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# An Optimal Control Approach to Semiconductor Design

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**Abstract**

The design problem for semiconductor devices is studied via an optimal control approach for the standard drift diffusion model. The solvability of the minimization problem is proved. The first–order optimality system is derived and the existence of Lagrange–multipliers is established. Further, estimates on the sensitivities are given. Numerical results concerning a symmetric n–p–diode are presented.

**Key words.** semiconductor design, drift diffusion, optimal control, existence, first–order necessary condition, Lagrange–multipliers, sensitivity, numerics.

**AMS(MOS) subject classification.** 35J50,49J20,49K20.

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# 1 Introduction

Due to the rapidly increasing demand for semiconductor technology lots of effort has been spend on the development of new semiconductor devices. Especially, the ongoing miniaturization revealed several challenging problems for electrical engineers and applied mathematicians, too. Numerical simulations proved to be the main tool for reducing the time of a design cycle. For this purpose a hierarchy of models is employed, which ranges from microscopic, like the Boltzmann–Poisson or the Wigner–Poisson model, to macroscopic models, like the energy transport, the hydrodynamic and the drift diffusion model (DD) [MRS90]. Most popular and widely used in commercial simulation packages is the DD, which allows for a very efficient numerical study of the charge transport in many cases of practical relevance.

Many performance properties of semiconductor devices can be derived from the so–called current–voltage characteristics (IVC), which relates the applied biasing voltage and the current density. Typically, such an ideal IVC is given and the engineer meets the following *design problem*: Adjust physical and/or geometrical parameters of a semiconductor device such that the given ideal IVC is matched optimally with respect to certain performance criteria.

In most applications one changes the geometry and the doping profile, which describes the the density of charged background ions. In the conventional design cycle simulation tools are employed to compute the IVC for a certain set of parameters and then, the parameters are adjusted empirically. Thus, the total design time depends crucially on the knowledge and experience of the electrical engineer.

Although this problem can be clearly tackled by an optimization approach, only recently efforts were made to solve the design problem via optimization techniques. In [LWT99] *Lee et al.* present a finite–dimensional least-squares approach for adjusting the parameters of a semiconductor to fit a given, ideal IVC. Their work is purely numerical and has its focus on testing different approaches to solve the least-squares problem. Recently, [BEMP00] addressed the identification problem for the doping profile from current–voltage data via the linearized drift diffusion model.

In standard applications a working point, i.e. a certain voltage–current pair, for the device is fixed [Sze81]. Especially for MOSFET devices in portable systems it is most important to have on the one hand a low leakage current, which maximizes the battery lifetime, and on the other hand to maximize the drive current [SSP+98]. Thus, in this paper we consider exemplarily the *modified design question*:

> Is it possible to gain an amplified current at the working point only by a slight change of the doping profile?

In the following we give a positive answer to this question by means of an optimal control problem for the DD. In [SSP+99] this problem was approached numerically by a blackbox optimization, which only required evaluations of a device simulator for different sets of doping parameters. The results are encouraging, although the blackbox optimizer yields high computational costs.

We focus on the DD due to fact that this model is today most widely used in simulation codes, since it allows for an accurate description of the underlying physics in combination with low computational costs. There exists a large amount of literature on this model, which covers questions of the mathematical analysis [Gaj85, Moc83, NW91] as well as of the numerical discretization and simulation [Gum64, Ker86]. For an excellent overview see [Mar86, MRS90].

The stationary standard drift diffusion model for semiconductor devices stated on a bounded domain $\Omega \subset \mathbb{R}^d$, $d = 1, 2$ and 3 reads

$$J_n = q\left(D_n \nabla n + \mu_n\, n\, \nabla V\right), \tag{1.1a}$$
$$J_p = -q\left(D_p \nabla p - \mu_p\, p\, \nabla V\right), \tag{1.1b}$$
$$\operatorname{div} J_n = R, \tag{1.1c}$$
$$\operatorname{div} J_p = -R, \tag{1.1d}$$
$$-\epsilon \Delta V = q(n - p - C). \tag{1.1e}$$

The variables are the densities of electrons $n(x)$ and holes $p(x)$, the current densities of electrons $J_n(x)$ and holes $J_p(x)$, respectively, and the electrostatic potential $V(x)$. The total current density is given by

$$J = J_n + J_p. \tag{1.1f}$$

The doping profile is denoted by $C(x)$. The parameters $D_n, D_p, \mu_n, \mu_p$ are the diffusion coefficients and mobilities of electrons and holes respectively. The physical constants are the elementary charge $q$ and the permittivity constant $\epsilon$. In the model generation–recombination processes are included via the recombination rate $R : \mathbb{R}^2 \to \mathbb{R}$. Commonly employed is the *Shockley–Read–Hall* term

$$R_{SRH}(n,p) = \frac{n\,p - n_i^2}{\tau_p(n + n_i) + \tau_n(p + n_i)},$$

where the physical constants are the carrier life times $\tau_n, \tau_p$ and the intrinsic density $n_i$. But also other recombination models are employed of which we only mention the *Auger* term and *impact ionization*, which models high field effects [Sze81].

In the folowing we will only consider regimes in which we can assume the Einstein relations

$$D_n = U_T\, \mu_n, \quad D_p = U_T\, \mu_p,$$

where $U_T = k_B\, T/q$ is the thermal voltage of the device and $T$ denotes its temperature and $k_B$ the Boltzmann constant. Especially in high field applications these mobilities depend crucially on the electric field $E = \nabla V$.

To get a well posed problem, system (1.1) has to be supplemented with appropriate boundary conditions. We assume that the boundary $\partial\Omega$ of the domain $\Omega$ splits into two disjoint parts $\Gamma_D$ and $\Gamma_N$, where $\Gamma_D$ models the Ohmic contacts of the device and $\Gamma_N$ represents the insulating parts of the boundary. Let $\nu$ denote the unit outward normal vector along the boundary. Firstly, assuming charge neutrality and thermal equilibrium at the Ohmic contacts $\Gamma_D$ and, secondly, zero current flow and vanishing electric field at the insulating part $\Gamma_N$ yields the following set of boundary data

$$n = n_D, \quad p = p_D, \quad V = V_D \quad \text{on } \Gamma_D, \tag{1.1g}$$

$$\nabla n \cdot \nu = \nabla p \cdot \nu = \nabla V \cdot \nu = 0 \quad \text{on } \Gamma_N, \tag{1.1h}$$

where $n_D, p_D, V_D$ are the $H^1(\Omega)$–extensions of

$$\begin{aligned} n_D &= \frac{C + \sqrt{C^2 + 4\,n_i^2}}{2}, \\ p_D &= \frac{-C + \sqrt{C^2 + 4\,n_i^2}}{2}, \\ V_D &= -U_T \,\log\left(\frac{n_D}{n_i}\right) + U, \qquad \text{on } \Gamma_D. \end{aligned}$$

Here, $U$ denotes the applied voltage.

