2.1 Towards the Optimization of On-chip Germanium Lasers

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Silicon photonics, combining electronics with photonics, has become a rapidly developing new field with a high potential for low-cost solutions to problems ranging from high-speed data transfer for optical on-chip communication to biosensing. The missing piece for the silicon photonics platform is an integrable active light source compatible to silicon technology. To fill this gap, various concepts based on silicon (Si) and germanium (Ge) are under consideration; cf., e.g., [1]. However, both Ge and Si are indirect semiconductors and therefore not capable of substantial light emission. But by applying mechanical strain to Ge, it is possible to improve its radiative efficiency due to a favorable shifting of the band structure under strain [1]. The pioneering work in this direction is the successful demonstration of an electrically pumped laser based on slightly tensile-strained Ge/Si heterostructures by Massachusetts Institute of Technology (MIT) researchers [2]. The extremely high lasing threshold currents observed in these devices lead to strong heating effects limiting their operation lifetime. This fact shows the strong demand for improvements, in particular, for a rigorous optimization of Ge semiconductor lasers.

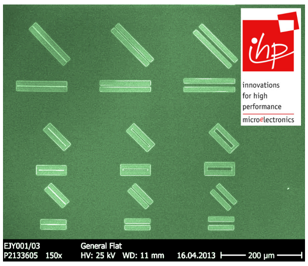


Fig. 1: *Ge microstrips with additional SiN stressor layer built at IHP provide higher biaxial strain compared to purely thermally strained Ge*

A first step in this direction was made by scientists at the *Leibniz-Institut für innovative Mikroelektronik IHP*, by proposing a manufacturing technique for strained Ge microstrips, which is superior to the purely thermally strained MIT device. Motivated by these promising results of our colleagues at IHP [3], we work on the mathematical optimization of mechanical strain and optical properties with the goal of finding a design for a Ge laser with a highly reduced threshold current. Finding this design is the goal of the ⊕**EC**Math funded MATHEON project D-OT1, which combines the long-standing expertise of WIAS regarding semiconductor modelling, analysis, and simulation with the expertise of *Humboldt-Universität zu Berlin* (Prof. M. Hintermüller, Prof. T. Surowiec) in nonsmooth partial differential equation optimization and algorithms. The quantity to be optimized is the stimulated emission, which depends on the doping through the carrier densities and on the band structure of Ge, which can be directly tuned by applying a mechanical strain. Our theoretical findings in simulations, e.g., with the software package `WIAS-TeSCA`, support the design of devices and interpretation of experiments at IHP.

Germanium as an optically active gain material

Light generation in a semiconductor is based on the radiative recombination of electrons with holes. In direct semiconductors, such as III-V materials, both electrons and holes occupy the Γ-valleys in the energy landscape possessing a similar momentum, which allows for an efficient radiative recombination. However, in unstrained Ge, the negatively charged electrons (n) mainly occupy the lower-lying conduction band L-valley, see Figure 2, thus making their momentum incompatible to that of the positively charged holes (p) in the valence band Γ-valley. Additional phonons are required to assist the optical transition, which makes radiative recombination much less likely.

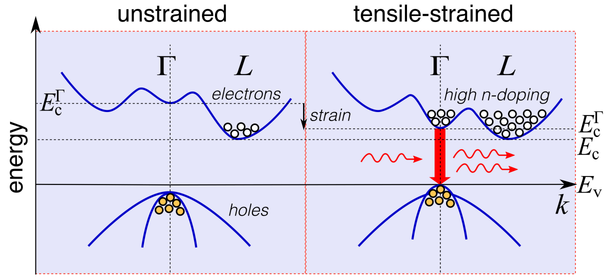


Fig. 2: *Schematic Ge band structure showing the occupation of electrons and holes in the conduction and valence band. The combined effect of tensile strain and n-doping resulting in an increase of stimulated emission by reducing the direct band gap $E_c^\Gamma - E_v$ (strain) and by filling the Γ-band (doping)*

