Doping optimization for optoelectronic devices

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***Abstract*—We present a mathematical framework and numerical simulations for the optimal doping design for optoelectronic devices using methods from mathematical optimization. With the goal to maximize light emission from an edge-emitting laser, we consider a model for semiconductor charge transport and include optical gain and losses into the cost functional for the optimization of its 2D cross sections. We present 1D and 2D results for exemplary setups that point out possible routes for device improvement.**

I. Introduction

Silicon photonics has a high potential for novel solutions in microelectronics, *e.g.*, for high-speed data transfer via optical on-chip communication or for bio-sensing. In this regard, the engineering of mechanical strains or of electronic doping provides feasible ways to enhance optoelectronic properties of semiconductor lasers in a desired direction. In the past, there have been several studies investigating the optimization of electronic transport in semiconductor devices with optimal control methods, *e.g.*, [1] and [2]. It is our goal to extend these mathematical methods systematically to *optoelectronic* devices.

It was shown that using a combination of tensile strain and high n-doping can transform germanium into a suitable optically active medium for an edge-emitting laser [3]. Additional design features, such as focussing the electron currents through an aperature, can still significantly lower lasing thresholds [4]. Motivated by this potential for further improvement, we study the problem of finding an optimal doping profile $c : \Omega \subset \mathbb{R}^d \to \mathbb{R}$ where $d \in \{1, 2\}$, aiming at enhanced laser light emission, *cf.* Fig. 1.

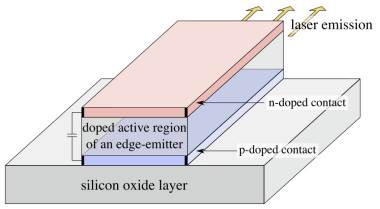

Figure 1: Sketch of a contacted edge-emitter, where the doping profile $c(x)$ in the optically active region is to be optimized.

II. Mathematical model and doping optimization

We seek the electrostatic potential $\psi(x)$, the electron and the hole densities $n(x), p(x)$, and the photon number γ, such that

$$0 = -\nabla \cdot (\epsilon_r \nabla \psi) - (c + p - n), \tag{1a}$$

$$0 = \dot{n} - \nabla \cdot \mathbf{j}_n + R_{\mathrm{nr}} + R_{\mathrm{rad}}, \tag{1b}$$

$$0 = \dot{p} + \nabla \cdot \mathbf{j}_p + R_{\mathrm{nr}} + R_{\mathrm{rad}}, \tag{1c}$$

$$0 = \dot{\gamma} - \frac{1}{|\Omega|} \int_\Omega (R_{\mathrm{rad}} - \Lambda |\Theta|^2), \tag{1d}$$

with charge fluxes $\mathbf{j}_n = -\mu_n n \nabla \phi_n$ and $\mathbf{j}_p = -\mu_p p \nabla \phi_p$, non-radiative and radiative recombination rates R_{nr} and R_{rad}, and extra losses Λ. Here, the quasi-Fermi potentials ϕ_n, ϕ_p are defined implicitly by the equation of state $n = N_c F\big(\frac{E_v - q(\psi - \phi_p)}{k_B T}\big)$ and $p = N_v F\big(\frac{q(\psi - \phi_n) - E_c}{k_B T}\big)$. Then, the standard drift-diffusion formulation is obtained by using Boltzmann statistics, *i.e.*, $F(s) = e^{-s}$. The model (1) is motivated by a publication of Gajewski et al. [5], for which we showed in [6] that it has a particular variational structure. The model (1) is supplemented with boundary conditions $\mathbf{j}_n \cdot \mathbf{n} = \mathbf{j}_p \cdot \mathbf{n} = \mathbf{n} \cdot \nabla \psi = 0$ on $\Gamma_N \subset \partial\Omega$ and Dirichlet conditions at standard Ohmic contacts Γ_D.

