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OPTIMAL DOPING PROFILES IN SEMICONDUCTOR DESIGN

C.R.Drago

Dipartimento di Matematica e Informatica,
Università di Catania Viale A. Doria, 6, I-95125 Catania, Italy
E-mail: drago@dmi.unict.it

R.Pinnau

Technische Universität Kaiserslautern
D-67663 Kaiserslautern, Germany
E-mail: pinnau@mathematik.uni-kl.de

Abstract.

This paper deals with the optimal design of doping profiles in a semiconductor device, based on the energy transport model. The objective is to slightly change the doping profile in order to get a gain in the outflow current. After introducing the optimal control approach in the framework of the mathematical theory for the control of systems governed by partial differential equations, some preliminary numerical results are shown for the $n^+ - n - n^+$ ballistic diode.

Keywords: Optimal semiconductor design; energy transport; doping profile; adjoints; numerics; descent algorithm

1. Introduction

The design of microelectronic devices becomes ever more demanding due to various factors such as the ever growing requirements regarding functionality and reliability. As a consequence, the design of a microelectronic devices requires advanced models and the improvement of their performances needs robust optimization algorithms.
In particular a typical goal, is to improve the device characteristics, in particular current flows over some contact by designing a suitable device doping profile (representing the density of ion impurities within the material). An alternative approach to standard black-box optimization algorithms that usually require a large number of function evaluations, is the adjoint method, recently proposed by Pinnau et al,[5] in the field of the optimal semiconductor design. Using techniques of control theory of systems governed by partial differential equations, the gradient can be determined indirectly by solving an adjoint system which has coefficients determined by the solution of the state equations. The computation of the gradient, by using the adjoint variables, needs a single run of the forward and adjoint model, independently from the dimension of the parameters space, reducing drastically the computational costs.
Once the gradient has been calculated, a descend method can be used to determine a doping profile change which will make an improvement in the design. The gradient can be recalculated and the whole process can be repeated until the design converges to an optimum solution, usually within 10-50 cycles.
The simulations of charge transport in semiconductor devices, on the other hand, have been addressed, during the last years, by using different types of models. Maybe, the most popular and widely used is the drift diffusion model, since it allows a good description of the physics

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combined with low computational costs. It is based on the assumption of isothermal motion. There exists a large amount of literature on this model, which covers questions of the mathematical analysis as well as of the numerical discretization and simulation.[9,10] However, in today semiconductor technology, with the semiconductor devices miniaturization, one comes closer to the limit of validity of the drift diffusion model. The presence of very high and rapidly varying electric fields, doesn't allow an accurate physical description of the semiconductor without considering the energy as dynamical variable. That's why more physically accurate models, like the energy transport one were introduced. For an overview see.[7]
In,[5] Pinnau et al. have presented and analyzed an optimal control approach based on the adjoint method for the standard drift diffusion model. Other analytical and numerical results for such an approach can be found also in,[1].[6] The same approach was extended to the energy transport model by C. Drago et al in,[2] where some analytical results on the existence of a minimizer and the adjoint states were presented.
In this paper we will present some preliminary numerical results based on the Chen energy transport model. The paper is organized as follows. In section 2 is shown the energy transport model for semiconductor devices. Section 3 contains the formulation of the optimization problem. In sections 4 the first order optimality system is given and finally in section 5 the numerical results are shown.

2. The Energy Transport Model

The dimensionless stationary energy-transport model for charge carriers in a semiconductor enclosed in a bounded domain $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$, is given, in the unipolar case, by the following equations for the electron density n and the temperature T, coupled to the Poisson equation for the electric potential V:[7]

$$\mathrm{div} J_1 = 0 \tag{1a}$$

$$\mathrm{div} J_2 = J_1 \cdot \nabla V + W \tag{1b}$$

$$\lambda^2 \triangle V = n - C(x)$$

where J_1 is the carrier flux density, J_2 the energy flux density, W the energy production, $C(x)$ the doping concentration and $\lambda^2 = \frac{\varepsilon_s U_T}{q C_m L^2}$ the Debye length.
Assuming the parabolic band approximation one has for the electron density $n(\mu, T) = T^{3/2} e^{\mu/T}$, where μ is the chemical potential and the constitutive equations can be written in term of n, T and V as:

$$J_1 = -\left(\nabla n - \frac{n}{T}\nabla V\right) \tag{1c}$$

$$J_2 = -\frac{3}{2}\left(\nabla(nT) - n\nabla V\right) \tag{1d}$$

Moreover the energy relaxation term is simply given by $W = -\frac{3}{2}\frac{n(T-T_L)}{\tau_w}$ where $\tau_w = \tau_0 \mu_0 U_t / L^2$ is the scaled energy relaxation time.
The energy transport model with the above relations is called the *Chen model*. The diffusion matrix in term of n, T reads:

$$L = n \begin{pmatrix} 1 & \frac{3}{2}T \\ \frac{3}{2}T & \frac{15}{4}T^2 \end{pmatrix}.$$