By applying a tensile mechanical strain to Ge, the energy difference $E_c^\Gamma - E_c$ between the Γ-valley and the L-valley conduction band edges can be decreased. For biaxial strains beyond 1.7% Ge even becomes a direct semiconductor, where $E_c^\Gamma < E_c$. Moreover, by adding a suitably high n-type doping, i.e., by implanting some impurities creating an excess of negative charges, the number of electrons available for optical emission can be highly increased. With this band-filling effect, it is possible to inject additional electrons into the Γ-valley enhancing the radiative recombination. If the radiative recombination rate is sufficiently high, light is amplified by stimulated emission. This amplification is measured by the so-called *optical gain*, which depends on carrier densities of electrons and holes, on the mechanical strain, and on the n-type doping.

The *optical gain* can be described by a quantum mechanical model where the modified band structure due to the mechanical strain e is used in the calculations [4]. The gain data obtained in this way are fitted in [5] to a macroscopic expression that we use for `WIAS-TeSCA` simulations with the afore-mentioned semiclassical optoelectronic laser model. The expression for the optical gain $g(\psi, n, p; \omega, e)$ obtained in [5] depends on the values of electron and hole densities n, p, as well as on the frequency of light ω, on the spatially inhomogeneous strain e, and on the doping density C.

The computed material gain spectra for the transverse electric (TE) polarization [5] and different values of the biaxial tensile strain ranging linearly from 0.35% to 0.70% and different excess carrier densities $\delta n = n - C$ for the n-type doped Ge are shown in the left panel of Figure 3. The right panel shows the corresponding fit to the analytic expression for g from [5] for the wavelength λ=1620 nm. As expected, the material gain increases with increasing strain and increasing excess density, which are our main quantities to use in the optimization.

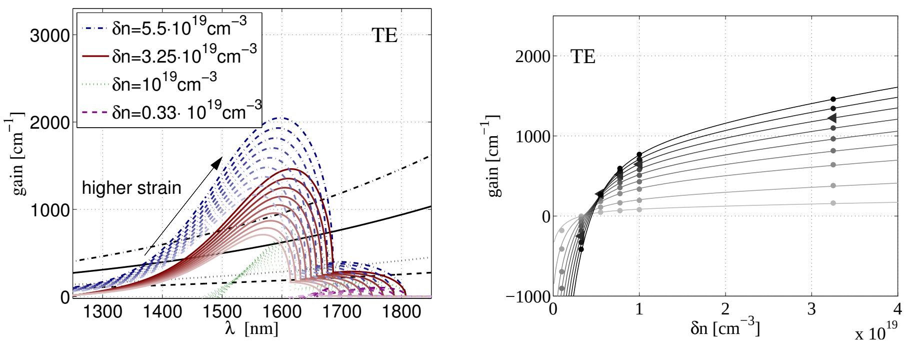


Fig. 3: *Left: Material gain for TE polarization computed for different excess densities δn and nine linearly increasing biaxial strains $0.35\% - 0.7\%$ for Ge with n-type doping $C = 5 \cdot 10^{19}\,\mathrm{cm}^{-3}$. Right: Fit to analytic expression for fixed wavelength λ = 1620 nm; see [5].*

Mathematical modeling and optimization strategy

We illustrate the approach for the optimization of a strained Ge microstrip, which is pursued in the MATHEON project D-OT1. Here, the optical gain depends on the mechanical strain e and on the carrier densities n, p for electrons and holes, making it sensitive to both the doping density C and the material distribution. When suitable physical optimization goals are identified, a mathematically rigorous optimization might generate producible improved laser designs.