The recombination rates in the model are of general the form $R_{\mathrm{nr}} = R\big(np - n_i^2\big)$ and contain contributions from spontaneous, Shockley-Read-Hall, and Auger recombination. The photon number γ in (1d) corresponds to an optical mode with frequency ω, which solves the Helmholtz equation

$$\Big[\Delta + \tfrac{\omega^2}{c^2}\, \epsilon_{\mathrm{opt}} - \xi^2\Big]\, \Theta = 0, \tag{2}$$

with $\epsilon_{\mathrm{opt}} = (n_r + i \frac{c}{2\omega} g)^2$. The radiative recombination R_{rad} can be written in terms of Θ and the imaginary part of ξ. Using a perturbation argument allows us to consider the radiative recombination a function $R_{\mathrm{rad}} \sim g|\Theta|^2$, where $g = g(n, p, \gamma)$ and Θ depends only implicitly on the doping profile c.

In order to find the optimal doping c_{opt}, we write the solutions of (1) in the compact form $\mathbf{u} = (\psi, n, p, \gamma)$. We are interested in low (treshold) currents Q_J through contacts $\Gamma_{\mathrm{c}} \subset \Gamma_D$ and high modal gain Q_R, where $Q_J(\mathbf{u}) = \int_{\Gamma_{\mathrm{c}}} |\mathbf{j}_n + \mathbf{j}_p|^2 \cdot \mathbf{n}$ and $Q_R(\mathbf{u}) = \int_\Omega (-R_{\mathrm{rad}} + \Lambda |\Theta|^2)$. This results in the constrained optimization problem

$$\min_{c, \mathbf{u}\ \text{s.t.}\ (1)} \Big(\alpha_J\, Q_J(\mathbf{u}) + \alpha_R\, Q_R(\mathbf{u}) + \beta\, \rho(c) \Big), \tag{3}$$

with suitable regularization $\rho(c)$, *e.g.*, $\rho(c) = \|\nabla(c - c_0)\|^2_{L^2}$, to guarantee existence of a minimizer c_{opt}. Below lasing threshold and due to the specific form of R_{rad} it is sufficient to consider (1a-c) with R_{rad} a function of n, p, where the photon number can be effectively absorbed into the coefficient α, and Θ is a given function.

III. Numerical Method and Discussion of Results

The numerical solution of the stationary solution of (1) relies on a finite element method, where we seek the electrostatic potential and the quasi-Fermi potentials (ψ, ϕ_n, ϕ_p), such that

$$\int \epsilon_r \nabla\psi \cdot \nabla w_1 = \int (c + p - n) w_1,$$
$$\int \mu_n n \nabla\phi_n \cdot \nabla w_2 = + \int (R_{\text{nr}} + R_{\text{rad}}) w_2,$$
$$\int \mu_p p \nabla\phi_p \cdot \nabla w_3 = - \int (R_{\text{nr}} + R_{\text{rad}}) w_3,$$

holds for all test functions (w_1, w_2, w_3). The densities n, p depend explicitly on the potentials via the before mentioned equation of state. For the doping optimization we apply a Newton scheme to the first order conditions of the constrained optimization problem (3). The function c_{opt} depends on the choice of ρ, γ, β. However, this ambiguity can be partially resolved by studying the limit $\beta \to 0$. Such an approach to device optimization is advantageous due to its fast convergence, which typically does not depend on the discretization. Here we present some results obtained for dimensions $d = 1$ and $d = 2$. The used gain model is motivated by [4] and [7], the numerical values have a reasonable order of magnitude but do not attempt to resemble any specific material or device setting. For the result in $d = 1$ in the domain $\Omega = [0, 1]\mu m$ with reference doping $N_0 = 10^{19} cm^{-3}$ and applied voltage $0.4V$ and $E_g = 0.24V$.

