0$ is the solution of (2.2) in this case, regardless of the values of $\kappa(\pm\psi)$. This observation is the basis of the proof of

Theorem 3.2. *Assume $\alpha = 1$ and*

$$|V| < m := \exp\left(-\|\psi_{bi}\|_\infty\right)\kappa(0) .$$

Then problem (1.1), (1.3), (1.7), (2.2) has a solution $(\psi, u, v) \in \left(H^1(\Omega) \cap L^\infty(\Omega)\right)^3$ with a contact voltage U satisfying

$$|U| \le -\ln\left(1 - \frac{|V|}{m}\right) . \tag{3.2}$$

Remark. *In [3], the bounds in the theorem have been computed in terms of the device length and the doping profile for the one dimensional case.*

Proof. The proof is very similar to the preceding one. We set

$$K = \|\psi_{bi}\|_\infty - \ln\left(1 - \frac{|V|}{m}\right)$$

and prove that T maps $\mathcal{S}_K$ into itself. The equation (2.2) for $\alpha = 1$ reads

$$(e^U - 1)\kappa(\psi) - (e^{-U} - 1)\kappa(-\psi) = V\,. \tag{3.3}$$

By (2.7) we have

$$\kappa(\pm\psi) \geq m - |V| \qquad \text{for } \psi \in \mathcal{S}_K\,. \tag{3.4}$$

The left hand side of (3.3) is the sum of two monotonically increasing functions which vanish for $U = 0$. Denoting the solutions of the equations

$$(e^U - 1)\kappa(\psi) = V \quad \text{and} \quad -(e^{-U} - 1)\kappa(-\psi) = V$$

by U_1 and U_2, respectively, this implies

$$\begin{aligned} U &\leq \min(U_1, U_2) \quad \text{for } V \geq 0 \quad \text{and} \\ U &\geq \max(U_1, U_2) \quad \text{for } V \leq 0 \end{aligned}$$

for the solution of (2.2). Thus, we get

$$U \leq U_1 = \ln\left(1 + \frac{V}{\kappa(\psi)}\right) \leq \ln\left(1 + \frac{V}{m - V}\right) = -\ln\left(1 - \frac{|V|}{m}\right)$$

for $V \geq 0$ and

$$U \geq U_2 = -\ln\left(1 - \frac{V}{\kappa(-\psi)}\right) \geq -\ln\left(1 - \frac{V}{m + V}\right) = \ln\left(1 - \frac{|V|}{m}\right)$$

for $V \leq 0$ where we have used (3.4). Since obviously sign(U) =sign(V) holds this proves the estimate (3.2). By applying (2.9) we obtain that T maps $\mathcal{S}_K$ into itself.

The proof is completed by an application of Schauder's fixed point theorem as above.#

Finally we consider the question of convergence of iterations based on the operator T. Similarly to Gummel's method for the voltage controlled case we can prove a convergence result close to thermal equilibrium. It is well known [2], [7] that for convergence proofs for Gummel's method some regularity is needed. This is also true in our situation. Therefore we assume

$$\|\nabla\phi_\psi\|_3 \leq C(K) \qquad \text{for } \psi \in \mathcal{S}_K\,. \tag{3.5}$$

This is a (not very restrictive) assumption on the boundary of Ω and in particular on the behaviour of $\partial\Omega$ close to the points where Dirichlet and Neumann segments meet. In [2], estimates of the form (3.5) have been proven for a typical geometry using general results for mixed boundary value problems. Additionally we need:

$$C_1 \text{ and } C_2 \text{ are of class } C^1. \tag{3.6}$$

Theorem 3.3. *Let (3.5), (3.6) and $U_0 > 0$ hold. Then there is a $V_0 > 0$ such that the operator T is a contraction on the set $\mathcal{S}_K$ with*

$$K = \|\psi_{bi}\|_\infty + U_0$$

for any V with $|V| \leq V_0$. The contraction property has to be understood with respect to the $L^6(\Omega)$-norm on $\mathcal{S}_K$.

Proof. The solution of the equation (2.2) can be written as

$$U = \Phi(V, \kappa(\psi), \kappa(-\psi))$$

with a smooth function Φ with the property $\Phi(0, \kappa_1, \kappa_2) = 0$. For $\psi \in \mathcal{S}_K$ the estimate (2.7) obviously implies

$$|\Phi(V, \kappa(\psi), \kappa(-\psi))| \leq \bar{\Phi}(V, U_0)$$

with another smooth function $\bar{\Phi}$ which satisfies $\bar{\Phi}(0, U_0) = 0$. This proves the existence of a positive $V_1 > 0$ such that

$$|\Phi(V, \kappa(\psi), \kappa(-\psi))| \leq U_0 \qquad \text{for } |V| \leq V_1 \text{ and } \psi \in \mathcal{S}_K .$$

Our above results imply that T maps $\mathcal{S}_K$ into itself for $|V| \leq V_1$.