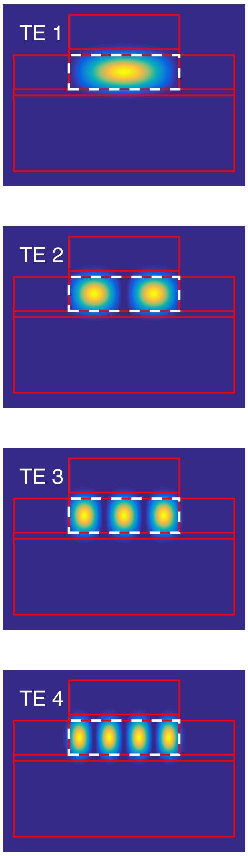
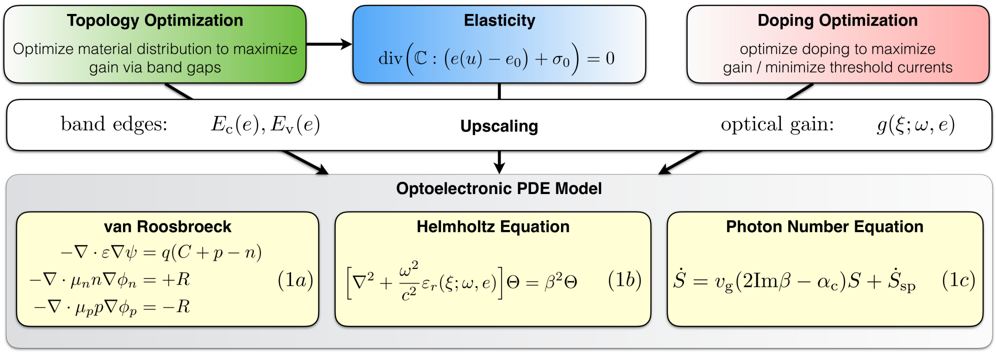


Fig. 4: Optical TE modes for $\lambda = 1.7\,\mu$m for an IHP geometry is concentrated in optically active Ge (dashed)



For a semiconductor occupying the domain $\Omega \subset \mathbb{R}^d$, charge transport is described by the *van Roosbroeck* system (1a), where, for a given doping profile C, one seeks the state $\xi = (\psi, \phi_n, \phi_p)$ consisting of the electric potential ψ, and the quasi-fermi potentials ϕ_n, ϕ_p for electrons and holes. With distribution function F, the carrier densities n, p are related to the potentials by

$$n = N_c F\left(\tfrac{q(\psi-\phi_n)-E_c}{k_B T}\right), \qquad p = N_v F\left(\tfrac{q(\phi_p-\psi)+E_v}{k_B T}\right), \tag{2}$$

with statistics F, where the energy levels $E_c(e), E_v(e)$ of the conduction band and valence band depend on the mechanical strain e. Additionally, the recombinations R in (1a) contain a contribution from stimulated emission of the form $R_{stim} \simeq gS|\Theta|^2$. The *Helmholtz equation* (1b) for the optical mode Θ couples to the van Roosbroeck system through the dependence of the permittivity

$$\varepsilon_r(\xi;\omega,e) = \Big(\mathsf{n}_r + \tfrac{ic}{2\omega}[g(\xi;\omega,e) - \alpha(\xi)]\Big)^2 \tag{3}$$

on the state ξ and on the strain e. The complex eigenvalue β of the Helmholtz equation (1b) enters the balance of *photon numbers* (1c), where $\mathrm{Im}\beta$ is typically increasing with increasing gain, so that a large gain results into a strong amplification of photon numbers, until, finally, the losses increase and balance the gain. The main effect of the material distribution on the strain is through the material-dependent thermal strains e_0 and stresses σ_0. Additionally, the refractive index n_r depends on the material. By creating a contrast of n_r within Ge with respect to the surrounding media, one creates confined optical modes with low losses outside the optically active Ge (Figure 4).

The main goal is to find such a doping and material distribution, so that the laser operates at a low threshold current, i.e., a sufficient amplification of $S \simeq$ "output power" at low electrical currents, i.e., with low heat production. In the following case study we explain different empirical strategies how this aim can be achieved, and how it can be translated into cost functionals.

Empirical case study

In [5], this modeling approach was used in order to identify promising starting geometries and feasible cost functionals for a doping and topology optimization. As an outcome, the case study underlined that a mathematically rigorous optimization may indeed be useful since the devices in fact show the possibility for a substantial lowering of the threshold currents. This observation is of great practical interest, because the device developed at MIT had a very short lifetime due to its high threshold currents.