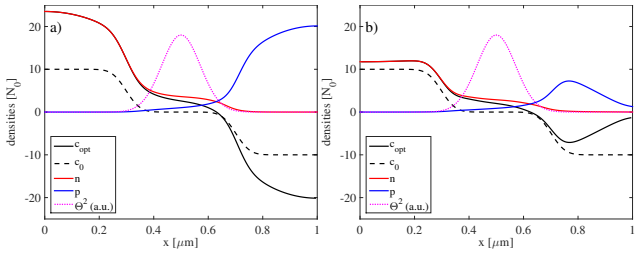

Figure 2: (left) optimal doping and electron/hole densities with $\alpha_R = 1$, $\alpha_J = 0$ and (right) or alternatively with $\alpha_R = 1$, $\alpha_J = 1/5$ and $\beta = 10^{-5}$

In Fig. 2 we show the optimal doping concentrations for $d = 1$ with different values of α_R, α_J. We observe a converging doping profile where the optical mode $|\Theta|^2$ is supported as $\beta \to 0$. Where the optical mode is small for $\alpha_J = 0$, the doping will depend on the choice of the regularization ρ, β (here $\beta = 10^{-5}$). When setting $\alpha_J = 1/5$ the optimal doping c_{opt} also converges where $|\Theta|^2$ is small. Also, using a combination of Q_J and Q_R as the optimization goal seems more reasonable. The shape of c_{opt} seems to suggest a fairly low doping with a slight gradient where the optical mode is located. Interestingly, the slight asymmetry in the free carrier absorbtion $f_p = 5 f_n$ in the gain model

$$g = \kappa \left(e^{\frac{-\hbar\omega}{k_B T}} - e^{\frac{-qU_F}{k_B T}} \right) \left(\frac{np}{N_0^2} \right)^{\gamma}, \quad \Lambda = f_n n + f_p p, \qquad (4)$$

with $qU_F = k_B T \big(F^{-1}(n/N_c) + F^{-1}(p/N_v) \big) + E_g$ leads to an asymmetric doping profile, so that for $x > 0.8\mu m$ the doping even decreases towards the Ohmic contact. At the other contact, for $x < 0.2\mu m$ the doping is nearly constant. The simulation result for $d = 2$ is shown in Fig. 3, where we have choosen the same physical parameters, except the bias is $0.2V$ and the geometry with the corresponding optical mode $\Theta \sim \sin\big(\pi x/(2\mu m)\big) \sin\big(\pi y/(0.5\mu m)\big)$. Near the contacts for $y \leq 0$ or $y \geq 0.5\mu m$ the doping is fixed, in all other places (including contacts) the doping is optimized. For better visibility, the result in Fig. 3 is shown on a coarse tensor-mesh with 6 016 vertices and 18 240 unknowns. Similar as for $d = 1$, there is only a slight gradient of c_{opt} where the optical mode is supported. Outside this region the behavior of the doping is again dependent on the regularization. In constrast to low-dimensional parameter studies, infinite-dimensional doping optimization provides valueable insights into the achievable optoelectronic performance. When designing such a toolbox, much implementation effort goes into computation higher-order derivatives of the model. However, this requires direct control over the solver implementation. Further improvement are viable by model improvement and validation.

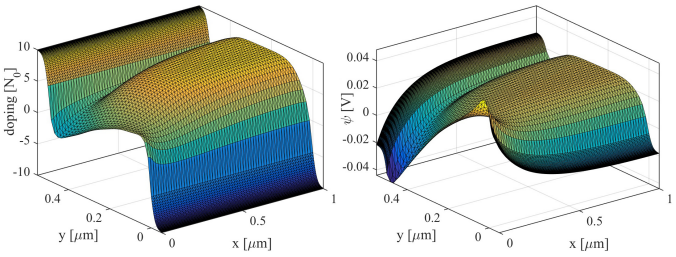

Figure 3: (left) optimal doping c_{opt} without low current goal $\alpha_R = 1$ and $\alpha_J = 0$ and (right) electrostatic potential ψ at $\beta = 10^{-5}$

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