For the sake of a smoother presentation we assume in the following that the device considered is operated near thermal equilibrium. Thus, we assume that no generation–recombination effects are present, i.e. $R \equiv 0$, and that the mobilities $\mu_n, \mu_p$ are constant. Further, we employ the following scaling

$$\begin{array}{lll} n \to C_m\,\tilde{n}, & p \to C_m\,\tilde{p}, & x \to L\,\tilde{x}, \\ C \to C_m\,\tilde{C}, & V \to U_T\,\tilde{V}, & J_{n,p} \to \dfrac{q\,U_T\,C_m\,\mu_0}{L}\tilde{J}_{n,p} \end{array}$$

where $L$ denotes a characteristic device length, $C_m$ the maximal absolute value of the background doping profile and $\mu_0$ a characteristic value for the mobilities. Defining the dimensionless *Debye length*

$$\lambda^2 = \frac{\epsilon\,U_T}{q\,C_m\,L^2}$$

the scaled equations read

$$\Delta n + \operatorname{div}(n\,\nabla V) = 0, \tag{1.2a}$$

$$\Delta p - \operatorname{div}(p\,\nabla V) = 0, \tag{1.2b}$$

$$-\lambda^2 \Delta V = n - p - C, \tag{1.2c}$$

where we eliminated the current densities and omitted the tilde for notational convenience. The boundary conditions transform to

$$n_D = \frac{C + \sqrt{C^2 + 4\,\delta^4}}{2}, \tag{1.2d}$$

$$p_D = \frac{-C + \sqrt{C^2 + 4\,\delta^4}}{2}, \tag{1.2e}$$

$$V_D = -\log\left(\frac{n_D}{\delta^2}\right) + U, \qquad \text{on } \Gamma_D, \tag{1.2f}$$

where $\delta^2 = n_i/C_m$ denotes the scaled intrinsic density.

To solve the modified design question we start from given a reference doping profile $\bar{C}$ and specify the working point $(\bar{U}, \bar{J})$. Let $\Gamma_O$ be a portion of the Ohmic contacts $\Gamma_D$ at which we can measure the total current $J$. At this contact we prescribe a gained current density $J_g$ and allow deviations of the doping profile from $\bar{C}$ in some suitable norm to gain this current flow.

Especially, we intend to minimize cost functionals of the form

$$Q(n,p,V,C) = \frac{1}{2}\,\|(J - J_g)\cdot\nu\|^2_{H^{-1/2}(\Gamma_O)} + \frac{\gamma}{2}\int_\Omega \left|C - \bar{C}\right|^2\,dx, \tag{1.3a}$$

and

$$Q(n,p,V,C) = \frac{1}{2}\,\|(J - J_g)\cdot\nu\|^2_{H^{-1/2}(\Gamma_O)} + \frac{\gamma}{2}\int_\Omega \left|\nabla(C - \bar{C})\right|^2\,dx, \tag{1.3b}$$

where the total current $J$ is given by the solution of (1.2). Clearly, the proposed evaluation of the total current along the boundary poses some restrictions on the regularity of the solutions to (1.2), which will be addressed below. Here, $\gamma > 0$ is a parameter which allows to balance the effective cost. Note that we penalize large deviations form the reference doping profile, which has the advantage that the overall structure of the device is retained after the optimization, i.e. a transistor is still a transistor.

The optimal control problem for the system (1.2) will be considered as a constrained optimization problem. The approach presented is closely related to that discussed by *Ito et al.* [IK96] for the control of nonlinear partial differential equations.

Further analytical results related to the work presented are given by *Fang et al.* in [FI92], where a mathematical model is developed for a non destructive optical testing technique for semiconductors called laser–beam–induced currents (LBIC), and by *Busenberg et al.* [BFI93], where the identifiability of defects in a semiconductor from its LBIC–image is mathematically studied.

The paper is organized as follows. In Section 2 we specify the optimal control problem and its analytical setting. We present an existence result in Section 3. The first–order optimality system is studied in Section 4. After its derivation we establish the existence and uniqueness of Lagrange–multipliers, and give estimates on the sensitivities. Lastly, numerical results for a symmetric n–p–diode are presented in Section 5.

## 2 Problem Formulation and Analytic Setting

We introduce a functional analytic framework which allows to deal with general optimization problems that in particular include those introduced in Section 1. This has the advantage that also cost functionals that meet different performance criteria can be used. The state equations (1.2) are considered as a constraint to the functional (1.3b) and the differentiability of this mapping is proved.

For the subsequent considerations we impose the following assumptions.

**A.1** Let $\Omega \subset \mathbb{R}^d$, $d = 1, 2$ or $3$ be a bounded domain with boundary $\partial\Omega \in C^{0,1}$. The boundary $\partial\Omega$ is piecewise regular and splits into two disjoint parts $\Gamma_N$ and $\Gamma_D$. The set $\Gamma_D$ has nonvanishing $(d-1)$–dimensional Lebesgue–measure. $\Gamma_N$ is closed.

**A.2** Let $\Gamma_D = \bigcup_{l=1}^{M} \Gamma_D^l$, $M \geq 2$ and $\mathrm{dist}(\Gamma_D^{l_1}, \Gamma_D^{l_2}) > 0$ for $l_1 \neq l_2$ and $l_1, l_2 \in \{1, \dots, M\}$. It holds $\Gamma_O = \bigcup_{k=1}^{N} \Gamma_D^{l_k}$ for $1 \leq N \leq M$.

**A.3** The boundary data fulfil $(n_D, p_D, V_D) \in H^1(\Omega)$. For the gained total current we require $J_g \cdot \nu \in H^{-1/2}(\partial\Omega)$ and $\bar{C} \in H^1(\Omega)$ for the reference doping profile.

**Remark 2.1.** Assumption **A.2** on the distance of two Ohmic contacts implies that they are pairwise separated by some part of the insulating boundary, which is physically reasonable since it prevents short-circuiting. On the other hand this is important for the regularity of solutions.

We introduce the space of states

$$X \stackrel{\text{def}}{=} x_D + X_0,$$

where $x_D \stackrel{\text{def}}{=} (n_D, p_D, V_D)$ denotes the boundary data introduced in (1.2) and $X_0 \stackrel{\text{def}}{=} \left(H_0^1(\Omega \cup \Gamma_N) \cap L^\infty(\Omega)\right)^3$ is equipped with the norm $\|x\|_{X_0} \stackrel{\text{def}}{=} \|x\|_{[H^1(\Omega)]^3} + \|x\|_{[L^\infty(\Omega)]^3}$. Let us recall that $H_0^1(\Omega \cup \Gamma_N)$ is the closure of $C_0^\infty(\Omega \cup \Gamma_N)$ with respect to the $H^1(\Omega)$–norm [Tro87]. The set of co–states will be $Z \stackrel{\text{def}}{=} [H^1(\Omega)]^3$ and the set of admissible controls is given by

$$\mathcal{C} \stackrel{\text{def}}{=} \{C \in H^1(\Omega) : C = \bar{C} \text{ on } \Gamma_D\}. \tag{2.1}$$

**Remark 2.2.** At a first glance this imposes a further restriction on the doping profile, since we freeze the boundary values of $C$. Nevertheless, considering the cost functional (1.3a) and deriving *formally* the first order optimality system under the assumption $C \in H^1(\Omega)$ yields exactly the additional restriction on the doping profile given in (2.1).

We abbreviate $x \stackrel{\text{def}}{=} (n, p, V)$ and rewrite the state equations (1.2) as $e(x, C) = 0$, where the nonlinear mapping $e : X \times \mathcal{C} \to Z^*$ is defined by

$$e(x, C) \stackrel{\text{def}}{=} \begin{pmatrix} \Delta n + \mathrm{div}(n \nabla V) \\ \Delta p - \mathrm{div}(p \nabla V) \\ -\lambda^2 \Delta V - n + p + C \end{pmatrix}. \tag{2.2}$$

Next we investigate the differentiability properties of the mapping $e$.

