INVERSE DOPING PROBLEMS FOR SEMICONDUCTOR DEVICES

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Abstract This paper is devoted to a class of inverse problems arising in the testing of semiconductor devices, namely the identification of doping profiles from indirect measurements of the current or the voltage on a contact. In mathematical terms, this can be modeled by an inverse source problem for the drift-diffusion equations, which are a coupled system of elliptic or parabolic partial differential equations.

We discuss these inverse problems in a stationary and a transient setting and compare these two cases with respect to their mathematical properties. In particular, we discuss the identifiability of doping profiles in the model problem of the unipolar drift-diffusion system. Finally, we investigate the important special case of a piecewise constant doping profile, where the aim is to identify the p-n junctions, i.e., the curves

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between regions where the doping profile takes positive and negative values.

1. Introduction

Due to their tremendous impact on modern electronics, the mathematical modeling of semiconductor devices has developed well in the last fifty years, since Van Roosbroeck (cf.[20]) first formulated the fundamental semiconductor device equations (see Section 2 for an overview). For a detailed expositions concerning the modeling, analysis and simulation of semiconductor devices we refer to the monographs [12, 14, 17] and for an overview of recent advances and hierarchies of models we refer to [9].

Although of increasing technological importance, optimal design and identification problems related to semiconductor devices seem to be poorly understood so far. Only recently, there was some effort in optimizing the performance of devices (cf. e.g. [8, 18, 19]) and in identifying relevant material properties (cf. [4, 10]). The position-dependent function $C = C(x)$ to be identified or optimized is the *doping profile*, which is the density difference of ionized donors and acceptors. In some cases (e.g. for the p-n diode discussed below), it may be assumed that the doping profile is piecewise constant over the device; the interesting quantities are then the curves or surfaces between the subdomains where the doping is constant. These curves are usually called *pn-junctions*, when they separate subdomains where the doping profile takes positive and negative values, respectively. In the most important doping technique of silicon devices, *ion implantation*, it is only possible to obtain a rough estimate of the doping profile by process modeling (cf. e.g. [17] for further details). In order to determine the real doping profile, reconstruction methods from indirect data have to be used. We shall use the notion *inverse doping problem* introduced in [4] for the identification of the doping profile in general.

2. Stationary and Transient Semiconductor Equations

In the following we review the drift-diffusion (DD) model for semiconductor devices, both in the stationary and transient case. The drift-diffusion model is a coupled system of nonlinear partial differential equations for the electrostatic potential V, the electron density n (≥ 0) and the hole density p (≥ 0) , which is solved in a domain $\Omega \subset \mathbf{R}^d$ ($d = 1, 2, 3$) representing the semiconductor device and in a time interval $[0, T]$ in the transient case.

2.1 The Transient DD-Model

The drift-diffusion equations in the *transient case* are given by (cf. [14])

$$\begin{aligned} 0 &= \operatorname{div}(\epsilon_s \nabla V) - q(n - p - C) && \text{in } \Omega \times (0,T) \\ \frac{\partial n}{\partial t} &= \operatorname{div}(D_n \nabla n - \mu_n n \nabla V) && \text{in } \Omega \times (0,T) \\ \frac{\partial p}{\partial t} &= \operatorname{div}(D_p \nabla p + \mu_p p \nabla V) && \text{in } \Omega \times (0,T) \end{aligned}$$

where ϵ_s denotes the semiconductor permittivity, q the elementary charge, μ_n and μ_p are the electron and hole mobility, D_n and D_p are the electron and hole diffusion coefficients. R denotes the *recombination-generation rate*, which generally depends on n and p. We assume that R is of the standard form

$$R = F(n,p,x)(np - n_i^2), \tag{2.1}$$

where F is a nonnegative smooth function, which holds e.g. for the frequently used *Shockley-Read-Hall* rate

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

The parameters ϵ_S and q are positive (dimensional) constants and $\mu_{n/p}$ and $D_{n/p}$ are modeled by positive functions.

