Optimal Control of the Drift Diffusion Model for Semiconductor Devices

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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.

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 the Boltzmann–Poisson or the Wigner–Poisson model, to macroscopic models, like the energy transport, the hydrodynamic and the drift diffusion model (DD) [10]. 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

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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 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 clearly be tackled by an optimization approach, only little efforts were yet made in semiconductor industry to solve the design problem via optimization techniques. As far as the authors know, up to now only one attempt has been made to address semiconductor design with mathematical optimization techniques. In [8] *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 has its focus on testing different approaches to solve numerically the least-squares problem.

In standard applications a working point, i.e. a certain voltage–current pair, for the device is fixed [14]. Thus, in this paper we consider 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?

We give an positive answer to this question by means of an optimal control problem for the DD. The focus on the DD is due to the 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 [11, 12] as well as of the numerical discretization and simulation [4, 7]. For an excellent overview see [9, 10]

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

$$J_n = \mu_n \left(\nabla n + n \nabla V\right), \tag{1.1a}$$

$$J_p = \mu_p \left(\nabla p - p \nabla V\right), \tag{1.1b}$$

$$\operatorname{div} J_n = 0, \tag{1.1c}$$

$$\operatorname{div} J_p = 0, \tag{1.1d}$$

$$-\lambda^2 \Delta V = n - p - C. \tag{1.1e}$$

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 doping profile is denoted by $C(x)$. The parameter λ is the scaled Debye length of the device and μ_n, μ_p denote the carrier mobilities. The total current

density is given by

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

Note that for the sake of simplicity we assume constant mobilities and that no generation–recombination processes occur [14].

Inserting the relations for the current densities into the continuity equations yields the system

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

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

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

which will be considered in the following.

To get a well posed problem, system (1.2) has to be supplemented with appropriate boundary conditions. We assume that the boundary $\partial\Omega$ of the domain Ω splits into two disjoint parts Γ_D and Γ_N, where Γ_D models the Ohmic contacts of the device and Γ_N represents the insulating parts of the boundary. Let ν denote the unit outward normal vector along the boundary. Firstly, assuming charge neutrality and thermal equilibrium at the Ohmic contacts Γ_D and, secondly, zero current flow and vanishing electric field and the insulating part Γ_N yields the following set of boundary data

$$n = n_D, \quad p = p_D, \quad V = V_D \qquad \text{on } \Gamma_D, \tag{1.2d}$$

$$\nabla n \cdot \nu = \nabla p \cdot \nu = \nabla V \cdot \nu = 0 \qquad \text{on } \Gamma_N, \tag{1.2e}$$

where n_D, p_D, V_D are the $H^2(\Omega)$–extensions of

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

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

$$V_D = -\log\left(\frac{C + \sqrt{C^2 + 4\,\delta^2}}{2\,\delta}\right) + U, \qquad \text{on } \Gamma_D.$$

Here, δ is the scaled intrinsic density and U is an applied voltage.

To solve the modified design question we start from given reference doping profile $\bar{C}$ and specify the working point $(\bar{U}, \bar{J})$. Let Γ_O be a portion of the Ohmic contacts Γ_D at which we can measure the total current J. At this contact we prescribe a gained current density J_g and allow for 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

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

and

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

where the total current J is given by the solution of (1.1). Here, $\gamma > 0$ is a parameter which allows to balance the effective cost. Clearly, the proposed evaluation of the total current along the boundary poses some restrictions on the regularity of the solutions to (1.1), which will be addressed below.

The optimal control problem for the system (1.1) will be considered as a constrained optimization problem. The approach presented is closely related to that discussed by *Ito et al.* [6] for the control of nonlinear partial differential equations.

Further analytical results related to the work presented are given by *Fang et al.* in [2], 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.* [1], where the identifiability of defects in a semiconductor from its LBIC–image is studied mathematically.

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 of Lagrange–multipliers, comment on their uniqueness 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 now introduce a functional analytic framework which allows to deal with general optimization problems that in particular include those introduced in Section 1. 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 $\partial\Omega \in C^{1,1}$. The boundary $\partial\Omega$ is piecewise regular and splits into two disjoint parts Γ_N and Γ_D. The set Γ_D has nonvanishing $(d-1)$–dimensional Lebesgue–measure. Γ_N is closed.

A.2 The boundary data fulfils $(n_D, p_D, V_D) \in H^2(\Omega)$. For the gained total current we require $J_g \in H^1(\Omega;\mathbb{R}^d)$ and $\bar{C} \in H^1(\Omega)$ for the reference doping profile.