**Theorem 2.3.** *The mapping $e$ defined in (2.2) is infinitely often Fréchet differentiable with derivatives vanishing for order greater than 2. The actions of the first derivatives at a point $(x, C) \in X \times \mathcal{C}$ in a direction $\hat{x} = (\hat{n}, \hat{p}, \hat{V}) \in X_0$ are given by*

$$\begin{aligned}\langle e_x(x, C)\hat{x}, z\rangle = \langle \Delta\hat{n} + \operatorname{div}(\hat{n}\nabla V), z^n\rangle \\ - \left\langle \hat{n}, z^V\right\rangle + \langle \Delta\hat{p} - \operatorname{div}(\hat{p}\nabla V), z^p\rangle + \left\langle \hat{p}, z^V\right\rangle \\ + \left\langle \operatorname{div}(n\nabla\hat{V}), z^n\right\rangle - \left\langle \operatorname{div}(p\nabla\hat{V}), z^p\right\rangle - \left\langle \lambda^2\Delta\hat{V}, z^V\right\rangle \qquad (2.3)\end{aligned}$$

*for all $z = (z^n, z^p, z^V) \in Z$ and*

$$\left\langle e_C(x, C)\hat{C}, z\right\rangle = \left\langle \hat{C}, z^V\right\rangle \qquad (2.4)$$

*for all $\hat{C} \in H^1_0(\Omega \cup \Gamma_N)$ and $z \in Z$. The second derivatives $e_{xC}(x, C)$, $e_{Cx}(x, C)$ and $e_{CC}(x, C)$ vanish, the action of the second derivative w.r.t. $x$ at a point $(x, C)$ in directions $\hat{x}_1 = (\hat{n}_1, \hat{p}_1, \hat{V}_1)$, $\hat{x}_2 = (\hat{n}_2, \hat{p}_2, \hat{V}_2) \in X_0$ is given by*

$$\begin{aligned}\langle e_{xx}(x, C)(\hat{x}_1, \hat{x}_2), z\rangle = \left\langle \operatorname{div}(\hat{n}_1\nabla\hat{V}_2), z^n\right\rangle - \left\langle \operatorname{div}(\hat{p}_1\nabla\hat{V}_2), z^p\right\rangle \\ + \left\langle \operatorname{div}(\hat{n}_2\nabla\hat{V}_1), z^n\right\rangle - \left\langle \operatorname{div}(\hat{p}_2\nabla\hat{V}_1), z^p\right\rangle \quad \textit{for all } z = (z^n, z^p, z^V) \in Z. \qquad (2.5)\end{aligned}$$

Here and in the following $\langle\cdot,\cdot\rangle$ denotes the dual pairing of $Z^*$ and $Z$.

**Proof.** Let $(x, C), (\tilde{x}, \tilde{C}) \in X \times \mathcal{C}$ and let $z \in Z$. By the definition of the mapping $e$ it holds

$$\begin{aligned}\left\langle e(x, C) - e(\tilde{x}, \tilde{C}), z\right\rangle = \left\langle \Delta(n - \tilde{n}) + \operatorname{div}\left((n\,\nabla V) - (\tilde{n}\,\nabla\tilde{V})\right), z^n\right\rangle \\ + \left\langle \Delta(p - \tilde{p}) - \operatorname{div}\left((p\,\nabla V) - (\tilde{p}\,\nabla\tilde{V})\right), z^p\right\rangle \\ + \left\langle -\lambda^2\Delta(V - \tilde{V}) - (n - \tilde{n}) + (p - \tilde{p}) + C - \tilde{C}, z^V\right\rangle.\end{aligned}$$

Since

$$\operatorname{div}\left((n\,\nabla V) - (\tilde{n}\,\nabla\tilde{V})\right) = \operatorname{div}((n - \tilde{n})\nabla V) + \operatorname{div}\left(\tilde{n}\nabla(V - \tilde{V})\right)$$

and

$$\operatorname{div}\left((p\,\nabla V) - (\tilde{p}\,\nabla\tilde{V})\right) = \operatorname{div}((p - \tilde{p})\nabla V) + \operatorname{div}\left(\tilde{p}\nabla(V - \tilde{V})\right)$$

after several integration by parts we can estimate

$$\begin{aligned}&\left|\left\langle e(x, C) - e(\tilde{x}, \tilde{C}), z\right\rangle\right| \le \\ &K\left\{\left[\|n - \tilde{n}\|_{H^1(\Omega)} + \|n - \tilde{n}\|_{L^\infty(\Omega)}\|V\|_{H^1(\Omega)} + \|\tilde{n}\|_{L^\infty(\Omega)}\|V - \tilde{V}\|_{H^1(\Omega)}\right]\|z^n\|_{H^1(\Omega)}\right. \\ &+ \left[\|p - \tilde{p}\|_{H^1(\Omega)} + \|p - \tilde{p}\|_{L^\infty(\Omega)}\|V\|_{H^1(\Omega)} + \|\tilde{p}\|_{L^\infty(\Omega)}\|V - \tilde{V}\|_{H^1(\Omega)}\right]\|z^p\|_{H^1(\Omega)} \\ &\left.+ \left[\lambda^2\|V - \tilde{V}\|_{H^1(\Omega)} + \|n - \tilde{n}\|_{L^2(\Omega)} + \|p - \tilde{p}\|_{L^2(\Omega)} + \|C - \tilde{C}\|_{L^2(\Omega)}\right]\|z^V\|_{H^1(\Omega)}\right\},\end{aligned}$$

where $K = K(\Omega) > 0$ denotes a strictly positive constant. Here we have utilized the continuity of the trace operator $\{\gamma_0, \gamma_1\} : H^1(\Omega) \to H^{1/2}(\partial\Omega) \times H^{-1/2}(\partial\Omega)$, $v \mapsto \{\gamma_0 v, \gamma_1 v\}$, where $\gamma_0 v := v_{|\partial\Omega}$, $\gamma_1 v := (\partial v/\partial\eta)_{|\partial\Omega}$ and $\eta$ denotes the unit outward normal to $\partial\Omega$, see [GR86, Theorem 1.6]. The previous estimate implies

$$\|e(x, C) - e(\tilde{x}, \tilde{C})\|_{Z^*} \leq K \left( \|x - \tilde{x}\|_{X_0} + \|C - \tilde{C}\|_{\mathcal{C}} \right)$$

and thus, the continuity of the nonlinear mapping $(x, C) \mapsto e(x, C)$. For the derivative w.r.t. $x$ one has

$$\begin{aligned}\langle e(x, C) - e(\tilde{x}, C) - e_x(x, C)(x - \tilde{x}), z\rangle = \left\langle \operatorname{div} \left( (\tilde{n} - n)\nabla(V - \tilde{V}) \right), z^n \right\rangle - \\ \left\langle \operatorname{div} \left( (\tilde{p} - p)(\nabla V - \tilde{V}) \right), z^p \right\rangle \quad \text{for all } z \in Z,\end{aligned}$$

so that similar estimation as above yields

$$\|e(x, C) - e(\tilde{x}, C) - e_x(x, C)(x - \tilde{x})\|_{Z^*} \leq K \, \|x - \tilde{x}\|^2_{X_0},$$

and thus, the existence and continuity of the mapping $(x, C) \mapsto e_x(x, C)$. Further, (2.4) is a simple consequence of the linearity of the mapping $(x, C) \mapsto e(x, C)$ w.r.t. $C$.

To finish the proof it remains to investigate the mapping $(x, C) \mapsto e_{xx}(x, C)$. Let $\hat{x}_1 \in X_0$ be arbitrary. Utilizing (2.3) and (2.5) one immediately gets

$$\langle e_x(x, C)\hat{x}_1 - e_x(\tilde{x}, C)\hat{x}_1 - e_{xx}(x, C) \left( (x - \tilde{x}), \hat{x}_1 \right), z\rangle = \langle 0, z\rangle \qquad \text{for all } z \in Z,$$

which completes the proof of the theorem. □

# 3 Existence of Solution

In this section we establish the existence of a solution to the optimal control problem. We require standard regularity properties of the cost functional $Q$.