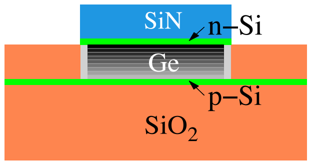


Fig. 5: *Cross section through* standard *Ge heterostructure similar to Fig. 1*

As in [5], we consider two competing designs: First, the standard design shown in Figure 5 consisting of a SiN stressor on top of the optically active Ge on an insulating SiO_2 layer. The doped silicon contacts are indicated by green layers in Figure 5. Second, the empirically improved aperture design shown in Figure 6, where electric currents are injected into the optically active Ge through a narrow opening near the center of the main mode (see insets in Figure 6). Both devices consist of a layered heterostructure based on an insulating SiO_2 substrate, with a Ge block sandwiched between the Si contacts (Si-n and Si-p) and a SiN layer on top, which, as experimentally and numerically verified in [3], induces a tensile strain to the Ge layer, linearly decreasing in vertical y-direction from top to bottom.

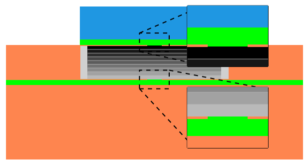


Fig. 6: *Cross section through* aperture *Ge heterostructure*

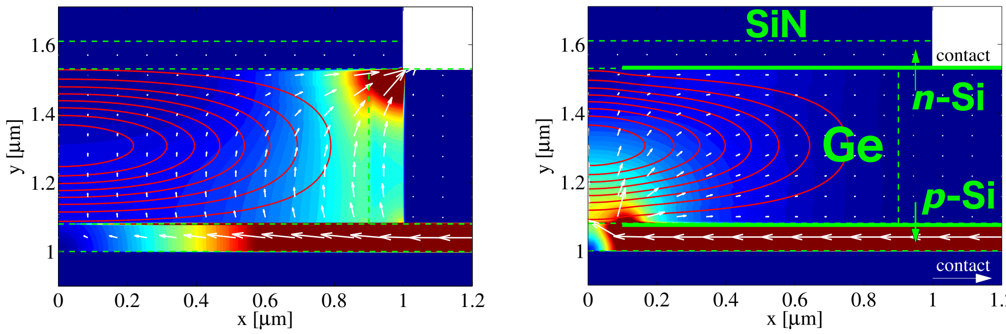


Fig. 7: *Hole current for left: standard device and right: aperture device above threshold. Red lines indicate the isolevels of Θ^2, whereas the white arrows and the colored background show the direction and magnitude of (the current) $j_p = -\mu_p p \nabla \phi_p$.*

For the standard device, which is considered a feasible and producible design by IHP, one observes significant leakage currents. They are very pronounced for the hole transport, cf. Figure 7 (left), where the carriers flow directly from the p-contact to the n-contact along the edges of the device without passing through the center of Ge, where the fundamental mode, indicated by the red isolines, is located. This observation is in contrast to the hole currents of the aperture device in Figure 7 (right), where the carriers are injected into the center of the fundamental mode, leading to a lower threshold thanks to a higher gain due to higher carrier densities and due to a more effective replenishment of carriers lost through stimulated recombination.

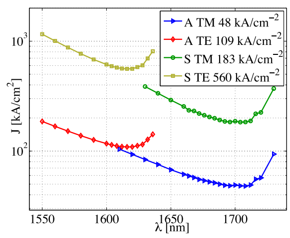


Fig. 8: *Threshold currents for aperture and standard design and TE/TM modes for different wavelengths*

The quantitative improvement of the aperture design over the standard design is shown in Figure 8, where one can see that the threshold current for the aperture device is lower than the threshold current for the standard device by a factor of almost four for transverse magnetic (TM) modes. The factor is even higher for TE modes; however, because of their lower gain, their threshold remains above that of TM modes.