A.3 There exists a constant $K = K(\Omega, \Gamma_D, \Gamma_N) > 0$ such that for $f \in L^2(\Omega)$ and $w_D \in H^2(\Omega)$ there exists a solution $w \in H^2(\Omega)$ of

$$\Delta w = f, \quad w - w_D \in H_0^1(\Omega \cup \Gamma_N),$$

which fulfils

$$\|w\|_{H^2(\Omega)} \le K \left(\|w_D\|_{H^2(\Omega)} + \|f\|_{L^2(\Omega)} \right).$$

Remark 2.1. Assumption **A.3** is essentially a restriction on the geometry of Ω. It is fulfilled in the case where the Dirichlet and the Neumann boundary do not meet, i.e. $\overline{\Gamma}_D \cap \Gamma_N = \emptyset$ [15]. In the two dimensional case it is fulfilled if Γ_D and Γ_N meet under angles larger than $\pi/2$ [3]. Let us recall that the space $H_0^1(\Omega \cup \Gamma_N)$ is the closure of $C_c^\infty(\Omega \cup \Gamma_N)$ with respect to the $H^1(\Omega)$–norm [15].

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 (1.1) and $X_0 \stackrel{\text{def}}{=} \left(H^2(\Omega) \cap H_0^1(\Omega \cup \Gamma_N)\right)^3$. 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).

According to the habits in control theory in the following doping profiles are denoted by the variable u. We abbreviate $x \stackrel{\text{def}}{=} (n, p, V)$ and rewrite the state equations (1.2) as $e(x, u) = 0$, where the nonlinear mapping $e : X \times \mathcal{C} \to (L^2(\Omega))^3$ is defined by

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

Next we state the differentiability properties of the mapping e.

Theorem 2.3. *The mapping e defined in (2.2) is infinitely often Fréchet differentiable with respect to the topology of $H^1(\Omega)$. Further, the derivatives vanish for order greater than or equal to 2. The actions of the first derivatives at a point $(x, u) \in X \times \mathcal{C}$ are given by*

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

for all $\tilde{x} = (\tilde{n}, \tilde{p}, \tilde{V}), z = (z^n, z^p, z^V) \in X_0$ and

$$\langle e_u(x,u)\tilde{u}, z\rangle = \left\langle \tilde{u}, z^V \right\rangle$$

for all $\tilde{u} \in \mathcal{C}$ and $z \in X_0$.

Here, $\langle \cdot, \cdot \rangle$ denotes the inner product in $L^2(\Omega)$. For a proof see [5].

3. Existence of Solutions

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 radially unbounded w.r.t. $\mathcal{C}$, bounded from below and weakly lower semi-continuous.

Remark 3.1. Clearly, the cost functional (1.3b) fits into this setting.

We now consider the minimization problem

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

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

Proposition 3.2. *Assume* **A.1**–**A.3**. *Then for each* $C \in H^1(\Omega)$ *there exists a solution* $(n,p,V) \in (H^2(\Omega))^3$ *of system* (1.2) *fulfilling* $(n,p) \geq (\underline{n},\underline{p}) > 0$.

For a proof see e.g. [9]. Note that uniqueness of solutions can only be expected for small potentials U, i.e. if the device is operated near thermal equilibrium.

Due to the $H^2(\Omega)$–regularity of (n,p,V) it holds $J \in H^1(\Omega;\mathbb{R}^d)$. Hence, the trace of the total current fulfils $trJ \in H^{1/2}(\partial\Omega)$. This implies that the functionals Q given by (1.3) are well defined.

The existence result reads

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

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

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

Since $\mathcal{C}$ is weakly closed w.r.t. the $H^1(\Omega)$-norm, $u^* \in \mathcal{C}$. By the continuous embedding $H^1(\Omega) \hookrightarrow L^p(\Omega)$ $(p \in [1,6))$ the sequence $\{u^n\}_{n\in\mathbb{N}}$ is also bounded in $L^p(\Omega)$. Now one can employ Stampaccia's method [13] to derive the following estimates [12]

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

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

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

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. Every solution (n^k, p^k, V^k) of (1.2) associated to u^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 [16] 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 (1.2), which satisfies

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

together with the boundary conditions in (1.1).

Lastly, we have to ensure $(n^*, p^*, V^*) \in X$, which is an easy consequence of assumption **A.3**. This completes the proof of the existence of a minimizer. □

Remark 3.4. The existence proof also works for less regular states in $H^1(\Omega)$. In this case one has to modify the cost functional and to investigate carefully the evaluation of the total current along the boundary. These techniques will be presented by the authors in [5].