**A.4** Let $Q : X \times \mathcal{C} \to \mathbb{R}$ denote a cost functional which is assumed to be twice continuously Fréchet differentiable with Lipschitz continuous second derivatives. Further, let $Q$ be of separated type, i.e. $Q(x, C) = Q_1(x) + Q_2(C)$ and radially unbounded w.r.t. $\mathcal{C}$ for every $x \in X$, bounded from below and weakly lower semi-continuous.

**Remark 3.1.** Clearly, the cost functional (1.3b) fits into this setting, while (1.3a) is excluded.

We now consider the minimization problem

$$\min_{X \times \mathcal{C}} Q(n, p, V, C) \quad \text{s.t.} \quad e(n, p, V, C) = 0. \tag{3.1}$$

The solvability of the state equations for every $C \in \mathcal{C}$ is a consequence of the following result.

**Proposition 3.2.** *Assume* **A.1**–**A.3**. *Then for each* $C \in H^1(\Omega)$ *and all data* $(n_D, p_D, V_D) \in X$ *with*

$$\frac{1}{K} \leq n_D(x), p_D(x) \leq K, \quad x \in \Omega, \quad \textit{and } \|V_D\|_{L^\infty(\Omega)} \leq K$$

*for some* $K \geq 1$*, there exists a solution* $(n, p, V) \in X$ *of system* (1.2) *fulfilling*

$$\frac{1}{L} \leq n(x), p(x) \leq L, \quad x \in \Omega, \quad \textit{and } \|V\|_{L^\infty(\Omega)} \leq L$$

*for some constant* $L = L(\Omega, K, \|C\|_{L^p(\Omega)}) \geq 1$*, where the embedding* $H^1(\Omega) \hookrightarrow L^p(\Omega)$ *holds.*

For a proof see e.g. [NW91], where Stampaccia's method [Sta58] is employed. We point out that standard a priori estimates relying on the maximum principle make use of the fact $C \in L^\infty(\Omega)$, which is much too strict for our purposes as we seek a minimizer in $H^1(\Omega)$. Nevertheless, also the proof in [NW91] uses the boundedness of $(n_D, p_D, V_D)$, which is another reason for the choice of the admissible set $\mathcal{C}$. Note that uniqueness of solutions can only be expected for small applied voltages $U$, i.e. if the device is operated near thermal equilibrium.

The existence result reads

**Theorem 3.3.** *Assume* **A.1**–**A.4**. *Then, the constrained minimization problem* (3.1) *admits a solution* $(n^*, p^*, V^*, C^*) \in X \times \mathcal{C}$.

**Proof.** Since $Q$ is bounded from below, $Q_0 \overset{\text{def}}{=} \inf_{(n,p,V,C) \in X \times \mathcal{C}} Q(n, p, V, C)$ is finite. Consider a minimizing sequence $\{(x^k, C^k)\}_{k \in \mathbb{N}} \subset X \times \mathcal{C}$. From the radial unboundedness of $Q$ we infer that $\{C^k\}_{k \in \mathbb{N}}$ is bounded in $\mathcal{C}$. Hence, there exists a weakly convergent subsequence, again denoted by $\{C^k\}_{k \in \mathbb{N}}$, such that

$$C^k \rightharpoonup C^*, \qquad \text{weakly in } \mathcal{C}.$$

Since $\mathcal{C}$ is weakly closed w.r.t. the $H^1(\Omega)$-norm, we have $C^* \in \mathcal{C}$. By the continuous embedding $H^1(\Omega) \hookrightarrow L^p(\Omega)$ $(p \in [1, 6))$ the sequence $\{C^k\}_{k \in \mathbb{N}}$ is also bounded in $L^p(\Omega)$. Now one can employ Stampaccia's method [Sta58] to derive the following estimates [NW91]

$$\left\|n^k\right\|_{H^1(\Omega)} + \left\|n^k\right\|_{L^\infty(\Omega)} \leq K \left( \|n_D\|_{L^\infty(\Gamma_D)} + \left\|C^k\right\|_{L^p(\Omega)} \right), \tag{3.2a}$$

$$\left\|p^k\right\|_{H^1(\Omega)} + \left\|p^k\right\|_{L^\infty(\Omega)} \leq K \left( \|p_D\|_{L^\infty(\Gamma_D)} + \left\|C^k\right\|_{L^p(\Omega)} \right), \tag{3.2b}$$

$$\left\|V^k\right\|_{H^1(\Omega)} + \left\|V^k\right\|_{L^\infty(\Omega)} \leq K \left( \|V_D\|_{L^\infty(\Gamma_D)} + \left\|C^k\right\|_{L^p(\Omega)} \right), \tag{3.2c}$$

for some constant $K = K(\Omega) > 0$. These are by far sufficient to pass to the limit in the state equations (1.2), which can be seen as follows. First note that $\|(n_D, p_D, V_D)\|_{(L^\infty(\Gamma_D))^3}$ is bounded independently of $k$ due to the definition of the admissible set (2.1). Every solution $(n^k, p^k, V^k)$ of (1.2) associated to $C^k$ satisfies the a priori estimates (3.2). Hence, there exists a subsequence, again denoted by $\{(n^k, p^k, V^k)\}_{k\in\mathbb{N}}$ such that

$$(n^k, p^k, V^k) \rightharpoonup (n^*, p^*, V^*) \quad \text{weakly in } (H^1(\Omega))^3,$$

which by Rellich's Theorem [Zei90] implies strong convergence of $\{(n^k, p^k, V^k)\}_{k\in\mathbb{N}}$ in $(L^2(\Omega))^3$. Further, the uniform $L^\infty(\Omega)$–bounds imply

$$(n^k, p^k, V^k) \rightharpoonup (n^*, p^*, V^*) \quad \text{weak-* in } L^\infty(\Omega).$$

Utilizing these convergences one can pass to the limit in the weak formulation of (1.2), which satisfies

$$\begin{aligned}
\Delta n^* + \operatorname{div}(n^* \nabla V^*) &= 0,\\
\Delta p^* - \operatorname{div}(p^* \nabla V^*) &= 0,\\
-\lambda^2 \Delta V^* &= n^* - p^* - C^*
\end{aligned}$$

together with the boundary conditions in (1.2). This completes the proof of the existence of a minimizer. □

**Remark 3.4.** Generally, we cannot expect the uniqueness of the minimizer for arbitrary biasing voltages due to several reasons. First, far from equilibrium the state equations may admit multiple solutions [Mar86]. Further, it is not clear, if different states yield different current densities, such that also the suggestive convexity of the cost functional cannot be used. Even worse, the admissible set of minimizers defined by the equality constraint $e(n, p, V, C) = 0$ might not be convex. We refer also to the discussion in [BEMP00], where the identification problem for the doping profile is treated with the linearized drift diffusion model. Therein, the authors point out that even for the linearized model uniqueness is hardly to achieve under very restrictive assumptions depending on the dimension of space, such as unipolarity, small biasing voltages and high regularity of the solution.

# 4 The First–order Optimality System

Next we derive the first–order optimality system, state a result on the existence and uniqueness of Lagrange–multipliers and give estimates on the sensitivities.