Afterward, introducing the dual entropy variables, or electro-chemical potentials (see[7] for a review):

$$w_1 = \mu/T - V/T \quad \text{and} \quad w_2 = -1/T$$

by elementary computations, one gets the equivalence of equations (1) and the following 'entropic' reformulation of the energy transport model:

$$\mathrm{div} I_1 = 0, \tag{2a}$$
$$\mathrm{div} I_2 = Q(w, V), \tag{2b}$$
$$\lambda^2 \Delta V = N(w, V) - C(x), \tag{2c}$$

$$I_1 = -\sum_{k=1}^{2} D_{1k}(w, V)\nabla w_k, \quad I_2 = -\sum_{k=1}^{2} D_{2k}(w, V)\nabla w_k. \tag{2d}$$

where $w = (w_1, w_2)$,

$$D_{11} = L_{11}, \qquad D_{12} = D_{21} = L_{12} - VL_{11}, \quad D_{22} = L_{22} - 2VL_{21} + V^2 L_{11},$$

$$Q(w, V) = W(\mu, T) \quad \text{and} \quad N(w, V) = (-1/w_2)^{3/2} \exp(w_1 - w_2 V).$$

To get a well posed problem, system (2) has to be supplemented with appropriate boundary conditions. We assume that the boundary $\partial\Omega$ of the domainΩ 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, we consider the following mixed boundary conditions:

$$w_1 = w_{1D}, \;\; w_2 = w_{2D}, \;\; V = V_D \qquad \text{on } \Gamma_D \tag{2e}$$
$$I_i \cdot \nu = \nabla V \cdot \nu = 0 \qquad i = 1, 2 \qquad \text{on } \Gamma_N \tag{2f}$$

where w_{1D}, w_{2D} and V_D are the $H^1(\Omega)$-extensions of fixed functions defined on Γ_D.

3. Formulation of the Design Problem as a Control Problem

Let $\overline{C}$ be a given reference doping profile and let Γ_O be a portion of the Ohmic contacts Γ_D, at which we can measure the density current I_1, obtained by solving the system (2). At the contact Γ_O we prescribe a gained current I_g and allow deviations, in some suitable norm, of the doping profile from $\overline{C}$ in order to gain this current flow. In other words we intend to minimize cost functionals of the form

$$F(w, V, C) = \frac{1}{2}\left|\int_{\Gamma_0} I_1 d\nu - I_g\right|^2 + \frac{\gamma}{2}\int_{\Omega} |\nabla(C - \bar{C})|^2 dx \tag{1}$$

where $\gamma > 0$ allows to balance the effective cost. C enters as a source term in the energy transport model (2), which can be interpreted as a constraint, to the minimization problem, determining the density current I_1, by the state variable (w_1, w_2, V).
This yields a constrained optimization problem in the framework of the mathematical theory for the control of systems governed by partial differential equations.[8] In order to get a solution to this problem let us introduce the state $y \stackrel{\text{def}}{=} (w_1, w_2, V)$ and an admissible set of controls

$$\mathcal{C} = \{C \in H^1(\Omega) \cap L^\infty(\Omega) : C = \bar{C} \text{ on } \Gamma_D\} \subset H^1(\Omega) \tag{2}$$

and let us rewrite the state equations (2) shortly as $f(y, C) = 0$.
In order to introduce a functional analytic framework let introduce the space of states

$$X = y_D + X_0 \tag{3}$$

where $y_D \stackrel{\text{def}}{=} (w_D, V_D)$ denotes the boundary data, introduced above, and $X_0 = \left[H_0^1(\Omega \cup \Gamma_N)\right]^2 \times \left(H_0^1(\Omega \cup \Gamma_N) \cap L^\infty\right)$, equipped with the norm $\|y\|_{X_0} \stackrel{\text{def}}{=} \|w\|_{[H^1(\Omega)]^2} + \|V\|_{H^1(\Omega)} + \|V\|_{L^\infty(\Omega)}$, as well as the space of co-states $Z \stackrel{\text{def}}{=} [H^1(\Omega)]^3$. Then the nonlinear mapping $f : X \times \mathcal{C} \to Z^*$ where

$$f(y, C) \stackrel{\text{def}}{=} \begin{pmatrix} div\left(\sum_{k=1}^2 D_{1k}(w, V)\nabla w_k\right) \\ div\left(\sum_{k=1}^2 D_{2k}(w, V)\nabla w_k\right) + Q(w, V) \\ \lambda^2 \triangle V - N(w, V) + C(x) \end{pmatrix}, \tag{4}$$

is well-defined.
In[2] the existence of a minimizer to the minimization problem

$$\min_{X \times \mathcal{C}} F(w, V, C) \qquad \text{s.t.} \qquad f(w, V, C) = 0 \tag{5}$$

has been established, under suitable hypothesis.