4. The First–order Optimality System

Next we derive the first–order optimality system and state a result on the existence of Lagrange–multipliers. Their uniqueness is commented and estimates on the sensitivities are given.

The Lagrangian $\mathcal{L} : X \times \mathcal{C} \times X_0 \to \mathbb{R}$ associated to the minimization problem (3.1) is defined by

$$\mathcal{L}(x, u, \xi) \stackrel{\text{def}}{=} Q(x, u) + \langle e(x, u), \xi \rangle . \tag{4.1}$$

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

$$\nabla_{(x,u,\xi)} \mathcal{L}(x, u, \xi) = 0. \tag{4.2}$$

All together we find that the first–order necessary optimality condition (4.2) is equivalent to the following nonlinear system of coupled equations for the state x,

the control u and the adjoint variable ξ. It consists of the state equations

$$\Delta n + \operatorname{div}(n \nabla V) = 0, \tag{4.3a}$$

$$\Delta p - \operatorname{div}(p \nabla V) = 0, \tag{4.3b}$$

$$-\lambda^2 \Delta V = n - p - u \tag{4.3c}$$

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

$$\Delta \xi^n - \nabla V \nabla \xi^n = \xi^V, \tag{4.4a}$$

$$\Delta \xi^p + \nabla V \nabla \xi^p = -\xi^V, \tag{4.4b}$$

$$-\lambda^2 \Delta \xi^V + \operatorname{div}(n \nabla \xi^n) - \operatorname{div}(p \nabla \xi^p) = 0, \tag{4.4c}$$

supplemented with boundary data

$$\xi^n = \xi^p = \begin{cases} 0 & \text{on } \Gamma_D \setminus \Gamma_O, \\ (J_g - J) \cdot \nu & \text{on } \Gamma_O, \end{cases} \tag{4.5a}$$

$$\xi^V = 0 \text{ on } \Gamma_D, \tag{4.5b}$$

$$\nabla \xi^n \cdot \nu = \nabla \xi^p \cdot \nu = \nabla \xi^V \cdot \nu = 0 \quad \text{on } \Gamma_N. \tag{4.5c}$$

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

$$\xi^V = -\gamma (u - \bar{C}) \tag{4.6}$$

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

$$\begin{aligned} \gamma \Delta (u - \bar{C}) &= \xi^V && \text{in } \Omega, \\ u &= \bar{C} && \text{on } \Gamma_D, \\ \nabla u \cdot \nu &= \nabla \bar{C} \cdot \nu && \text{on } \Gamma_N. \end{aligned} \tag{4.7}$$

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 existence of the Lagrange–multipliers.

For the following investigations it is most convenient to write system (4.4) in symmetric form. This is accomplished by multiplying the first two equations of (4.4) with e^{-V} and e^V, respectively.

$$\operatorname{div}\left(e^{-V} \nabla \xi^n\right) = e^{-V} \xi^V, \tag{4.8a}$$

$$\operatorname{div}\left(e^{V} \nabla \xi^p\right) = -e^{V} \xi^V, \tag{4.8b}$$

$$-\lambda^2 \Delta \xi^V + (n + p) \xi^V = -J_n \nabla \xi^n + J_p \nabla \xi^p. \tag{4.8c}$$

Note, that $J_n, J_p \in H^1(\Omega; \mathbb{R}^d)$ due to Proposition 3.2. Now we are in the position to state the existence theorem for the Lagrange–multipliers.

Theorem 4.1. *Assume* **A.1**–**A.3**. *Then there exists a constant* $j = j(\Omega, \lambda, V) > 0$ *such that for*

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

there exists a solution $(\xi^n, \xi^p, \xi^V) \in (H^1(\Omega))^3$ *of system* (4.8) *supplemented with the boundary data* (4.5).

The proof is done by means of Schauder's fixed point theorem by decoupling the equations appropriately and deriving a priori estimates ensuring the compactness of the fixed point mapping. The existence of Lagrange–multipliers also holds for less regular states $(n, p, V) \in \left[H^1(\Omega) \cap L^\infty(\Omega)\right]^3$, see [5].

4.2. Sensitivity

Testing (4.4) with appropriate test functions and using the following estimate on the extension operator

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

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

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

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

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

Further, we get

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

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

Theorem 4.2. *Under the assumptions of Theorem 4.1 it holds*

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

In analogy one proves the following sensitivity bounds.