The Lagrangian $\mathcal{L} : X \times \mathcal{C} \times Z \to \mathbb{R}$ associated to the minimization problem (3.1) is defined by

$$\mathcal{L}(x, C, \xi) \stackrel{\text{def}}{=} Q(x, C) + \langle e(x, C), \xi \rangle \,.$$

For the subsequent investigations we write $\xi \stackrel{\text{def}}{=} (\xi^n, \xi^p, \xi^V)$. By Theorem 2.3 and **A.4** the Lagrangian $\mathcal{L}$ is twice continuously Fréchet differentiable with Lipschitz continuous second derivatives. The first order optimality system corresponding to problem (3.1) is given by

$$\nabla_{(x,C,\xi)} \mathcal{L}(x, C, \xi) = 0. \tag{4.1}$$

In the following we rewrite this equations in a more concise form. First, we note that variations of $\mathcal{L}$ w.r.t. $\xi \in Z$ yield the state equations

$$e(x, C) = 0.$$

Secondly, taking variations of $\mathcal{L}$ w.r.t. the control $C \in \mathcal{C}$ leads to the optimality condition

$$e_C^*(x, C)\xi = -Q_C(x, C) \quad \text{in } \mathcal{C}^*, \tag{4.2}$$

and finally, the co–state or adjoint equations satisfied by $\xi$ are obtained by taking variations of $\mathcal{L}$ w.r.t. the state $x$. This leads to

$$e_x^*(x, C)\xi = -Q_x(x, C) \quad \text{in } X^*. \tag{4.3}$$

Here, $e_C^*(x, C) \in L(Z, \mathcal{C}^*)$ and $e_x^*(x, C) \in L(Z, X^*)$ denote the adjoint operators associated to $e_C(x, C)$ and $e_x(x, C)$, respectively.

A short computation shows that for the cost functionals given by (1.3a),(1.3b) the optimality condition (4.2) is due to the assumption **A.4** equivalent to

$$\xi^V = -\gamma \left(C - \bar{C}\right)$$

in the case of (1.3a), and

$$\xi^V = \gamma\Delta \left(C - \bar{C}\right)$$

in the case of (1.3b).

The derivation of the co–state equations is more involved. To begin with let $\tilde{x} \in X_0$, with $\tilde{x} = (\tilde{n}, \tilde{p}, \tilde{V})$, denote a test function. Since $\tilde{x}$ vanishes on $\Gamma_D$

$$\begin{aligned} \langle Q_x(x, C), \tilde{x}\rangle &= \langle (J(x) - J_g) \cdot \nu, w\rangle_{H^{-1/2}(\Gamma_O), H^{1/2}(\Gamma_O)} \\ &= \langle J_x(x)\tilde{x} \cdot \nu, \varphi\rangle_{H^{-1/2}(\Gamma_O), H^{1/2}(\Gamma_O)} \end{aligned} \tag{4.4}$$

holds, where $\varphi$ and $w$ are the $H^1(\Omega)$–solutions of

$$-\Delta\varphi + \varphi = 0 \quad \text{in } \Omega \tag{4.5a}$$

$$\varphi = 0 \quad \text{on } \Gamma_N \tag{4.5b}$$

$$\nabla\varphi \cdot \nu = \begin{cases} \langle (J(x) - J_g) \cdot \nu, \cdot\rangle_{H^{-1/2}(\Gamma_O), H^{1/2}(\Gamma_O)} & \text{on } \Gamma_O \\ 0 & \text{on } \Gamma_D \setminus \Gamma_O, \end{cases} \tag{4.5c}$$

and

$$\begin{aligned} -\Delta w + w &= 0 \quad \text{in } \Omega \\ w &= 0 \quad \text{on } \Gamma_N \\ \nabla w \cdot \nu &= \begin{cases} \langle J_x(x)\tilde{x} \cdot \nu, \cdot\rangle_{H^{-1/2}(\Gamma_O), H^{1/2}(\Gamma_O)} & \text{on } \Gamma_O \\ 0 & \text{on } \Gamma_D \setminus \Gamma_O, \end{cases} \end{aligned}$$

respectively. Here we have utilized the variational characterization of the $H^{-1/2}$-norm [BF91, p.90].

Next, we consider $\langle e_x(x,C)\tilde{x},\xi\rangle$ for test functions $\tilde{x}\in X_0\cap C_0^\infty(\Omega)$. After several applications of Green's formula to remove all derivatives from the test function $\tilde{x}$ we conclude with the adjoint system

$$\Delta\xi^n - \nabla V\,\nabla\xi^n = \xi^V, \tag{4.6a}$$
$$\Delta\xi^p + \nabla V\,\nabla\xi^p = -\xi^V, \tag{4.6b}$$
$$-\lambda^2\Delta\xi^V + \operatorname{div}(n\,\nabla\xi^n) - \operatorname{div}(p\,\nabla\xi^p) = 0. \tag{4.6c}$$

Now, we derive the boundary data for (4.6). Due to $\tilde{x}\in X_0$ we can choose $\tilde{x}$ arbitrarily on $\Gamma_N$, and $\nabla\tilde{x}\cdot\nu$ can be chosen arbitrarily on $\Gamma_D$. First, let $\tilde{x}$ be arbitrary on $\Gamma_N$ and $\nabla\tilde{x}\cdot\nu = 0$ on $\partial\Omega$. This together with $\lambda^2 > 0$ gives

$$\nabla\xi^n\cdot\nu = \nabla\xi^p\cdot\nu = \nabla\xi^V\cdot\nu = 0 \quad \text{on } \Gamma_N. \tag{4.7a}$$

Secondly, let $\nabla\tilde{x}\cdot\nu$ be arbitrary on $\Gamma_D$. Then we conclude that

$$\xi^V = 0 \text{ on } \Gamma_D \quad\text{ and }\quad \xi^n = \xi^p = \begin{cases} 0 & \text{on } \Gamma_D\setminus\Gamma_O, \\ -\varphi & \text{on } \Gamma_O. \end{cases} \tag{4.7b}$$

All together we find that the first–order necessary optimality condition (4.1) is equivalent to the following nonlinear system of coupled equations for the state $x$, the control $u$ and the adjoint variable $\xi$. It consists of the state equations

$$\begin{aligned} \Delta n + \operatorname{div}(n\,\nabla V) &= 0, \\ \Delta p - \operatorname{div}(p\,\nabla V) &= 0, \\ -\lambda^2\Delta V &= n - p - C \end{aligned}$$

with boundary data given in (1.2) and the adjoint system

$$\begin{aligned} \Delta\xi^n - \nabla V\,\nabla\xi^n &= \xi^V, \\ \Delta\xi^p + \nabla V\,\nabla\xi^p &= -\xi^V, \\ -\lambda^2\Delta\xi^V + \operatorname{div}(n\,\nabla\xi^n) - \operatorname{div}(p\,\nabla\xi^p) &= 0, \end{aligned}$$

supplemented with boundary data (4.7).

Moreover, the adjoint and the control are coupled via the equation

$$\xi^V = -\gamma\,(C-\bar{C}) \tag{4.8}$$

in the case of cost functional (1.3a), and via

$$\gamma\Delta\left(C-\bar{C}\right) = \xi^V \quad \text{in } \Omega, \tag{4.9a}$$
$$C = \bar{C} \quad \text{on } \Gamma_D, \tag{4.9b}$$
$$\nabla C\cdot\nu = \nabla\bar{C}\cdot\nu \quad \text{on } \Gamma_N. \tag{4.9c}$$

in the case of cost functional (1.3b).

## 4.1 Existence of Lagrange–multipliers

In Section 3 we proved that the minimizer satisfies the state equations. Now, we want to establish the unique existence of the Lagrange–multipliers in the case of states which are near to the thermal equilibrium.

For the following investigations it is most convenient to write system (4.6) in symmetric form. This is accomplished by multiplying the first two equations of (4.6) with $e^{-V}$ and $e^{V}$, respectively.

$$\operatorname{div}\left(e^{-V}\nabla\xi^n\right) = e^{-V}\,\xi^V, \tag{4.10a}$$

$$\operatorname{div}\left(e^{V}\nabla\xi^p\right) = -e^{V}\,\xi^V, \tag{4.10b}$$

$$-\lambda^2\Delta\xi^V + (n+p)\,\xi^V = -J_n\,\nabla\xi^n + J_p\,\nabla\xi^p. \tag{4.10c}$$

**Remark 4.1.** This is exactly the form of the adjoint system which would be derived from the linearization of the state equations written in terms of the so–called *Slotboom variables* (compare [Mar86]).

