Combining Asymptotic Analysis and Optimization in Semiconductor Design

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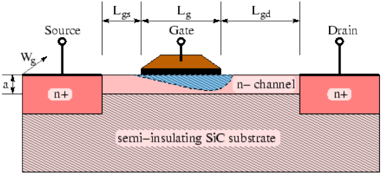
Once Upon a Time...

Optimal Semiconductor Design

- Miniaturization
- Switching–times
- Energy Consumption

The Design Problem

Higher/lower current density
in the **on/off state**
by changing the **doping profile**



(©T. Ayalew, TU Vienna)

(Selberherr, et al. 1998)

Classical Semiconductor Models

Model Hierarchy

Boltzmann Equation

Hydrodynamic Equations

Energy Transport Model

Drift Diffusion Model

State of the Art

- Fang, Ito (1992):
  Identification of doping profiles from LBIC images
- Selberherr, Stockinger, et al. (1998 –):
  Optimization of MOSFET doping profiles using a black box gradient method
- Wang, et al. (1999):
  Optimization of doping profiles using finite dimensional least squares
- Burger, Engl, Markowich, Pietra (2001 –):
  Identification of doping profiles
- Hinze, Pinnau (2001 –):
  Optimal control approach to semiconductor design
- Burger, Pinnau (2002 –):
  Gummel–type algorithms
- Drago, Anile, Pinnau (2005 –):
  Optimization based on the energy–transport model, space mapping
- Unterreiter, Volkwein (2006):
  Optimal control for QDD
- Burger, Fuego, Pinnau, Rau (2011–):
  Optimal control of self-consistent classical and quantum particle systems
- Liu (2014):
  Optimization of solar cell performance
- Peschka, Rotundo, Thomas (2016):
  Doping optimization of semiconductor lasers

A Simple Design Problem

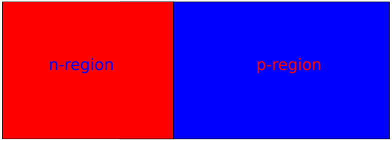


Figure: np-junction

$$\min_{(V,C)} J(V,C) = \frac{1}{2}\|n(V) - n_d\|_{L^2} + \frac{1}{2}\|p(V) - p_d\|_{L^2} + \frac{\gamma}{2}\|\nabla(C - \bar{C})\|_{L^2}$$

subject to the Drift Diffusion equations in Equilibrium

$$e_\lambda(V,C) := -\lambda^2 \Delta V - n(V) + p(V) + C = 0$$

space charge $n(V) - p(V) - C$

Separate Blocks of Research

We can

optimize on different levels of the model hierarchy!

provide analysis for the different models!

can link the models via asymptotic analysis!

Can we

also find an asymptotic link for the different optimization problems?

E.g. Zero Space Charge Approximation $\lambda = 0$

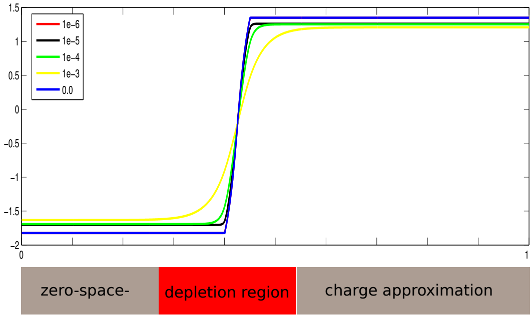


Figure: potential V for different λ

away from the junction, potential is linear and behaves like the zero space charge solution, different approximation in depletion region

Limit $\lambda \to 0$ combined with optimization

$$
\begin{array}{ccc}
(V_\lambda, C_\lambda) = \arg\min\limits_{(V,C)} J(V,C) & \text{subject to} & e_\lambda(V_\lambda, C_\lambda) = 0 \\
?\Big\downarrow & \lambda \to 0 & \Big\downarrow {\scriptstyle L^r,\ r \in [1,\infty)} \\
(V_0, C_0) = \arg\min\limits_{(V,C)} J(V,C) & \text{subject to} & e_0(V_0, C_0) = 0\,[1]
\end{array}
$$

[1] Andreas Unterreiter, "The Thermal Equilibrium Solution of a Generic Bipolar Quantum Hydrodynamic Model", Commun. Math. Phys.,1997

Limit $\lambda \to 0$ combined with optimization

$$(V_\lambda, C_\lambda) = \arg\min_{(V,C)} J(V,C) \quad \text{subject to} \quad e_\lambda(V_\lambda, C_\lambda) = 0$$

$$\Gamma \Big\downarrow \qquad \lambda \to 0 \qquad \Big\downarrow \begin{array}{c} L^r \\ r \in [1,\infty) \end{array}$$

$$(V_0, C_0) = \arg\min_{(V,C)} J(V,C) \quad \text{subject to} \quad e_0(V_0, C_0) = 0$$

convergence of minima and minimizers

Forward problem - Drift Diffusion Equations

Considering a semiconductor in thermal equilibrium, without recombination and generation processes.
The classical Drift Diffusion equations

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

with boundary conditions $\nu \cdot \nabla n = \nu \cdot \nabla p = \nu \cdot \nabla V = 0$ on $\partial\Omega$ can be condensed to

$$-\lambda^2 \Delta V = n(V) - p(V) - C$$

where $n(V) = \alpha e^{-V}$, $p(V) = \beta e^{V}$ are written in Slotboom variables and the additional conditions

$$\nu \cdot \nabla V = 0 \text{ on } \partial\Omega, \int n = N, \int p = P, \int V = 0.$$

Variational Approach (dual to Unterreiter)