4. The First-order Optimality System

In order to write the first-order optimality system let consider the Lagragian $\mathcal{L} : X \times \mathcal{C} \times Z \to \mathbb{R}$, associated to the minimization problem (5), defined by

$$\mathcal{L}(y, C, \xi) \stackrel{\text{def}}{=} F(y, C) + < f(y, C), \xi >_{Z^*, Z}$$

where $\xi \stackrel{\text{def}}{=} (\xi^{w_1}, \xi^{w_2}, \xi^V)$ denotes the adjoint variables. The Lagrangian $\mathcal{L}$ is continuously Fréchet differentiable.[2] The first order optimality system related to problem are given by

$$\nabla_{(y,C,\xi)} \mathcal{L}(y, C, \xi) = 0. \tag{1}$$

which can be rewrite in the following form:

$$f(y, C) = 0 \qquad \text{in } Z^* \tag{2}$$
$$f_C^*(y, C)\xi + F_C(y, C) = 0 \qquad \text{in } C^* \tag{3}$$
$$f_y^*(y, C)\xi + F_y(y, C) = 0 \qquad \text{in } X^* \tag{4}$$

where $f_C^*(y, C) \in L(Z, \mathcal{C}^*)$ and $f_y^*(y, C) \in L(Z, X^*)$ denote the adjoint operators associated to $f_C(y, C)$ and $f_y(y, C)$ respectively.
By a short computation, the optimality condition (3), for the cost functional (1) can be written as

$$\xi^V = \gamma \triangle (C - \bar{C}), \tag{5a}$$

with the following boundary conditions

$$C = \bar{C} \qquad \text{on } \Gamma_D \tag{5b}$$
$$\nabla C \cdot \nu = \nabla \bar{C} \cdot \nu \qquad \text{on } \Gamma_N \tag{5c}$$

For the adjoint system we refer to.[2]

5. Optimization procedure and numerical results

In this section we show some numerical results for the optimization procedure applied on a one-dimensional n+ n n+ ballistic silicon diode, which is a simple model for the channel of a MOS transistor. The semiconductor domain is given by the interval $\Omega = (0, L)$ with $L > 0$. In the n^+-regions the maximal doping concentration is $C_m = 5 \cdot 10^{17}$ cm^{-3}. In the n-channel the minimal doping profile is $2 \cdot 10^{15}$ cm^{-3}. The length of the n^+-regions is $0.1\mu m$, whereas the length of the channel region equals $0.4\mu m$. The physical parameters for silicon are given in the following table:

Parameter	Physical meaning	Numerical value
q	elementary charge	$1.6 \cdot 10^{-19} As$
ε_s	permittivity constant	$10^{-12} AsV^{-1}cm^{-1}$
μ_0	(low field) mobility constant	$1.4 \cdot 10^3 cm^2 V^{-1} s^{-1}$
U_T	thermal voltage at $T_0 = 300K$	$0.026V$
τ_0	energy relaxation time	$0.4 \cdot 10^{-12} s$
L	length of the device	$0.6\mu m$

For the numerical solution of (5) we have performed the following gradient algorithm. Starting from a reference doping profile (which is depicted in fig 1a with a solid line), we solve in a first step the energy transport model as the underlying semiconductor model and in a next step the adjoint system for the Lagrange-multipliers and update the doping profile via (5a). In other words we perform the following:

Algorithm 1. ([6])

1. Choose $C_0 \in \mathcal{C}$
2. For $k = 1, 2, ...$ compute $C_k = C_{k-1} - \alpha_k \hat{F}'(C_{k-1})$

Here, $\hat{F}(C) = F(y(C), C)$ denotes the reduced cost functional and $\hat{F}'(C_{k-1})$ is the Riesz representative of its first variation.
The evaluation of

$$\hat{F}'(C) = F_C(y, C) + e_C^* \xi$$

requires the solution of the nonlinear state system (2) as well as a solution of the *linear* adjoint system and finally a linear solve of a Poisson problem (5a) to get the correct Riesz representative. In the following results we have chosen a constant step–size $\alpha = 10^{-2}$ and $\gamma = 10^{-3}$. The iteration stops when the difference of two consecutive doping profiles is below some specified threshold.
The state system was discretized by an exponentially fitted scheme. The computations were performed on a uniform grid of 301 points. For the biasing voltage at the working point we choose $\bar{U} = 1V$ and try to gain an amplification of the current J by 50%, i.e. we set $I_g = \bar{I} \cdot 1.50$. The numerical results can be found in Figure 1. One can observe that the desided amplification in the current is already achieved by a very slight change in doping profile, i.e. an increase of background charges in the channel. The overall performance of the algorithm is very promising, since only 30 gradient steps are sufficient for the optimization. For the convenience of the reader we show also how both parts of the cost functional (1), i.e. the observation and the penalizing (energy) term, evolve during the iterations. Further, we depict in Figure 1 the densities, velocities and temperatures before and after the optimization. They almost coincide due to the very small change in the doping density. Nevertheless, we reach our objective as can be also seen from the given current-voltage characteristics (IVC).