Now we are in the position to state the existence and uniqueness theorem for the Lagrange–multipliers.

**Theorem 4.2.** *Assume* **A.1**–**A.4**. *Then there exists a constant* $j = j(\Omega,\lambda,V) > 0$ *such that for each state* $(n,p,V) \in X$ *with*

$$\left\|\frac{J_n^2}{n}\right\|_{L^\infty(\Omega)} + \left\|\frac{J_p^2}{p}\right\|_{L^\infty(\Omega)} \le j$$

*system* (4.10) *supplemented with boundary conditions* (4.7) *possesses a unique solution* $(\xi^n,\xi^p,\xi^V) \in Z$.

**Remark 4.3.** The smallness condition on the current densities inherits also a assumption on their regularity. Physically, it is common believe that the current densities behave well throughout the whole device [Moc83]. Analytically, we can assure this regularity in our weak setting only in one space dimension, where the current densities are constants. Nevertheless, assuming a more regular domain and data this can also be achieved in dimensions larger than one due to the regularizing effect of the elliptic operators, see e.g. [Tro87] and [Gri85].

**Proof.** For the proof we reduce the linear system (4.10) to a single elliptic equation. To this purpose we define $\bar{\xi^n}, \bar{\xi^p} \in H^1(\Omega)$ as the unique solution of

$$\begin{aligned}
\operatorname{div}\left(e^{-V}\nabla\bar{\xi^n}\right) &= 0,\\
\operatorname{div}\left(e^{V}\nabla\bar{\xi^p}\right) &= 0,\\
\bar{\xi^n} = \bar{\xi^p} &= \begin{cases} 0 & \text{on } \Gamma_D\setminus\Gamma_O,\\ -\varphi & \text{on } \Gamma_O,\end{cases}\\
\nabla\bar{\xi^n}\cdot\nu = \nabla\bar{\xi^p}\cdot\nu &= 0 \quad \text{on } \Gamma_N,
\end{aligned}$$

where $\varphi$ is the solution of (4.5). Further, we introduce the solution operators $T_{n,p} : L^2(\Omega) \to H_0^1(\Omega \cup \Gamma_N)$ by

$$\begin{gathered}
\operatorname{div}\left(e^{-V} \nabla T_n(\xi^V)\right) = e^{-V}\, \xi^V, \\
\operatorname{div}\left(e^{V} \nabla T_p(\xi^V)\right) = -e^{V}\, \xi^V, \\
T_n(\xi^V),\ T_p(\xi^V) \in H_0^1(\Omega \cup \Gamma_N)
\end{gathered}$$

Then system (4.10) can be equivalently written as

$$-\lambda^2 \Delta \xi^V + (n+p)\, \xi^V + J_n\, \nabla T_n(\xi^V) - J_p\, \nabla T_p(\xi^V) = -J_n\, \nabla \bar{\xi^n} + J_p\, \nabla \bar{\xi^p}, \tag{4.11}$$

subject to $\xi^V \in H_0^1(\Omega \cup \Gamma_N)$, and $\xi_n, \xi_p$ are given by

$$\xi^n = \bar{\xi^n} + T_n(\xi^V), \quad \xi^p = \bar{\xi^p} + T_p(\xi^V). \tag{4.12}$$

¿From elliptic estimates [Tro87] we know

$$\left\|T_n(\xi^V)\right\|_{H^1(\Omega)} + \left\|T_p(\xi^V)\right\|_{H^1(\Omega)} \le c_1 \left\|\xi^V\right\|_{L^2(\Omega)},$$

for some constant $c_1 = c_1(\Omega, V) > 0$.

In the following we show the solvability of (4.11) by means of the Lax–Milgram Lemma. We define the bilinear form $b : H_0^1(\Omega \cup \Gamma_N) \times H_0^1(\Omega \cup \Gamma_N) \to \mathbb{R}$ and the functional $G : H_0^1(\Omega \cup \Gamma_N) \to \mathbb{R}$ by

$$\begin{aligned}
b(\xi^V, \phi) &= \lambda^2 \int_\Omega \nabla \xi^V\, \nabla \phi\, dx + \int_\Omega (n+p) \xi^V\, \phi\, dx \\
&\quad + \int_\Omega J_n \nabla T_n(\xi^V)\, \phi\, dx - \int_\Omega J_p \nabla T_p(\xi^V)\, \phi\, dx \\
G(\phi) &= \int_\Omega -J_n\, \nabla \bar{\xi^n}\, \phi + J_p\, \nabla \bar{\xi^p}\, \phi\, dx
\end{aligned}$$

Clearly, $b$ and $G$ are continuous. The coercivity of $b$ is a consequence of

$$\begin{aligned}
b(\xi^V, \xi^V) \ge \lambda^2 &\int_\Omega \left|\nabla \xi^V\right|^2\, dx + \int_\Omega (n+p) \left|\xi^V\right|^2\, dx \\
&- \left\|\frac{J_n}{\sqrt{n}}\right\|_{L^\infty(\Omega)} \left\|\nabla T_n(\xi^V)\right\|_{L^2(\Omega)} \left\|\sqrt{n}\, \xi^V\right\|_{L^2(\Omega)} \\
&- \left\|\frac{J_p}{\sqrt{p}}\right\|_{L^\infty(\Omega)} \left\|\nabla T_p(\xi^V)\right\|_{L^2(\Omega)} \left\|\sqrt{p}\, \xi^V\right\|_{L^2(\Omega)}
\end{aligned}$$

and by Young's inequality

$$
\begin{aligned}
&\geq \lambda^2 \int_\Omega \left|\nabla \xi^V\right|^2 \, dx + \int_\Omega (n+p) \left|\xi^V\right|^2 \, dx \\
&\quad - \frac{1}{4} \left\| \frac{J_n^2}{n} \right\|_{L^\infty(\Omega)} \left\|\nabla T_n(\xi^V)\right\|_{L^2(\Omega)}^2 - \frac{1}{4} \left\| \frac{J_p^2}{p} \right\|_{L^\infty(\Omega)} \left\|\nabla T_p(\xi^V)\right\|_{L^2(\Omega)}^2 \\
&\quad - \int_\Omega n \left|\xi^V\right|^2 \, dx - \int_\Omega p \left|\xi^V\right|^2 \, dx \\
&\geq \lambda^2 \int_\Omega \left|\nabla \xi^V\right|^2 \, dx - c_1^2(\Omega, V) \left( \left\| \frac{J_n^2}{n} \right\|_{L^\infty(\Omega)} + \left\| \frac{J_p^2}{p} \right\|_{L^\infty(\Omega)} \right) \left\|\xi^V\right\|_{L^2(\Omega)}^2 \\
&\geq \kappa \left\|\xi^V\right\|_{H^1(\Omega)}^2 ,
\end{aligned}
$$

for some constant $\kappa = \kappa(\Omega, \lambda, V, j) > 0$ provided we have

$$
\left\| \frac{J_n^2}{n} \right\|_{L^\infty(\Omega)} + \left\| \frac{J_p^2}{p} \right\|_{L^\infty(\Omega)} \leq j
$$

for $j = j(\Omega, \lambda, V) > 0$ small enough.

Now the existence of a unique solution $\xi^V \in H_0^1(\Omega \cup \Gamma_N)$ follows directly from the Lax–Milgram Lemma and $\xi^n, \xi^p$ are uniquely determined by (4.12).