Corollary 4.3. *Under the conditions of Theorem 4.1 it holds*

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

Remark 4.4.

a) As expected the sensitivities are small in the case of small deviations from the desired state and for small current densities, i.e. if the device is operated near thermal equilibrium.

b) Under the conditions of Theorem 4.2 the Lagrange–multipliers prove to be unique. We cannot expect their uniqueness without less restrictions. Compare the uniqueness results for the DD [9].

5. Numerical Results

In this section we solve the 1–d first–order optimality system numerically on the domain $\Omega = (0,1)$ to gain an improved performance of a symmetric n–p–diode. The reference doping profile can be found in Figure 5.1 and the corresponding current–voltage characteristic is depicted in Figure 5.2. The Si–diode is 500nm long and operated at 300K. The maximum doping density is $10^{22}\mathrm{m}^{-3}$.

For the biasing voltage at the working point we choose $\bar{U} = 0.39\mathrm{V}$ and try to gain an amplification of the total current $\bar{J}$ by 50%, i.e. we set $J_g = \bar{J} \cdot 1.5$.

For the simulations we employ the cost functionals given by (1.3) and decouple the state system from the adjoint system, i.e. starting with some C_0 we compute the corresponding state via (4.3), solve the adjoint system (4.4) for the Lagrange–multipliers and update the doping profile via (4.6) and (4.7), respectively. Note that these updates do not require $\bar{C} \in H^1(\Omega)$. The iteration stops, if the difference of two consecutive doping profiles is below some specified threshold. The advantage of this approach is that during the iteration an existing fast solver for the state system can be used. To stabilize the numerics we use a continuation method in γ, starting with $\gamma = 16$ which is bisected in each step. Clearly, the convergence of the iteration depends crucially on the size γ as it slows down for decreasing γ.

The state system was discretized using an exponentially fitted mixed finite element method suitable for convection dominated equations [9], while the adjoint system was discretized in its symmetric form (4.8) using standard techniques. The nonlinear discrete state system was solved by a full Newton method, while for the linear adjoint system a GMRES–solver was employed.

The numerical results show that the system it not controllable into the desired state. Nevertheless, for $\gamma = 1/16$ the minimizer of (1.3b) yields a current gain of approximately 20%. The minimizing doping density can be found in Figure 5.1,

where also minimizing doping density for (1.3a) is shown, which also yields an amplification of 20%. 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.

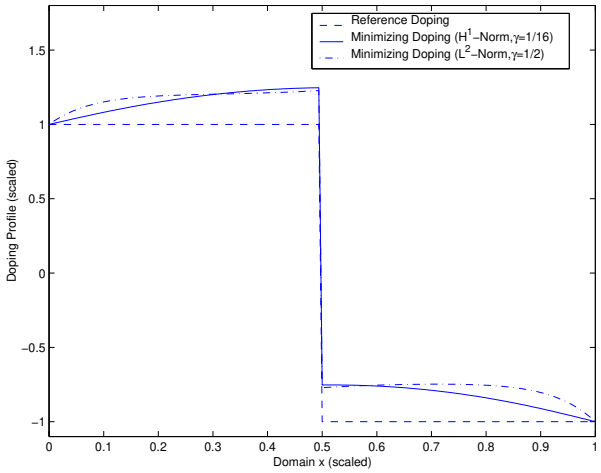

FIGURE 5.1. Doping Profiles

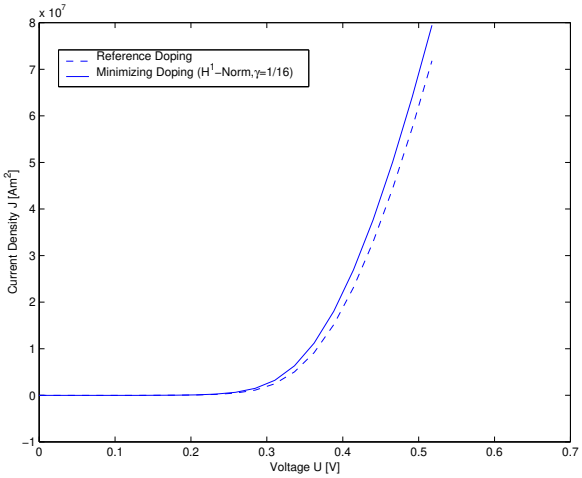

FIGURE 5.2. Current–Voltage Characteristics

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