For $\psi_1, \psi_2 \in \mathcal{S}_K$ we set $\phi_1 = \phi_{\psi_1}$ and $\phi_2 = \phi_{\psi_2}$. Taking the difference of the equations (2.3) for ϕ_1 and ϕ_2, multiplication by $\phi_1 - \phi_2$ and integration by parts yields

$$\int_\Omega e^{\psi_1} |\nabla(\phi_1 - \phi_2)|^2 \, dx = - \int_\Omega (e^{\psi_1} - e^{\psi_2}) \nabla \phi_2 \cdot \nabla(\phi_1 - \phi_2) \, dx .$$

The estimate

$$\|\nabla(\phi_1 - \phi_2)\|_2 \leq e^{2K} \|\nabla \phi_2\|_3 \|\psi_1 - \psi_2\|_6 \tag{3.7}$$

follows from the above equation by employing Hölder's inequality. Considering (3.5) this implies the Lipschitz continuity of the map $\psi \mapsto \phi_\psi$ from $\mathcal{S}_K$ to $H^1(\Omega)$ with a Lipschitz constant depending on U_0.

For the map $\psi \mapsto \kappa(\psi)$ from $\mathcal{S}_K$ to $\mathbf{R}$ we have

$$\kappa(\psi_1) - \kappa(\psi_2) = \int_\Omega e^{\psi_1} \left(|\nabla \phi_1|^2 - |\nabla \phi_2|^2 \right) \, dx + \int_\Omega \left(e^{\psi_1} - e^{\psi_2} \right) |\nabla \phi_2|^2 \, dx$$

and, thus, by the Hölder inequality the estimate

$$|\kappa(\psi_1) - \kappa(\psi_2)| \leq C \|\nabla(\phi_1 + \phi_2)\|_2 \|\nabla(\phi_1 - \phi_2)\|_2 + C \|\nabla \phi_2\|_{12/5}^2 \|\psi_1 - \psi_2\|_6 .$$

Using (3.5) and (3.7) this implies the Lipschitz continuity of the map $\kappa(\psi)$. Obviously, we also get Lipschitz continuous dependence of $\phi_{-\psi}$ and $\kappa(-\psi)$ on ψ.

Since $\kappa(\psi)$ and $\kappa(-\psi)$ vary in bounded sets the map $\Phi(V, \kappa_1, \kappa_2)$ defined above, is Lipschitz continuous with respect to the second and third variables with a Lipschitz constant which tends to zero as $V \to 0$.

It is straightforward to show that $u, v \in H^1(\Omega)$ determined by (2.1) depend Lipschitz continuously on $\psi \in \mathcal{S}_K$ where again the Lipschitz constant is arbitrarily small for small V.

If U_1, u_1, v_1 and U_2, u_2, v_2 denote the results of the first three steps in the definition of $T(\psi_1)$ and $T(\psi_2)$, respectively, then $w_i = T(\psi_i)$ solves the problem (2.4) with U, u, v replaced by U_i, u_i, v_i for $i = 1, 2$. The difference of the respective differential equations reads

$$\begin{aligned}\Delta(w_1 - w_2) =& \left(e^{w_1} - e^{w_2}\right)u_1 - \left(e^{-w_1} - e^{-w_2}\right)v_1 \\ &+ e^{w_2}(u_1 - u_2) - e^{-w_2}(v_1 - v_2)\,.\end{aligned} \tag{3.8}$$

By applying standard results about traces (see e.g. [11]) the assumption (3.6) is sufficient for guaranteeing the existence of a function $w_D \in H^1(\Omega)$ with $w_D|_{C_1} = 0$, $w_D|_{C_2} = U_1 - U_2$ and

$$\|w_D\|_{H^1(\Omega)} \leq C|U_1 - U_2|\,. \tag{3.9}$$

Multiplication of (3.8) by $w_1 - w_2 + w_D$ and integration by parts gives

$$\begin{aligned}&\int_\Omega |\nabla(w_1 - w_2)|^2\,dx + \int_\Omega \left(\left(e^{w_1} - e^{w_2}\right)u_1 - \left(e^{-w_1} - e^{-w_2}\right)v_1\right)(w_1 - w_2)\,dx \\ &= -\int_\Omega \nabla(w_1 - w_2)\cdot\nabla w_D\,dx + \int_\Omega \left(\left(e^{w_1} - e^{w_2}\right)u_1 - \left(e^{-w_1} - e^{-w_2}\right)v_1\right) w_D\,dx \\ &\quad + \int_\Omega \left(e^{w_2}(u_1 - u_2) - e^{-w_2}(v_1 - v_2)\right)(w_1 - w_2 - w_D)\,dx\,.\end{aligned}$$

