THE OPEN UNIVERSITY OF SRI LANKA
BACHELOR OF TECHNOLOGY (level 05)
ECX 5239
PHYSICAL ELECTRONICS
FINAL EXAMINATION 2005

DATE : 30th April 2006 **TIME : 9.30 – 12.30 hours**

Answer the question given in **SECTION A** and select any **four** questions from **SECTION B.**

SECTION A:

1. By using the concepts of drift diffusion model/energy band model or as needed of both models, derive the mathematical model of **ONE** of the following devices:

   (a) diode
   (b) BJT
   (c) MOSFET

SECTION B:

Select **ANY FOUR** questions

The pages 3 to 7 of the article 'An optimal control approach to semiconductor design' by Michael Hinze and Rene Pinnau is attached for your reference. Read these pages and answer following questions.

2. Describe in your own words the problem considered in this article.

3. State the physical meaning of each equation (1.1a), (1.1b), (1.1c), (1.1d) and (1.1e). Name the five unknown variables in the above set of equations.

4 To find solutions to the system of differential equations (1.1) it is necessary to specify boundary conditions. What sort of boundaries is considered for this particular device.

5. Derive the system of equations (1.2) i.e. equations (1.2a), (1.2b) and (1.2c) from the system of equations (1.1). State the boundary conditions for the system of equations (1.2) and all assumptions made during derivation (if any) clearly.

6. Briefly explain (in point form) the basic concepts of the drift diffusion model.

7. Briefly explain (in point form) the underlying scientific theory of the drift diffusion model.

8. In the context of the given article why is it desirable to simulate the behavior of semiconductor devices? What are microscopic and macroscopic device models?

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

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

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

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

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

$$-\epsilon \Delta V = q(n - p - C). \tag{1.1e}$$

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, μ_n, μ_p are the diffusion coefficients and mobilities of electrons and holes respectively. The physical constants are the elementary charge q and the permittivity constant ϵ. 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 τ_n, τ_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 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 at the insulating part Γ_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

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

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 μ_n, μ_p are constant. Further, we employ the following scaling

$$n \to C_m \bar{n}, \qquad p \to C_m \bar{p}, \qquad x \to L \bar{x},$$
$$C \to C_m \bar{C}, \qquad V \to U_T \bar{V}, \qquad J_{n,p} \to \frac{q\,U_T\,C_m\,\mu_0}{L} \bar{J}_{n,p}$$

where L denotes a characteristic device length, C_m the maximal absolute value of the background doping profile and μ_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 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 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

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

and

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

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.

$e = 1.6 \times 10^{-19}$ C

$m_e = 9.108 \times 10^{-31}$ kg

$h = 6.625 \times 10^{-34}$ Js

$c = 3 \times 10^8\ ms^{-2}$

$P_n = nh/2\pi r \quad \lambda = h/p \quad \Delta x.\Delta p \geq h \quad \Delta E.\Delta t \geq h$

$\sqrt{\overline{c^2}} = \sqrt{(3KT/m_e)} \quad J = -ne\overline{v}$

$R_H = -(1/ne) = (1/pe)$

$p_n = n_i^2/N_D \quad n_p = n_i^2/N_A$

$D_e/\mu_e = KT/e \quad E = hc/\lambda$

$J_e = ne\mu_e E + eD_e\ (dn/dx)$

$n = N_c \exp -(E_c - E_F)/KT$

$n_i = \sqrt{N_c N_v} \exp-(Eg/2KT)$

$V_0 - V = (D_e/\mu_e).\ \ln(n_n/n_p)$

$I_s = A\ [\ (D_e e n_p/L_p) + (D_h e p_n/L_n)]$

$W_{n0}^2 = (2\varepsilon V_0/e).\ [N_A/(N_A N_D + N_D^2)]$

$k = 1.38 \times 10^{-23}$ J/k

$1\ eV = 1.6 \times 10^{-19}$ J

$\varepsilon o = 8.854 \times 10^{-12}$ F/m

$I = N_- n_- e + N_+ n_+ e$

$R = \rho.l/A \quad \rho = 1/\sigma \quad J = \sigma E$

$\overline{v} = e\tau E/m_e$

$\mu_e = e\tau/m_e \quad \mu_h = e\tau/m_h$

$\lambda = \tau\sqrt{\overline{c^2}} \quad D = (\lambda/3).\sqrt{\overline{c^2}}$

$\sigma = \mu_e ne = \mu_h pe$

$J_h = pe\mu_h E - eD_h\ (dp/dx)$

$p = N_v \exp -(E_F - E_c)/KT$

$V_0 = (KT/e).\ \ln(N_D N_A/n_i^2)$

$I = I_s\ [\ \exp\ (eV/KT) - 1]$

$W_n^2 = W_{n0}^2\ (1 - V/V_0) \quad W = W_n + W_p$

$W_{p0}^2 = (2\varepsilon V_0/e).\ [N_D/(N_A N_D + N_A^2)]$