This system is supplemented by homogeneous Neumann boundary conditions on a part $\partial\Omega_N$ (open in $\partial\Omega$) of the boundary. On the remaining part $\partial\Omega_D$ (with positive $(d-1)$-dimensional Lebesgue-measure), the following Dirichlet conditions are imposed:

$$\begin{aligned} V(x,t) &= V_D(x,t) = U(x,t) + V_{bi}(x) = U(x) + U_T \ln\left(\frac{n_D(x)}{n_i}\right) \\ n(x,t) &= n_D(x) = \frac{1}{2}\left(C(x) + \sqrt{C(x)^2 + 4n_i^2}\right) \\ p(x,t) &= p_D(x) = \frac{1}{2}\left(-C(x) + \sqrt{C(x)^2 + 4n_i^2}\right) \end{aligned}$$

on $\partial\Omega_D \times (0,T)$, where n_i is the intrinsic carrier density, U_T (≥ 0) the thermal voltage and U is the applied potential. Moreover, the initial conditions

$$n(x,0) = n_0(x) \geq 0, \qquad p(x,0) = p_0(x) \geq 0 \qquad \text{in } \Omega \tag{2.2}$$

have to be supplied.

2.2 The Stationary DD-Model

The *stationary drift-diffusion model* is obtained from the transient case by setting

$$\frac{\partial n}{\partial t} = \frac{\partial p}{\partial t} = 0$$

and omitting the initial conditions. Using the Einstein relations, which are standard assumptions about the mobilities and diffusion coefficients of the form

$$D_n = \mu_n U_T, \qquad D_p = \mu_p U_T, \tag{2.3}$$

we may transform the system using the so-called *Slotboom variables* u and v defined by

$$n = C_0 \delta^2 e^{V/U_T} u, \qquad p = C_0 \delta^2 e^{-V/U_T} v, \tag{2.4}$$

where $\delta^2 = \frac{n_i}{C_0}$ with a typical value C_0 for the doping profile, which is also scaled by C_0. Rescaling all quantities to non-dimensional analogues (cf. [14] for further details) we obtain the system

$$\lambda^2 \Delta V = \delta^2 (e^V u - e^{-V} v) - C \qquad \text{in } \Omega \tag{2.5}$$

$$\mathrm{div} J_n = \delta^4 Q(u, v, V, x)(uv - 1) \qquad \text{in } \Omega \tag{2.6}$$

$$\mathrm{div} J_p = -\delta^4 Q(u, v, V, x)(uv - 1) \qquad \text{in } \Omega \tag{2.7}$$

$$J_n = \mu_n \delta^2 e^V \nabla u \qquad \text{in } \Omega \tag{2.8}$$

$$J_p = -\mu_p \delta^2 e^{-V} \nabla v \qquad \text{in } \Omega \tag{2.9}$$

where λ^2 is a positive constant and Q is defined via the relation $F(n, p, x) = Q(u, v, V, x)$. The new variables J_n and J_p are the scaled electron and hole current densities; the above mixed formulation seems to be natural for cases where one is interested in these quantities, since it contains them explicitly. Unless specified otherwise, we shall set δ to 1 in the sequel.

The Dirichlet boundary conditions can be written as

$$V = U + V_{bi} = U + \ln\left(\frac{1}{2\delta^2}(C + \sqrt{C^2 + 4\delta^2})\right) \qquad \text{on } \partial\Omega_D \tag{2.10}$$

$$u = e^{-U} \qquad \text{on } \partial\Omega_D \tag{2.11}$$

$$v = e^{U} \qquad \text{on } \partial\Omega_D. \tag{2.12}$$

On the remaining part $\partial\Omega_N = \partial\Omega - \partial\Omega_D$, the homogeneous Neumann conditions can be formulated in terms of J_n and J_p, i.e.,

$$\frac{\partial V}{\partial \nu} = J_n.\nu = J_p.\nu = 0 \qquad \text{on } \partial\Omega_N \tag{2.13}$$

We note that the mobilities μ_n and μ_p generally depend on the electric field strength, i.e, on $|\nabla V|$ in a realistic model. Such a dependence could be incorporated in our subsequent analysis. However, since the technical details one has to deal with in this general case do not contribute to the understanding of inverse doping problems and their solution, we will assume that μ_n and μ_p are positive constants in the following.Also, for the sake of simplicity we shall henceforth use $F \equiv 0$, i.e., no recombination-generation.