□

## 4.2 Sensitivity

After we established the unique existence of the Lagrange–multipliers, we derive now estimates, which give insight into the sensitivity of the problem. Testing (4.10) with appropriate test functions and using the following estimate on the extension operator [Tro87]

$$
\|\xi_D^n\|_{H^1(\Omega)} \leq c \, \|\varphi\|_{H^{1/2}(\Gamma_O)} \leq c \, \|(J_g - J) \cdot \nu\|_{H^{-1/2}(\Gamma_O)} ,
$$

for some constant $c = c(\Omega) > 0$, yields

$$
\|\xi^n\|_{H^1(\Omega)} \leq K e^{V_{max} - V_{min}} \left\{ \left\|\xi^V\right\|_{L^2(\Omega)} + \|(J_g - J) \cdot \nu\|_{H^{-1/2}(\Gamma_O)} \right\} , \tag{4.13a}
$$

for some constant $K = K(\Omega) > 0$ and in analogy

$$
\|\xi^p\|_{H^1(\Omega)} \leq K e^{V_{max} - V_{min}} \left\{ \left\|\xi^V\right\|_{L^2(\Omega)} + \|(J_g - J) \cdot \nu\|_{H^{-1/2}(\Gamma_O)} \right\} . \tag{4.13b}
$$

Further, we get

$$
\lambda^2 \left\|\xi^V\right\|_{H^1(\Omega)}^2 \leq \frac{K}{4} \left\{ \left\| \frac{J_n^2}{n} \right\|_{L^\infty(\Omega)} \|\xi^n\|_{H^1(\Omega)}^2 + \left\| \frac{J_p^2}{p} \right\|_{L^\infty(\Omega)} \|\xi^p\|_{H^1(\Omega)}^2 \right\} . \tag{4.14}
$$

These are the key estimates for the proof of the next theorem, which states the bound on the sensitivity of the electrostatic potential.

**Theorem 4.4.** *Assume* **A.1**–**A.4**. *Then there exists a constant* $j = j(\Omega, \lambda, V) > 0$ *such that for*

$$\left\| \frac{J_n^2}{n} \right\|_{L^\infty(\Omega)} + \left\| \frac{J_p^2}{p} \right\|_{L^\infty(\Omega)} \le j$$

*it holds*

$$\|\xi^V\|^2_{H^1(\Omega)} \le j \left( \lambda^2 - \frac{K^3}{4} e^{2(V_{max} - V_{min})} j \right)^{-1} \frac{K^3}{2} e^{2(V_{max} - V_{min})} \|(J_g - J) \cdot \nu\|^2_{H^{-1/2}(\Gamma_O)},$$

*for some constant* $K = K(\Omega) > 0$.

**Proof.** Combining the estimates (4.13) and (4.14) yields

$$\left\{ \lambda^2 - \frac{K^3}{4} e^{2(V_{max} - V_{min})} \left( \left\| \frac{J_n^2}{n} \right\|_{L^\infty(\Omega)} + \left\| \frac{J_p^2}{p} \right\|_{L^\infty(\Omega)} \right) \right\} \|\xi^V\|^2_{H^1(\Omega)} \le$$
$$\frac{K^3}{2} e^{2(V_{max} - V_{min})} \left( \left\| \frac{J_n^2}{n} \right\|_{L^\infty(\Omega)} + \left\| \frac{J_p^2}{p} \right\|_{L^\infty(\Omega)} \right) \|(J_g - J) \cdot \nu\|^2_{H^{-1/2}(\Gamma_O)}$$

and choosing $j = j(\Omega, \lambda, V) > 0$ small enough we get the desired estimate. □

In analogy one proves the following sensitivity bounds.

**Corollary 4.5.** *Under the conditions of Theorem 4.4 it holds*

$$\|\xi^n\|^2_{H^1(\Omega)} + \|\xi^p\|^2_{H^1(\Omega)} \le$$
$$4K\, e^{2(V_{max} - V_{min})} \left( 1 - \frac{K^2}{\lambda^2} e^{2(V_{max} - V_{min})} j \right)^{-1} \|(J_g - J) \cdot \nu\|^2_{H^{-1/2}(\Gamma_O)}.$$

**Remark 4.6.** As expected the sensitivities are small in the case of small deviations from the desired state. Furthermore, for small current densities, i.e. if the device is operated near thermal equilibrium, also the sensitivity $\xi^V$ for the potential is small.

# 5 Numerical Results

In this section we propose an algorithm for the solution of the the first–order optimality system, which can be easily adapted to existing simulation codes for semiconductor devices. The method generalizes the well–known *Gummel–iteration* for the drift diffusion model [Gum64, MRS90].

Starting with some doping profile $C_0$, we decouple the state system (1.2) from the adjoint system, solve in a next step the adjoint system (4.6) for the Lagrange–multipliers and update the doping profile via (4.8) or (4.9), respectively. The iteration stops, if the difference of two consecutive doping profiles is below some specified threshold. To stabilize the numerics we use a continuation method in $\gamma$, starting with $\gamma = 2^{-7}$ which is bisected in each step.

The advantage of this decoupling approach is that during the iterative process an existing fast solver for the state system can be employed and in each iteration only one additional *linear* system has to be solved.

We test this numerical scheme for a symmetric n–p–diode and try to gain an amplified total current at the working point. The reference doping profile of the device can be found in Figure 5.1 and the corresponding current–voltage characteristic is depicted in Figure 5.2. The Si–diode is $1\mu$m long and operated at 300K. The maximum doping density is $10^{22}\text{m}^{-3}$.

**Remark 5.1.** Note, that it holds only $\bar{C} \in L^\infty(\Omega)$, in contrast to our assumptions. Nevertheless, the algorithm still works, since we can solve (4.9) for $W = C - \bar{C}$ and update the doping profile via $C = W + \bar{C}$.

For the biasing voltage at the working point we choose $\bar{U} = 0.5$V and try to gain an amplification of the total current $\bar{J}$ by 75%, i.e. we set $J_g = \bar{J} \cdot 1.75$. In the simulations we employ both cost functionals given in (1.3).

The numerical results show that the system is not controllable into the desired state. Nevertheless, for $\gamma = 2^{-23}$ the minimizer of (1.3b) yields a current gain of approximately 20%. The minimizing doping density can be found in Figure 5.1. The corresponding current–voltage characteristics are depicted in Figure 5.2.

Note, that the position of the junction is identical with the one of the reference profile and also the height of the junction did only change slightly, which becomes clear in view of the updates (4.8) and (4.9). In a future work different cost functionals will be applied, which allow also for a change in the position and height of the junction.

| $\gamma$ | $Q$ | $(J_g - J)^2$ | $\left\|C - \bar{C}\right\|_{L^2}^2$ |
|---|---|---|---|
| $2^{-13}$ | $1.2 \cdot 10^{-9}$ | $3.1 \cdot 10^{-8}$ | 0 |
| $2^{-15}$ | $4.6 \cdot 10^{-9}$ | $2.9 \cdot 10^{-8}$ | $3 \cdot 10^{-4}$ |
| $2^{-17}$ | $1.7 \cdot 10^{-8}$ | $2.6 \cdot 10^{-8}$ | $5 \cdot 10^{-3}$ |
| $2^{-19}$ | $4.9 \cdot 10^{-8}$ | $2 \cdot 10^{-8}$ | $5 \cdot 10^{-2}$ |