The second integral on the left hand side is nonnegative because of the nonnegativity of u_1 and v_1. By employing this and a Poincare estimate for $w_1 - w_2$ we obtain

$$\begin{aligned}\|w_1 - w_2\|^2_{H^1(\Omega)} \leq& C_1\left(\|w_D\|_{H^1(\Omega)} + \|u_1 - u_2\|_2 + \|v_1 - v_2\|_2\right)\|w_1 - w_2\|_{H^1(\Omega)} \\ &+ C_2\left(\|u_1 - u_2\|_2 + \|v_1 - v_2\|_2\right)\|w_D\|_{H^1(\Omega)}\end{aligned}$$

for $V \leq V_1$ (This condition provides a priori estimates for w_1, w_2 in $L^\infty(\Omega)$).

Considering (3.9) and our knowledge about the dependence of U, u, v on ψ, the above inequality implies

$$\|w_1 - w_2\|_{H^1(\Omega)} \leq L(V, U_0)\|\psi_1 - \psi_2\|_6$$

with a Lipschitz constant L tending to zero as $V \to 0$. The continuous imbedding $H^1(\Omega) \hookrightarrow L^6(\Omega)$ holds for the space dimensions $n = 1, 2, 3$ which we consider. This implies

$$\|T(\psi_1) - T(\psi_2)\|_6 \leq CL(V, U_0)\|\psi_1 - \psi_2\|_6$$

completing the proof.#

4. Nonvanishing recombination-generation

In this section we assume that the recombination-generation rate is of the form (1.2). For our analysis we need the following assumptions:

(4.1) The function $Q(u,v,\psi)$ is twice continuously differentiable.
(4.2) The equilibrium potential ψ_e is in $H^2(\Omega)$.
(4.3) There is a function $\phi \in H^2(\Omega)$ with

$$\phi|_{C_1} = 0, \quad \phi|_{C_2} = 1, \quad \nabla\phi\cdot\nu|_{\partial\Omega_N} = 0\,.$$

(4.4) For $f \in L^2(\Omega)$ the solution u of the problem

$$\Delta u = f\,, \quad u|_{C_1\cup C_2} = \nabla u\cdot\nu|_{\partial\Omega_N} = 0$$

satisfies $\|u\|_{H^2(\Omega)} \le c\|f\|_2$.

The assumptions (4.2), (4.3), (4.4) are in essence requirements on the geometry. Particularly (4.4) is very restrictive. In two dimensions it requires that contacts and insulating segments meet at angles smaller than $\pi/2$. We can prove the following local existence result:

Theorem 4.1. *Let (4.1), (4.2), (4.3), (4.4) hold. Then for $|V|$ small enough the problem (1.1), (1.3), (1.7), (1.8) has a locally unique solution $(\psi,u,v,U) \in (H^2(\Omega))^3 \times \mathbb{R}$ which depends continuously differentiably on V.*

Proof. We set

$$\begin{aligned} &\psi_D(U) = \psi_e - U\phi\,,\\ &u_D(U) = (e^U-1)\phi + 1\,, \quad v_D(U) = (e^{-U}-1)\phi + 1\,, \end{aligned}$$

where ϕ is the function described in (4.3). The new variables

$$w = \psi - \psi_D\,, \qquad y = u - u_D\,, \qquad z = v - v_D$$

satisfy homogeneous boundary conditions, i.e. they will be required to be elements of

$$H^2_\partial(\Omega) = \{u \in H^2(\Omega) :\ u|_{C_1\cup C_2} = \nabla u\cdot\nu|_{\partial\Omega_N} = 0\}\,.$$