3. Available Data

In a typical experiment, measurements are always taken on the boundary of the device, more precisely on a contact $\Gamma_1 \subset \partial\Omega_D$. In the following we will therefore use the notation

$$\Sigma_1 := \begin{cases} \Gamma_1 & \text{in the stationary case} \\ \Gamma_1 \times (0,T) & \text{in the transient case} \end{cases}$$

For general semiconductor devices, two different types of data can be measured, namely:

- *Voltage-Current Data* (denoted by I_U) are given by measurements of the normal component of the current density $J := (J_n + J_p)$ on Σ_1, i.e.,
$$I_U := (J_n + J_p)|_{\Sigma_1} \tag{3.1}$$
for all applied voltages $U \in \mathcal{U}$, where $\mathcal{U}$ is an appropriate class of functions on $\partial\Omega_D$ in the stationary and on $\partial\Omega_D \times (0,T)$ in the transient case.

- *Capacitance Data* (denoted by Q_Φ) around the voltage U are measurements of the variation of the electric flux in normal outward direction ($\frac{\partial V}{\partial \nu}$ on Σ_1) with respect to the voltage Φ, i.e.,
$$Q_\Phi := \lim_{s \to 0} s^{-1} \left(\frac{\partial V^{s\Phi+U}}{\partial \nu} - \frac{\partial V^U}{\partial \nu}\right)|_{\Sigma_1} \tag{3.2}$$
for all voltages $\Phi \in \mathcal{U}$, where V^Φ denotes the solution of the Poisson equation with $U = \Phi$ and $\mathcal{U}$ is as above. For simplicity we assume that $U \equiv 0$ in the following, i.e., we are interested in capacitance data around equilibrium.

Using well-posedness and regularity results for the solutions of the stationary and transient DD-model, one can show that for given doping profile C, both current and capacitance are well-defined outputs for appropriate choices of the applied voltage U. In the stationary case,

"appropriate" means smoothness (e.g. $U \in H^{\frac{3}{2}}(\partial\Omega_D)$) and we assume (for linearized stability of the DD system) smallness of U (cf. [4]), since hysteresis might occur for large voltages (cf. [14] for examples of non-unique solutions). In the transient case, a smallness assumption on U is not necessary, which is due to the fact the transient DD-model and its linearization are invertible for arbitrarily large applied voltage (cf. [13]).

The computation of the current consists of solving the DD-equations and evaluation of a trace type operator, which can be realized numerically by standard tools. The computation of the capacitance is more involved, since it requires the solution of the DD-model and its linearization. At equilibrium, i.e., $U \equiv 0$, the electron and hole density are given by $n^0 = e^V$, $p^0 = e^{-V}$ with the corresponding Slotboom variables $u^0 = v^0 = 1$. The potential V^0 solves the Poisson equation

$$\lambda^2 \Delta V^0 = \delta^2 (e^{V^0} - e^{-V^0}) - C \tag{3.3}$$

subject to the boundary conditions given above with $U \equiv 0$ (note that this holds both in the transient as in the stationary case). The capacitance can now be computed by a linearization of the drift-diffusion model with respect to the applied voltage, i.e., it is given by

$$Q_\Phi = \frac{\partial \hat{V}}{\partial \nu}|_{\Sigma_1}, \tag{3.4}$$

where in the transient case $(\hat{V}, \hat{n}, \hat{p})$ solves the linearized equations (given here after scaling)

$$\begin{aligned} 0 &= \lambda^2 \Delta \hat{V} - q(\hat{n} - \hat{p}) && (3.5)\\ \frac{\partial \hat{n}}{\partial t} &= \operatorname{div}\left(\mu_n(\nabla \hat{n} - \hat{n}\nabla V^0 - e^{V^0}\nabla \hat{V})\right) && (3.6)\\ \frac{\partial \hat{p}}{\partial t} &= \operatorname{div}\left(\mu_p(\nabla \hat{p} + \hat{p}\nabla V^0 + e^{-V^0}\nabla \hat{V})\right) && (3.7) \end{aligned}$$

in $\Omega \times (0,T)$, subject to homogenous initial conditions, homogeneous Neumann boundary conditions on $\partial\Omega_N$, and the Dirichlet boundary conditions

$$\hat{V} = \Phi, \qquad \hat{n} = \hat{p} = 0, \tag{3.8}$$

on $\partial\Omega_D$. Again, in the stationary case, the boundary conditions remain the same and the corresponding differential equations are obtained from the transient ones by setting $\frac{\partial n}{\partial t} = \frac{\partial p}{\partial t} = 0$.