Table 1: Numerical Results for cost functional (1.3a)

| $\gamma$ | $Q$ | $(J_g - J)^2$ | $\left\|\nabla(C - \bar{C})\right\|_{L^2}^2$ |
|---|---|---|---|
| $2^{-13}$ | $1 \cdot 10^{-10}$ | $3 \cdot 10^{-8}$ | $0$ |
| $2^{-16}$ | $8 \cdot 10^{-10}$ | $3 \cdot 10^{-8}$ | $1 \cdot 10^{-4}$ |
| $2^{-19}$ | $6 \cdot 10^{-9}$ | $2.9 \cdot 10^{-8}$ | $7 \cdot 10^{-3}$ |
| $2^{-23}$ | $5 \cdot 10^{-8}$ | $8 \cdot 10^{-9}$ | $9 \cdot 10^{-1}$ |

Table 2: Numerical Results for cost functional (1.3b)

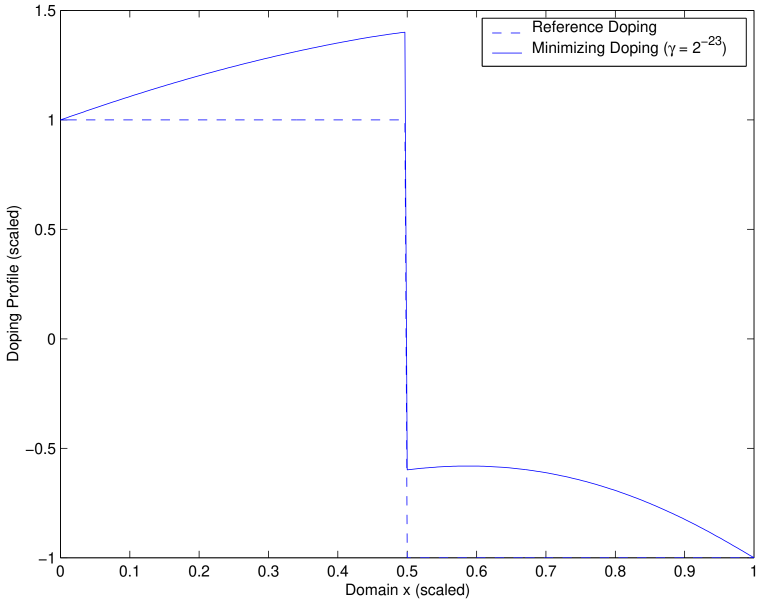


Figure 5.1: Doping Profiles

# References

[BEMP00] M. Burger, H. W. Engl, P. A. Markowich, and P. Pietra. Identification of doping profiles in semiconductor devices. *In preparation*, 2000.

[BF91] F. Brezzi and M. Fortin. *Mixed and Hybrid Finite Element Methods.* Springer Series in Computational Mathematics 15, 1991.

[BFI93] S. Busenberg, W. Fang, and K. Ito. Modeling and analysis of laser-beam-induced current images in semiconductors. *SIAM J. Appl. Math.*, 53:187–204, 1993.

[FI92] W. Fang and K. Ito. Identifiability of semiconductor defects from LBIC images. *SIAM J. Appl. Math.*, 52:1611–1625, 1992.

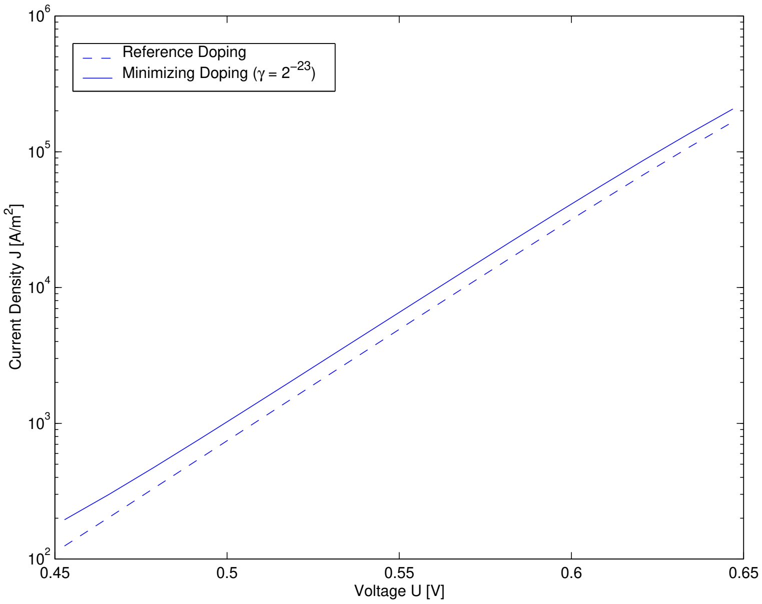


Figure 5.2: Current–Voltage Characteristics


[Gaj85] H. Gajewski. On existence, uniqueness and asymptotic behavior of solutions of the basic equations for carrier transport in semiconductors. *Z. Angew. Math. Mech.*, 65(2):101–108, 1985.

[GR86] V. Girault and P.A. Raviart. *Finite Element Methods for the Navier-Stokes Equations*. Springer Series in Computational Mathematics 5, 1986.

[Gri85] P. Grisvard. *Elliptic Problems in Nonsmooth Domains*. Pitman, Boston, first edition, 1985.

[Gum64] H. K. Gummel. A self–consistent iterative scheme for one–dimensional steady state transistor calculations. *IEEE Trans. Elec. Dev.*, ED–11:455–465, 1964.

[IK96] K. Ito and K. Kunisch. Augmented Lagrangian-SQP-methods for nonlinear optimal control problems of tracking type. *SIAM J. Control and Optimization*, 34:874–891, 1996.

[Ker86] T. Kerkhoven. A proof of convergence of Gummel's algorithm for realistic device geometries. *SIAM J. Numer. Anal.*, 23(6):1121–1137, December 1986.

[LWT99] W.R. Lee, S. Wang, and K.L. Teo. An optimization approach to a finite dimensional parameter estimation problem in semiconductor device design. *Journal of Computational Physics*, 156:241–256, 1999.

[Mar86] P. A. Markowich. *The Stationary Semiconductor Device Equations.* Springer–Verlag, Wien, first edition, 1986.

[Moc83] M. S. Mock. *Analysis of Mathematical Models of Semiconductor Devices.* Boole Press, Dublin, first edition, 1983.

[MRS90] P. A. Markowich, Ch. A. Ringhofer, and Ch. Schmeiser. *Semiconductor Equations.* Springer–Verlag, Wien, first edition, 1990.

[NW91] J. Naumann and M. Wolff. A uniqueness theorem for weak solutions of the stationary semiconductor equations. *Appl. Math. Optim.*, 24:223–232, 1991.

[SSP+98] M. Stockinger, R. Strasser, R. Plasun, A. Wild, and S. Selberherr. A qualitative study on optimized MOSFET doping profiles. In *Proceedings SISPAD 98 Conf.*, pages 77–80, 1998.

[SSP+99] M. Stockinger, R. Strasser, R. Plasun, A. Wild, and S. Selberherr. Closed–loop MOSFET doping profile optimization for portable systems. In *Proceedings Intl. Conf. on Modelling and Simulation of Microsystems, Semiconductors and Sensors*, pages 395–398, 1999.

[Sta58] G. Stampaccia. Contributi alla regolarizzazione delle soluzioni dei problemi al contorno per secondo ordine ellittiche. *Ann. Scuola Norm. Suo. Pisa*, 12:223–245, 1958.

[Sze81] S. M. Sze. *Physics of Semiconductor Devices.* Wiley, New York, second edition, 1981.

[Tro87] G. M. Troianiello. *Elliptic Differential Equations and Obstacle Problems.* Plenum Press, New York, first edition, 1987.

[Zei90] E. Zeidler. *Nonlinear Functional Analysis and its Applications*, volume II/A and II/B. Springer–Verlag, Berlin, first edition, 1990.