Towards rigorous device optimization

The major difference between the IHP device concept and the purely thermally strained devices of MIT is the spatially nonuniform strain of the first, which is experimentally verified to increase

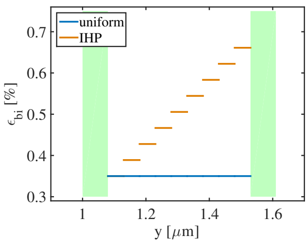


***Fig. 9:** Strain in Ge along y-direction is constant or linearly increasing 0.35%– 0.7% as achievable at IHP [5]*

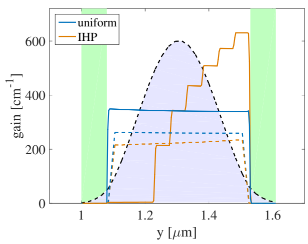


***Fig. 10:** Gain g (full lines) and losses α (dashed lines) for strains from Fig. 9 with optical mode Θ^2 in blue-shaded area*

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linearly with y as shown in Figure 9, leading to a substantial spatial variation of the band gaps and the gain shown in Figure 10. This property should be exploited in the topology optimization and in the doping optimization. The band gaps and the gain thereby depend on the y-coordinate from bottom to top, which, so far, were realized in the `WIAS-TeSCA` simulations by introducing nine artificial material layers in the Ge block with piecewise constant strain. The layering is indicated by regions of constant gray color in Figure 5 and by the section through the device center in Figure 9, where two different realizations of strain distributions through Ge are shown.

Figure 10 shows that, in contrast to the uniform strain, the strong *IHP strain* results in a very non-uniform gain, with the strongest enhancement in regions of highest strain. It is interesting to note that the main term responsible for photon amplification in (1c) can be approximated by lowest-order perturbation theory as

$$\mathrm{Im}\beta \approx \int_\Omega \big(g(\xi;\omega,e) - \alpha(\xi)\big)\,\Theta^2\,\mathrm{d}x \tag{4}$$

and, therefore, is called *modal gain*. For spatially constant densities, uniform gain, and a normalized confined mode, leading to $\mathrm{Im}\beta \approx (g-\alpha)$, with g and α constant throughout Ge. However, for spatially nonuniform gain, the optimization goal implied by (4) is to engineer a device so that the mode coincides with regions for large gain. For doping optimization, where the optical mode Θ is given, which implies optimizing the doping C so that $(g-\alpha)$ weighted with Θ^2 is maximal. In the context of topology optimization, we have to distribute the material such that the regions of large tensile strains and the shape of the optical mode overlap in an optimal way.

We refer to this concept as *overlap engineering* and, together with threshold currents, consider it a feasible cost functional for a rigorous doping and topology optimization of such an optoelectronic device.

References

[1] R. Geiger, T. Zabel, H. Sigg, *Group IV direct band gap photonics: Methods, challenges, and opportunities*, Front. Mater., **2** (2015), pp. 52/1–52/18.

[2] R.E. Camacho-Aguilera, Y. Cai, N. Patel, J.T. Bessette, M. Romagnoli, L.C. Kimerling, J. Michel, *An electrically pumped germanium laser*, Opt. Express, **20**:10 (2012), pp. 11316–11320.

[3] G. Capellini, C. Reich, S. Guha, Y. Yamamoto, M. Lisker, M. Virgilio, A. Ghrib, M. El Kurdi, P. Boucaud, B. Tillack, T. Schroeder, *Tensile Ge microstructures for lasing fabricated by means of a silicon complementary metal-oxide-semiconductor process*, Opt. Express, **22**:1 (2014), pp. 399–410.

[4] M. Virgilio, C.L. Manganelli, G. Grosso, G. Pizzi, G. Capellini, *Radiative recombination and optical gain spectra in biaxially strained n-type germanium*, Phys. Rev. B., **87**:23 (2013), pp. 235313/1–235313/11.

[5] D. Peschka, M. Thomas, A. Glitzky, R. Nürnberg, K. Gärtner, M. Virgilio, S. Guha, T. Schroeder, G. Capellini, T. Koprucki, *Modeling of edge-emitting lasers based on tensile strained germanium microstrips*, IEEE Photon. J., **7**:3 (2015), pp. 1502115/1–1502115/16.

[6] U. Bandelow, H. Gajewski, R. Hünlich, *Fabry–Perot lasers: Thermodynamics-based modeling*, in: Optoelectronic Devices – Advanced Simulation and Analysis, J. Piprek, ed., Springer, New York, 2005, pp. 63–85.