The above formulation of the data set is a rather general one, in specific applications one usually has to deal with some of the following choices for the function class $\mathcal{U}$:

- *Full data:* here $\mathcal{U}$ denotes a linear function space of admissible applied voltages, e.g., $\mathcal{U} = H^{\frac{3}{2}}(\partial\Omega_D)$ in the stationary case. This case is a mathematical idealization of a situation with a very large number of measurements. For full data, the identification problem has many analogies to the important field of impedance tomography (cf. [6, 11]).

- *Parameterized data set:* in this case $\mathcal{U}$ is a special function class that can be parametrized using parameters $s_j \in (-S, S)$, $j = 1, \ldots, m$, with some $S \in \mathbf{R}_+$. Of particular importance is the case where U is piecewise constant on some disjoint sets $\Gamma_j \subset \partial\Omega_D$, which represent different ohmic contacts. The parameter s_j denotes the voltage applied on the j-th contact.

- *Finite number of measurements:* here $\mathcal{U}$ consists of a finite number N of functions U_j, $j = 1, \ldots, N$ on $\partial\Omega_D$ (and possible in the time interval $(0, T)$).

A frequently appearing special case is the one with a *single measurement*, i.e., the preceding case with $N = 1$.

An immediate observation for all cases of data is that the amount of available data is much larger in the transient case than in the stationary case. Together with the simpler mathematical analysis, this clearly makes the transient case favourable. However, under practical conditions it is not always possible to obtain meaningful transient measurements, since the time variation only occurs in a small initial time layer. Therefore one has to use either the stationary or the transient model dependent on the specific application.

For the sake of simplicity, we restrict our attention here to the case of a finite number of applied potentials, with measured current or capacitance (or both of them). Under the standard conditions on the applied potential U and the domain Ω one can show that current and capacitance are well-defined on a contact $\Gamma \subset \partial\Omega_D$.

4. Identification of Doping Profiles

In the following we discuss some mathematical problems concerned with the identification of spatially varying doping profiles. The domain of admissible doping profiles C is given by

$$\mathcal{D} := \left\{ C \in L^2(\Omega) \mid \underline{C} \leq C \leq \overline{C} \text{ a.e. in } \Omega \right\} \tag{4.1}$$

for some constants $\underline{C}, \overline{C} \in \mathbf{R}$.

All the above cases can be transformed to the standard form for an inverse problem, namely the nonlinear operator equation

$$F(C) = Y^\delta, \tag{4.2}$$

where F stands for the parameter-to-output map

$$\begin{array}{rccc} F: & \mathcal{D} & \to & L^2(\Sigma_1)^N \\ & C & \mapsto & (I_{U_j})_{j=1,\dots,N} \end{array} \tag{4.3}$$

for current measurements, and

$$\begin{array}{rccc} F: & \mathcal{D} & \to & L^2(\Sigma_1)^N \\ & C & \mapsto & (Q_{\Phi_j})_{j=1,\dots,N} \end{array} \tag{4.4}$$

for capacitance measurements. The right-hand side Y^δ represents noisy current or capacitance data, and we assume that the data error is bounded by δ, i.e.,

$$\|Y^\delta - Y\|_{L^2(\Sigma_1)^N} \leq \delta \tag{4.5}$$

for the exact data Y.

We are now able to state the following result on the parameter-to-output operator, for a proof in the stationary case we refer to [4] and in the transient case to [5]:

Theorem 1. *The parameter-to-output map F is well-defined by* (4.3) *respectively* (4.4) *and Frèchet-differentiable on $\mathcal{D}$.*

The well-definedness and differentiability of the operator F enables the application of *iterative regularization methods* for the solution of the identification problem, such as the Landweber iteration

$$C_{k+1} = C_k - \omega F'(C_k)^*(F(C_k) - Y^\delta), \tag{4.6}$$

with appropriate damping parameter $\omega \in \mathbf{R}_+$, or Newton-type methods, e.g., the *Levenberg-Marquardt method*

$$C_{k+1} = C_k - (F'(C_k)^* F'(C_k) + \alpha_k)^{-1} F'(C_k)^*(F(C_k) - Y^\delta), \tag{4.7}$$

where $(\alpha_k)_{k\in\mathbf{N}}$ is a sequence of positive real numbers. We mention that the evaluation of the directional derivative $F'(C)\hat{C}$ and of the adjoint $F'(C_k)^*\hat{Y}$ require the solution of a linear system similar to the original drift-diffusion equations, which causes a high effort in the numerical solution of the identification problem. We refer to Burger et al [4] for the iterative regularization of the inverse doping problem (4.2) and to [7] for a unified overview of iterative regularization methods.