In terms of the new variables the problem reads

$$\begin{aligned} &\Delta w - e^{w+\psi_D}(y+u_D) + e^{-w-\psi_D}(z+v_D) + e^{\psi_e} - e^{-\psi_e} = 0\,,\\ &\nabla\cdot\big(e^{w+\psi_D}\nabla(y+u_D)\big) - Q(y+u_D, z+v_D, w+\psi_D)\big((y+u_D)(z+v_D)-1\big) = 0\,,\\ &\nabla\cdot\big(e^{-w-\psi_D}\nabla(z+v_D)\big) - Q(y+u_D, z+v_D, w+\psi_D)\big((y+u_D)(z+v_D)-1\big) = 0\,,\\ &(1-\alpha)U + \alpha\int_{C_2}\big(e^{w+\psi_D}\nabla(y+u_D) - e^{-w-\psi_D}\nabla(z+v_D)\big)\cdot\nu\, ds - V = 0 \end{aligned} \tag{4.5}$$

with $(w,y,z,U) \in \left(H^2_\partial(\Omega)\right)^3 \times \mathbb{R}$. Formally the problem can be written as $F_V(w,y,z,U) = 0$ where the operator $F_V: \left(H^2_\partial(\Omega)\right)^3 \times \mathbb{R} \to \left(L^2(\Omega)\right)^3 \times \mathbb{R}$ is defined by the left hand sides of the above equations. Note that we need the continuous imbedding $H^2(\Omega) \hookrightarrow C(\bar{\Omega})$ and the estimate

$$\|u\|_4 \le \varepsilon \|\nabla u\|_2 + c_\varepsilon \|u\|_2 \tag{4.6}$$

(see [4, p. 69]) for F_V to be well defined. (4.6) is needed for estimates of the form

$$\|\nabla w \cdot \nabla y\|_2 \le \|\nabla w\|_4 \|\nabla y\|_4 \le c\|w\|_{H^2(\Omega)} \|y\|_{H^2(\Omega)} \,.$$

Considering the thermal equilibrium problem we have $F_0(0,0,0,0) = 0$. For an application of the implicit function theorem we shall show that $D_{(w,y,z,U)}F_0(0,0,0,0)$, the Frechet derivative of F_0 evaluated at $(w,y,z,U) = (0,0,0,0)$, is boundedly invertible. The problem

$$D_{(w,y,z,U)}F_0(0,0,0,0)(\hat{w} + W\phi, \hat{y} - W\phi, \hat{z} + W\phi, W) = (f_1, f_2, f_3, f_4)$$

can be written as

$$\begin{aligned} &\Delta \hat{w} = \left(e^{\psi_e} + e^{-\psi_e}\right)\hat{w} + e^{\psi_e}\hat{y} - e^{-\psi_e}\hat{z} + f_1 \,, \\ &\hat{w}|_{C_1} = 0 \,, \quad \hat{w}|_{C_2} = -W \,, \quad \nabla \hat{w} \cdot \nu|_{\partial\Omega_N} = 0 \,, \end{aligned} \tag{4.7}$$

$$\begin{aligned} &\nabla \cdot \left(e^{\psi_e} \nabla \hat{y}\right) = Q_0(\hat{y} + \hat{z}) + f_2 \,, \\ &\nabla \cdot \left(e^{-\psi_e} \nabla \hat{z}\right) = Q_0(\hat{y} + \hat{z}) + f_3 \,, \\ &\hat{y}|_{C_1} = \hat{z}|_{C_1} = \nabla \hat{y} \cdot \nu|_{\partial\Omega_N} = \nabla \hat{z} \cdot \nu|_{\partial\Omega_N} = 0 \,, \quad \hat{y}|_{C_2} = -\hat{z}|_{C_2} = W \,, \end{aligned} \tag{4.8}$$

$$(1-\alpha)W + \alpha \int_{C_2} \left(e^{\psi_e}\nabla \hat{y} - e^{-\psi_e}\nabla \hat{z}\right) \cdot \nu \, ds = f_4 \,. \tag{4.9}$$

where $Q_0 = Q(1,1,\psi_e)$ holds.

Our first observation is that the problem is partially decoupled. The solution component $\hat{w}$ can be obtained from (4.7) after having solved (4.8), (4.9) for $(\hat{y}, \hat{z}, W)$. It can be shown (see [6, p. 46f]) that for given W the problem (4.8) has a unique solution $(\hat{y}, \hat{z}) = (Wy_0 + y_f, Wz_0 + z_f) \in \left(H^1(\Omega)\right)^2$ where (y_0, z_0) solves a version of (4.8) with $f_2 = f_3 = 0$ and $W = 1$. The pair (y_f, z_f) is obtained from (4.8) with W replaced by zero, and satisfies

$$\|y_f\|_{H^1(\Omega)}, \|z_f\|_{H^1(\Omega)} \le c\left(\|f_2\|_2 + \|f_3\|_2\right). \tag{4.10}$$