Let $\Sigma_0 = \{V \in L^1(\Omega) \colon |V| \le K \text{ a.e.}, \int_\Omega V = 0\}$ with $K > 0$. Define

$$F(V) = \begin{cases} N \log(\int_\Omega e^{-V}\,\mathrm{d}x) + P \log(\int_\Omega e^{V}\,\mathrm{d}x) + \int_\Omega CV\,\mathrm{d}x, & \text{if } V \in \Sigma_0 \\ +\infty, & \text{otherwise} \end{cases}$$

and

$$F_\lambda(V) = \frac{\lambda^2}{2}\int_\Omega |\nabla V|^2\,\mathrm{d}x + F(V) \quad \text{for } V \in \Sigma_0 \cap H^1 =: \Sigma_1.$$

Then one obtains the nonlocal(!) Euler-Lagrange equation $F_\lambda'(V)[\varphi] = 0$

$$\int_\Omega \lambda^2 \nabla V \cdot \nabla \varphi\,\mathrm{d}x - \int_\Omega \frac{N}{\int e^{-V}\,\mathrm{d}x} e^{-V}\varphi\,\mathrm{d}x + \int_\Omega \frac{P}{\int e^{V}\,\mathrm{d}x} e^{V}\varphi\,\mathrm{d}x + \int_\Omega C\varphi\,\mathrm{d}x = 0.$$

Theorem

The functional F_λ is strictly convex and possesses a unique minimizer V_λ.

Further, we get uniform bounds allowing for the extraction of convergent subsequences $V_\lambda \to V_0$, where V_0 is the unique minimizer of F_0.

The dual approach also allows to consider weaker assumptions on the doping profile C.

Lemma

The constrained optimization problem

Find (V, C) such that

$$j = \min_{(V,C)} J(V, C) \text{ s.t. } e_\lambda(V, C) = 0$$

is solvable for every given $C \in H^1(\Omega)$. In general, no uniqueness!

The adjoint system is given by

$$\begin{aligned} -\lambda^2 \Delta \Psi_V &= \alpha e^{-V} \Psi_n + \beta e^V \Psi_p, \\ -\Psi_V + \Psi_n &= (n - n_d), \\ \Psi_V + \Psi_p &= (p - p_d), \end{aligned}$$

with boundary conditions $\nu \cdot \nabla \Psi_i = 0$ and integral conditions $\int \Psi_i = 0$ for $i = n, p, V$ and the optimality condition reads

$$\begin{aligned} \gamma \Delta (C - \bar{C}) &= \Psi_V \\ \nu \cdot \nabla C &= 0 \quad \text{on } \partial\Omega. \end{aligned}$$

Proposition (Γ-convergence[2])

Let X be a topological space, let $\{F_n\}$ be a sequence of functions from X into $\overline{R}$, then $\{F_n\}$ Γ-converges to F if and only if the following conditions are satisfied:

$$\liminf -\mathit{inequality}: \quad \forall x \in X \quad \forall x_n \to x \in X : F(x) \le \liminf_{n\to\infty} F_n(x_n),$$
$$\limsup -\mathit{inequality}: \quad \forall x \in X \quad \exists x_n \to x \in X : F(x) \ge \lim_{n\to\infty} F_n(x_n).$$

To obtain Γ-convergence we include the PDE constraint in the cost functional

$$J_\lambda(V,C) = J(V,C) + \chi_{\mathcal{E}_\lambda},$$

where

$$\chi_{\mathcal{E}_\lambda} = \begin{cases} 0, & \text{if } (V,C) \in \mathcal{E}_\lambda \\ +\infty, & \text{else} \end{cases}$$

and

$$\mathcal{E}_\lambda := \{(V,C) \in \mathcal{V} \times U_{ad} : e_\lambda(V,C) = 0\} \text{ with } U_{ad} = \{u \in H^1 : |u| \le K\}.$$

[2] Gianni Dal Maso, "An Introduction to Γ-convergence", Birkhäuser

Properties required to obtain the Γ-convergence

We use $X = H^1(\Omega) \times H^1(\Omega)$ endowed with its weak topology.

Lemma

- *uniqueness of the solution of the forward problem for* $\lambda \geq 0$
- *strong* L^2 *convergence of the solutions* $V_\lambda \to V_0$, $n(V_\lambda) \to n(V_0)$, $p(V_\lambda) \to p(V_0)$ *as* $\lambda \to 0$ *and uniform boundedness of* $\{V_\lambda\}$ *in* $H^1(\Omega)$ *depending on* $\|C\|_{H^1}$
- $J(V,C) = J_1(V) + J_2(C)$, J_1 *weakly continuous,* J_2 *weakly lower semicontinous and radially unbounded.*

Definition

Let X be a metric space. A sequence of functionals $\{F_n\}$ is said to be **equi-coercive** on X, if for every $t \in \mathbb{R}$ there exists a compact subset K_t of X such that $\{F_n \leq t\} \subset K_t$ for every $n \in \mathbb{N}$.

Convergence of Minima and Minimizers

Theorem

J_λ is an equi-coercive sequence of functionals.

Idea: Let $(V_t, C_t) \in \{J_\lambda(V_t, C_t) \leq t\}$. Due to $\chi_{\mathcal{E}_\lambda}$ in the definition of J_λ, V_t is a solution of DD equations with doping C_t. $\|C_t\| \leq K$ since J_λ is radially unbounded w.r.t C, this yields uniform boundedness of V_t. Therefore $\|V_t\|_{H^1} + \|C_t\|_{H^1}$ bounded.

Proposition

Γ-convergence + equi-coercivity ⇒ convergence of minima and minimizers [3]

[3] Gianni Dal Maso, "An Introduction to Γ-convergence", Birkhäuser

Numerical results