In the remaining part of this section we focus on a fundamental question in the identification of parameters from indirect measurements:

> *Do the data determine the doping profile uniquely, respectively which set of data is suffficient for uniquely determining the doping profile ?*

The mathematical equivalent of this question is called *identifiabilty* (cf. [1]) and means to investigate the injectivity of the parameter-to-output map F, which is a difficult task for inverse doping problems as we shall see below. Therefore we restrict our attention to the special case of unipolarity, where a rigorous analysis can be carried out. The unipolar drift diffusion equations arise from the original DD-system by setting $p \equiv 0$ in Ω. We start this discussion in the stationary case, where a large amount of data is necessary in order to ensure identifiability. In the transient case we shall show that even a single measurement of capacitance and current can determine the doping profile uniquely.

4.1 Stationary Inverse Doping

We start our investigation of stationary inverse doping problems with the spatially one-dimensional case, i.e., $\Omega = (0, L)$. We assume without restriction of generality that the voltage is applied at $x = 0$ and the measurements of current and capacitance are taken at $x = L$. Even if we are able to measure both, a single measurement consists only of two real numbers, which can clearly not suffice to identify the doping profile as a function of the spatial variable x. Full data in this case means to measure current and capacitance as a function of the applied voltage $U \in (-r, r)$ with appropriate $r \in \mathbf{R}^+$, respectively the variation of the voltage $\Phi \in \mathbf{R}$.

At a first glance it seems possible to identify the doping profile from full data, since the data are now a function of one variable and, roughly speaking, of the same dimensionality as the parameter to be identified. However, the information content in the data is much smaller, which can be seen very easily for capacitance measurements. Here the map $\Phi \mapsto Q_\Phi$ is affinely linear because it only consists in solving the linearized drift-diffusion equations and evaluating a linear trace operator. Since an affinely linear function of one variable can be characterized by two real numbers, the information content is the same as if one would measure the capacitance at only two different values $\Phi \in \mathbf{R}$ and hence cannot suffice to determine the doping profile uniquely. For current measurements a similar argument holds, since it can be shown that the current behaves around $U = 0$ like an exponential function of U (cf. [14]).

In two spatial dimensions, the situation is different. Here a single measurement of current or capacitance is given by a function of one spatial variable over the contact Γ_1. Of course, a single measurement is again not sufficient for identifiability of the doping profile, which is a function over the two-dimensional domain Ω, but by exploiting similarities to electrical impedance tomography (cf. [6, 15]) we may argue that full data are sufficient, which we shall rigourously prove in a special case below.

As a starting point for the analysis we investigate the unipolar drift-diffusion system around equilibrium, i.e., its linearization with respect to the voltage at $U = 0$. Since $p = 0$, this implies $u \equiv 1$, $v \equiv 0$ and the linearization $\hat{v}$ solves the elliptic differential equation

$$\text{div } (e^{V^0} \nabla \hat{u}) = 0 \qquad \text{in } \Omega \tag{4.8}$$

subject to the boundary conditions

$$\hat{u} = \Phi \quad \text{on } \partial\Omega_D, \qquad \frac{\partial \hat{u}}{\partial \nu} = 0 \quad \text{on } \partial\Omega_N. \tag{4.9}$$

The function V^0 is the solution of the Poisson equation at equilibrium, i.e.,

$$\Delta V^0 = e^{V^0} - C \qquad \text{in } \Omega \tag{4.10}$$

with the boundary conditions

$$V^0 = V_{bi} \quad \text{on } \partial\Omega_D, \qquad \frac{\partial V^0}{\partial \nu} = 0 \quad \text{on } \partial\Omega_N. \tag{4.11}$$