For proving $H^2(\Omega)$-regularity of $\hat{y}$ we write the differential equation for $\hat{y}$ as

$$\Delta \hat{y} = -\nabla \psi_e \cdot \nabla \hat{y} + e^{-\psi_e} Q_0(\hat{y} + \hat{z}) + e^{-\psi_e} f_2$$

and use (4.6) for estimating the first term on the right hand side. With assumption (4.4) we have

$$\|\hat{y}\|_{H^2(\Omega)} \le \varepsilon \|\nabla \psi_e\|_4 \|\hat{y}\|_{H^2(\Omega)} + c\left(|W| + \|f_2\|_2 + \|f_3\|_2\right),$$

which implies an $H^2(\Omega)$ estimate for $\hat{y}$ by choosing ε small enough. For $\hat{z}$ we proceed analogously.

With the above representation for $\hat{y}$ and $\hat{z}$, the equation (4.9) for W becomes

$$W\left[1-\alpha+\alpha\int_{C_2}\left(e^{\psi_e}\nabla y_0 - e^{-\psi_e}\nabla z_0\right)\cdot\nu\, ds\right] = f_4 - \alpha\int_{C_2}\left(e^{\psi_e}\nabla y_f - e^{-\psi_e}\nabla z_f\right)\cdot\nu\, ds\,.$$

With the aid of the divergence theorem the integrals over the contact C_2 can be rewritten as volume integrals:

$$W\left[1-\alpha+\alpha\int_{\Omega}\left(e^{\psi_e}|\nabla y_0|^2 + e^{-\psi_e}|\nabla z_0|^2 + Q_0(y_0+z_0)^2\right)\, dx\right] = f_4 - \alpha\int_{\Omega}\left(\nabla\phi\cdot(e^{\psi_e}\nabla y_f - e^{-\psi_e}\nabla z_f) + \phi(f_2 - f_3)\right)\, dx\,,$$

where ϕ is the function from assumption (4.3). Obviously, the coefficient of W is positive. Thus, W is determined uniquely, and the estimates (4.10) imply

$$|W| \le c\left(\|f_2\|_2 + \|f_3\|_2 + |f_4|\right).$$

Having determined $\hat{y}$, $\hat{z}$ and W, we can compute $\hat{w}$ from (4.7). The assumption (4.4) implies $\hat{w} \in H^2(\Omega)$ and the continuous dependence on the data.#

References

[1] H.K. GUMMEL, A self consistent iterative scheme for one dimensional steady state transistor calculations, *IEEE Trans. on Electron Devices* **ED-11**, pp. 455–465 (1964).

[2] T. KERKHOVEN, A proof of convergence of Gummel's algorithm for realistic device geometries, *SIAM J. Numer. Anal.* **23**, pp. 1121–1137 (1986).

[3] T. KERKHOVEN, On the one-dimensional current driven semiconductor equations, *SIAM J. Appl. Math.* **51**, pp. 748–774 (1991).

[4] O.A. LADYZHENSKAYA, V.A. SOLONNIKOV, and N.N. URAL'TSEVA, *Linear and Quasilinear Equations of Parabolic Type*, AMS Transl. vol. 23, New York, 1968.

[5] O.A. LADYZHENSKAYA and N.N. URAL'TSEVA, *Linear and Quasilinear Elliptic Equations*, Academic Press, New York, 1968.

[6] P.A. MARKOWICH, A nonlinear eigenvalue problem modelling the avalanche effect in semiconductor diodes, *SIAM J. Math. Anal.* **16**, pp. 1268–1283 (1985).

[7] P.A. MARKOWICH, *The Stationary Semiconductor Device Equations*, Springer-Verlag, Wien, 1986.

[8] P.A. MARKOWICH, C. RINGHOFER, and C. SCHMEISER, *Semiconductor Equations*, Springer-Verlag, Wien, 1990.

[9] P.A. MARKOWICH, C. RINGHOFER, and A. STEINDL, Computation of current-voltage characteristics in a semiconductor device using arc-length continuation, *IMA J. Appl. Math.* **33**, pp. 175–187 (1984).

[10] M.S. MOCK, *Analysis of Mathematical Models of Semiconductor Devices*, Boole Press, Dublin, 1983.

[11] G.M. TROIANIELLO, *Elliptic Differential Equations and Obstacle Problems*, Plenum Press, New York, 1987.