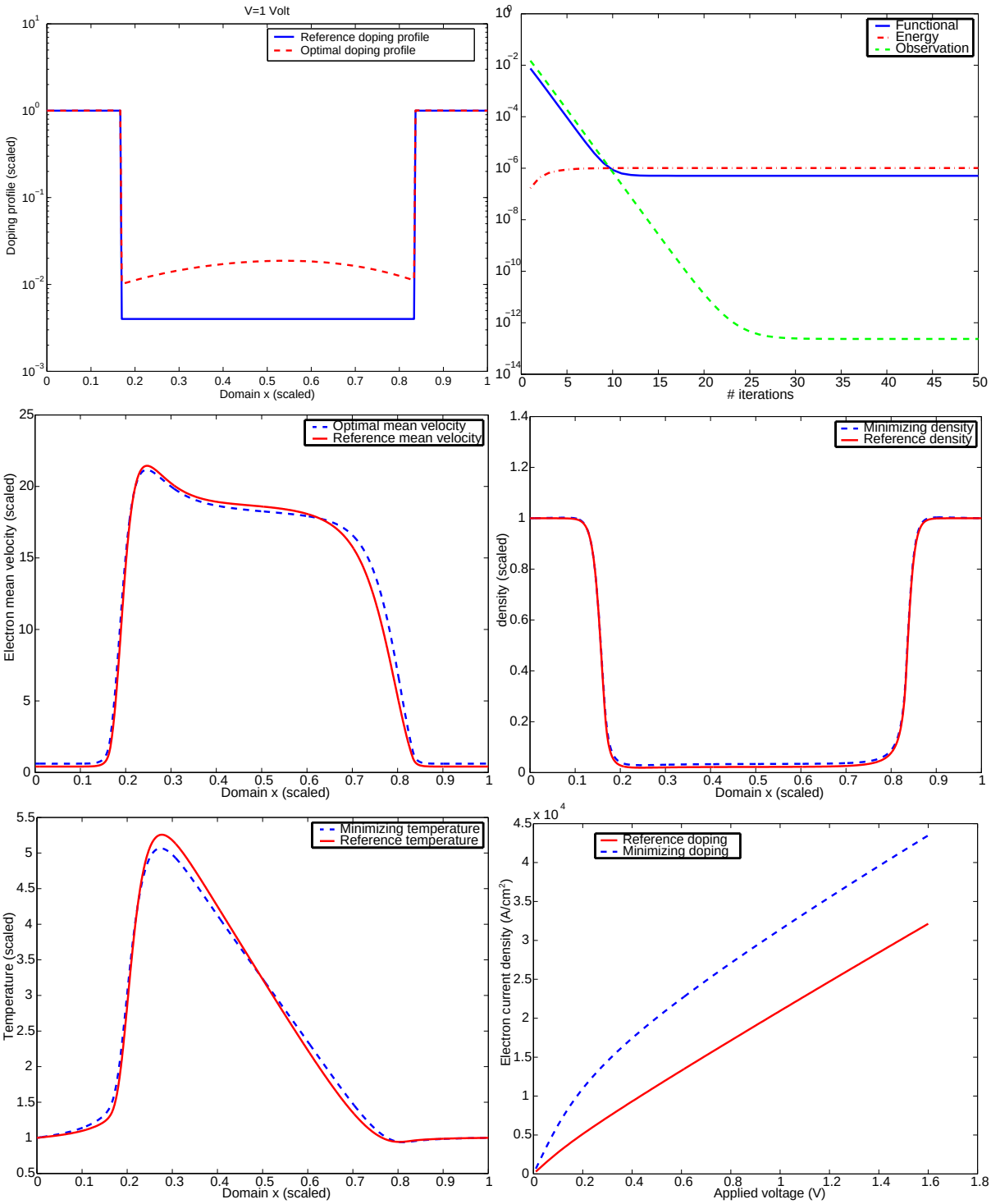

Fig. 1. Optimized doping profile, evolution of the cost functional, electron mean velocity, electron density and temperature for a biasing voltage of 1 V

Conclusions

Here, we have presented some first numerical results for doping profile optimal design based on the energy transport semiconductor model. Unlike the standard drift diffusion model, this takes into account temperature and mobility effects of the electrons transport. The optimization procedure, based on a descent algorithm and the adjoint calculus is tested on a $n^+ - n - n^+$

ballistic diode.

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