The output current in this case can be identified after rescaling with the Neumann boundary data of $\hat{u}$, i.e.,

$$I_\Phi := \frac{\partial \hat{u}}{\partial \nu}|_{\Gamma_1}. \tag{4.12}$$

From the standard theory of elliptic differential equations one may conclude that for a domain Ω with regular boundary, there is a one-to-one relation between functions $V^0 \in H^2(\Omega)$ satisfying the Poisson equation and potentials $C \in L^2(\Omega)$. This motivates the investigation of the identifiability of $V^0 \in H^2(\Omega)$ in (4.8) directly, since for known potential V^0 the doping profile is determined uniquely by (4.10). The identifiability of the potential V^0 in (4.8), respectively the identifiability of the conductivity $a = e^{V^0}$ has been investigated by Nachman [15] with a positive answer only in the case of full data, which leads to the following result:

Theorem 2. *Let $\Omega \subset \mathbf{R}^2$ be a bounded Lipschitz domain, $\Gamma_1 = \partial\Omega_D = \partial\Omega$, and let for two doping profiles C_1 and C_2 in $\mathcal{D}$ denote their output currents by I^1_Φ and I^2_Φ obtained from linearization around equilibrium. Then the equality*

$$I^1_\Phi = I^2_\Phi, \qquad \forall\ \Phi \in H^{\frac{3}{2}}(\partial\Omega)$$

implies $C_1 = C_2$.

4.2 Transient Inverse Doping

We have seen in the previous section that the identification in the stationary case makes no sense for spatial dimension one. In the transient case, the situation is different, because a second dimension is added via the time variable. If we measure current and capacitance over a time interval $(0, T)$, the dimensionality of the data is the same as of the doping profile, namely that of functions over an interval. Since there are many examples of parabolic identification problems, where a measurement on the boundary over some time interval determines a spatially distributed parameter uniquely (cf. [11] and the references therein), it seems reasonable that one can identify the doping profile from a single transient measurement.

For a rigorous justification of the identifiability, we consider the model problem of the unipolar transient drift-diffusion equations in $\Omega = (0, L)$. After appropriate scaling (setting $\mu_n = 1$), they are given by

$$0 = \lambda^2 \frac{\partial^2 V}{\partial x^2} - n + C \qquad \text{in } (0, L) \times [0, T] \tag{4.13}$$

$$\frac{\partial n}{\partial t} = \frac{\partial}{\partial x}\left(\frac{\partial n}{\partial x} - n\frac{\partial V}{\partial x}\right) \qquad \text{in } (0, L) \times [0, T], \tag{4.14}$$

subject to appropriate Dirichlet boundary conditions for n and V at $x = 0$ and $x = L$, and the initial condition

$$n(x, 0) = n_0(x) \geq 0. \tag{4.15}$$

We assume that the potential $U = U(t)$ is applied at $x = 0$, i.e.,

$$V(0, t) = U(t) + V_D(0), \qquad V(1, t) = V_D(1). \tag{4.16}$$

Introducing the antiderivatives N and D determined by

$$\frac{\partial N}{\partial x} = n, \quad N(L, .) = 0, \qquad D_x = C, \quad D(L) = 0 \tag{4.17}$$

for all $t \in [0, T]$, we can integrate (4.13) to

$$\lambda^2 \frac{\partial V}{\partial x} = N - D + \alpha, \tag{4.18}$$

where $\alpha = \alpha(t)$. Thus, the system (4.13), (4.14) can be reduced to the single equation

$$\frac{\partial N}{\partial t} = J + \beta = \frac{\partial^2 N}{\partial x^2} - \lambda^{-2}\frac{\partial N}{\partial x}(N - D) - \frac{\partial N}{\partial x}\alpha + \beta, \tag{4.19}$$

where α and β are functions of time only, which have to be determined from boundary data. Using the boundary values of N and D at $x = L$, we deduce $\alpha(t) = \lambda^2 \frac{\partial V}{\partial x}(L,t)$. Moreover, the current J at $x = 1$ determines β, since

$$0 = \frac{\partial N}{\partial t}(L,t) = J(L,t) + \beta(t).$$

I.e., under the knowledge of $\frac{\partial V}{\partial x}(L,t)$ and $J(L,t)$, the reconstruction of the doping profile C in the unipolar case reduces to the identification of the spatially varying source D in the parabolic equation (4.19) from the overposed boundary data for $\frac{\partial N}{\partial x}$ at $x = 0, L$ and N at $x = L$. Using results for parabolic inverse problems based on Carleman estimates, we may derive the following result (cf. [5]):

Theorem 3. *Let $C \in C^{1,1}(\Omega)$, $\frac{dU}{dt}(s) \neq 0$ for some $s \in (0,T)$ and assume that $\frac{\partial V}{\partial x}(L,t)$ and*

$$J(L,t) = \frac{\partial n}{\partial x}(L,T) - n(L,T)\frac{\partial V}{\partial x}(L,t)$$

are known in a finite time interval $(0,T)$ and $\frac{\partial V}{\partial x}(L,.) \in C^{1,1}(0,T)$. Then the solution (n,V,C) of the unipolar identification problem is uniquely determined.

In two spatial dimensions, the situation is similar, since we want to identify a function on $\Omega \subset \mathbf{R}^2$ from a measurement on $\Gamma_1 \times (0,T) \subset \mathbf{R}^2$. However, there are no rigorous results on the multi-dimensional inverse doping profile yet. Nonetheless, there is hope to derive uniqueness results at least in special cases, which raises important problems for future research.

5. Identification of P-N Junctions

Finally, we consider the case, where the doping profile is a piecewise constant function of position. We assume that there exists a decomposition $\overline{\Omega} = \overline{\Omega_P} \cup \overline{\Omega_N}$ and values $C_+ \in \mathbf{R}_+$, $C_- \in \mathbf{R}_-$, such that

$$C \equiv C_+ \quad \text{in } \Omega_P, \qquad C \equiv C_- \quad \text{in } \Omega_N. \tag{5.1}$$

Both Ω_N and Ω_P shall only consist of a finite number of connected components. Under this a-priori information it seems now reasonable to consider also the stationary case with a finite number of measurements.

In the case of one spatial dimension, we only have to identify a finite number of points $x_j \in (0, L)$ that mark the location of the p-n junction. This seems possible from voltage and capacitance measurements if the number of junctions is not too large. E.g., for a p-n diode, which is a device where the Ω_N and the Ω_P region consist of only one connected component each, one only seeks the location of one junction, i.e., a single real value in the interval $(0, L)$, which seems reasonable to be determined from a single measurement of the current or the capacitance. We will rigorously prove the identifiability of the p-n junction for a unipolar p-n diode in the following section.

In two spatial dimensions one may argue again that a single measurement on a contact is sufficient for identifiability of the p-n diode, which is now a curve, i.e., a function of one variable (the arclength parameter). We will investigate the identification in a special case, namely a p-n diode with zero space charge and low injection below; for this problem the identification of the p-n junction reduces to an inverse boundary problem for the Laplace equation and one can rigorously prove identifiability. However, it is well-known that such inverse problems are *severely ill-posed*, i.e., measurement errors are amplified dramatically. Typically, stability estimates for the unknown boundaries in such problems are only of logarithmic type with respect to the data error δ (cf. e.g. [2]).

5.1 A Unipolar P-N Diode in $\mathbf{R^1}$

In the following we investigate a simple identification problem for a one-dimensional p-n diode ($\Omega = (0, L)$) in the unipolar case. The linearization around equilibrium ($U = 0$, as a system for the equilibrium potential V^0 and the perturbation $\hat{u}$ of u) in Slotboom variables reads

$$\lambda^2 \frac{\partial^2 V^0}{\partial x^2} = e^{V^0} - C \qquad \frac{\partial}{\partial x}\left(e^{V^0}\frac{\partial \hat{u}}{\partial x}\right) = 0, \tag{5.2}$$

in Ω, with Dirichlet boundary conditions for V^0 and $\hat{u}$ at $x = 0$ and $x = L$. If we are given the linearized current $J = e^{V^0}\frac{\partial \hat{u}}{\partial x}$ at $x = 0$, we may conclude that

$$\frac{\partial \hat{u}}{\partial x} = e^{-V^0} J \qquad \text{in } \Omega.$$

With the given Dirichlet boundary values $u(0)$ and $u(L)$ we can reduce the identification of the p-n junction to the identification of the p-n junc-

tion in the equilibrium Poisson equation with the additional condition

$$\hat{u}(L) - \hat{u}(0) = J \int_0^L e^{-V^0(x)}\, dx. \tag{5.3}$$

For the solution of this identification problem we can now prove an identifiability result:

Theorem 4. *Let $C_+ > 0$ and $C_- \leq 0$ be given and let C_1 and C_2 be two doping profiles satisfying*

$$C_i = \begin{cases} C_+ & \text{for } x < p_i \\ C_- & \text{for } x > p_i \end{cases} \tag{5.4}$$

for $p_i \in (0, L)$, $i = 1, 2$. Denote by $(V_i^0, \hat{u}_i)$ the corresponding solutions of (5.2) with doping profile C_i. If the output currents $J_i = e^{V_i^0(0)} \frac{\partial \hat{u}_i}{\partial x}(0)$ are equal, then $C_1 = C_2$ in Ω.

Proof. We have seen above that we may equivalently consider the identification of C in the Poisson equation with the additional integral condition (5.3). Let in the following w.r.o.g. $p_1 \leq p_2$ and set $w := V_1^0 - V_2^0$, then by the mean value theorem we may deduce the existence of bounded functions a and b such that w satisfies

$$\begin{aligned} -\lambda^2 \frac{\partial^2 w}{\partial x^2} + e^a w = C_1 - C_2 = (C_+ - C_-)1|_{(p_1,p_2)} &\geq 0, \\ \int_0^L e^{b(x)} w(x)\, dx &= 0. \end{aligned}$$

Moreover, w satisfies homogeneous Dirichlet boundary conditions at $x = 0$ and $x = L$. Using the maximum principle for elliptic differential equations we deduce that $w \geq 0$ in Ω and hence, the above integral identity can only hold for $w \equiv 0$, which implies also $\chi_(p_1, p_2) \equiv 0$. Thus, we have $p_1 = p_2$ and consequently $C_1 \equiv C_2$. □

5.2 A P-N Diode with Zero Space Charge and Low Injection

The case of zero space charge and low injection means to let first tend $\lambda \to 0$ and then $\delta \to 0$ in the stationary drift-diffusion equations. It has been shown by Schmeiser [16] that the arising limiting problem for u and v can be solved explicitely and identifiability can be shown in two space dimensions (cf . [4]) using tools from the theory of harmonic functions.

In [4], numerical test have been performed for the identification of the p-n junction in this special case. The data where generated by numerically solving the stationary drift-diffusion equations with appropriate

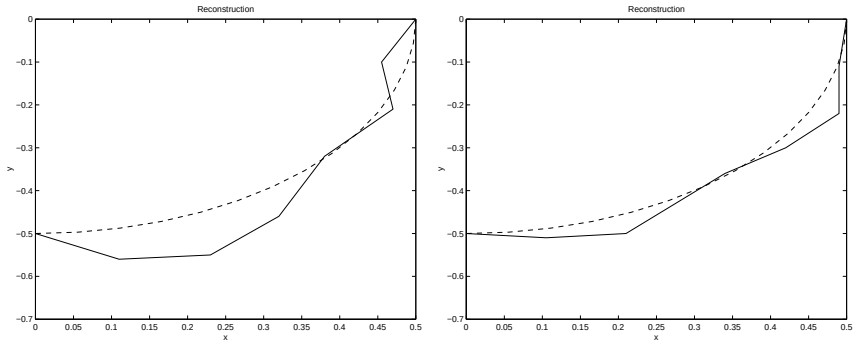

Figure 1. Reconstruction using data from the full drift-diffusion model for $C_0 = 10^{20} m^{-3}$ (left) and $C_0 = 10^{21} m^{-3}$ (right) compared to the exact junction (dotted).

parameter choices (cf. [3] for details on the numerical scheme employed) and subsequently evaluating the current over the contact. The inverse problem was solved using an iterative regularization method for the simplified model. The results for two different values of $C_0 = C_+ = |C_-|$, which can be interpreted as two different noise levels in the current measurements, are shown in Figure 1. One observes that the quality of the reconstruction improves with increasing C_0, which is related to the better approximation of the reduced equation to the original drift-diffusion model. The results obtained indicate that the doping profile is not only identifiable, but can be reconstructed with reasonable precision also from noisy data obtained in practice.

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