Weierstrass Institute for
Applied Analysis and Stochastics

Leibniz Association

Towards the optimization of Ge micro-bridges

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M. Virgilio[4], K. Gärtner[5], R. Nürnberg[1]

1) WIAS, 2) Humboldt-University, 3) IHP Frankfurt (Oder), 4) Uni. Pisa, 5) USI Lugano

19th European Conference for Mathematics for Industry
ECMI 2016

ECMath
Einstein Center
for Mathematics Berlin

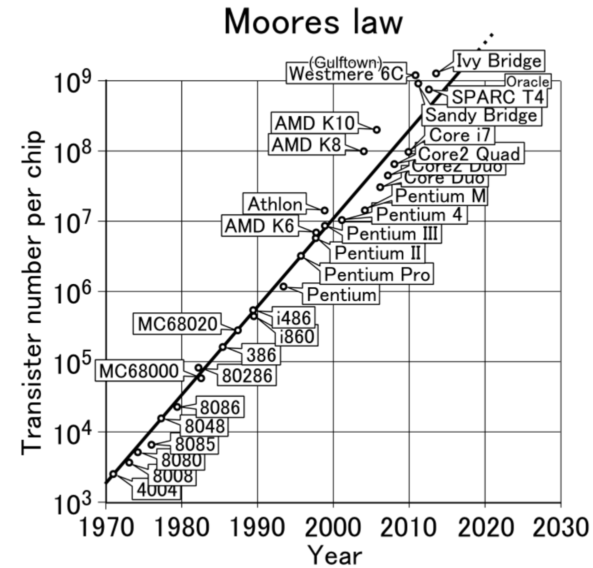
Research Center Matheon
Mathematics for Key Technologies

Outline

1. Motivation
2. Heuristic Improvement
3. Doping Optimization
4. Topology Optimization

1. Motivation

Moore’s law comes to an end …

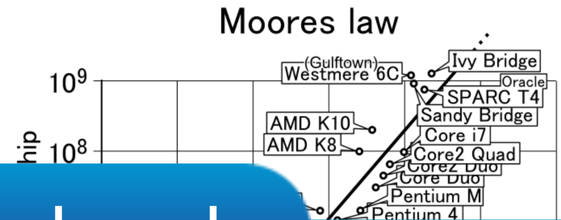


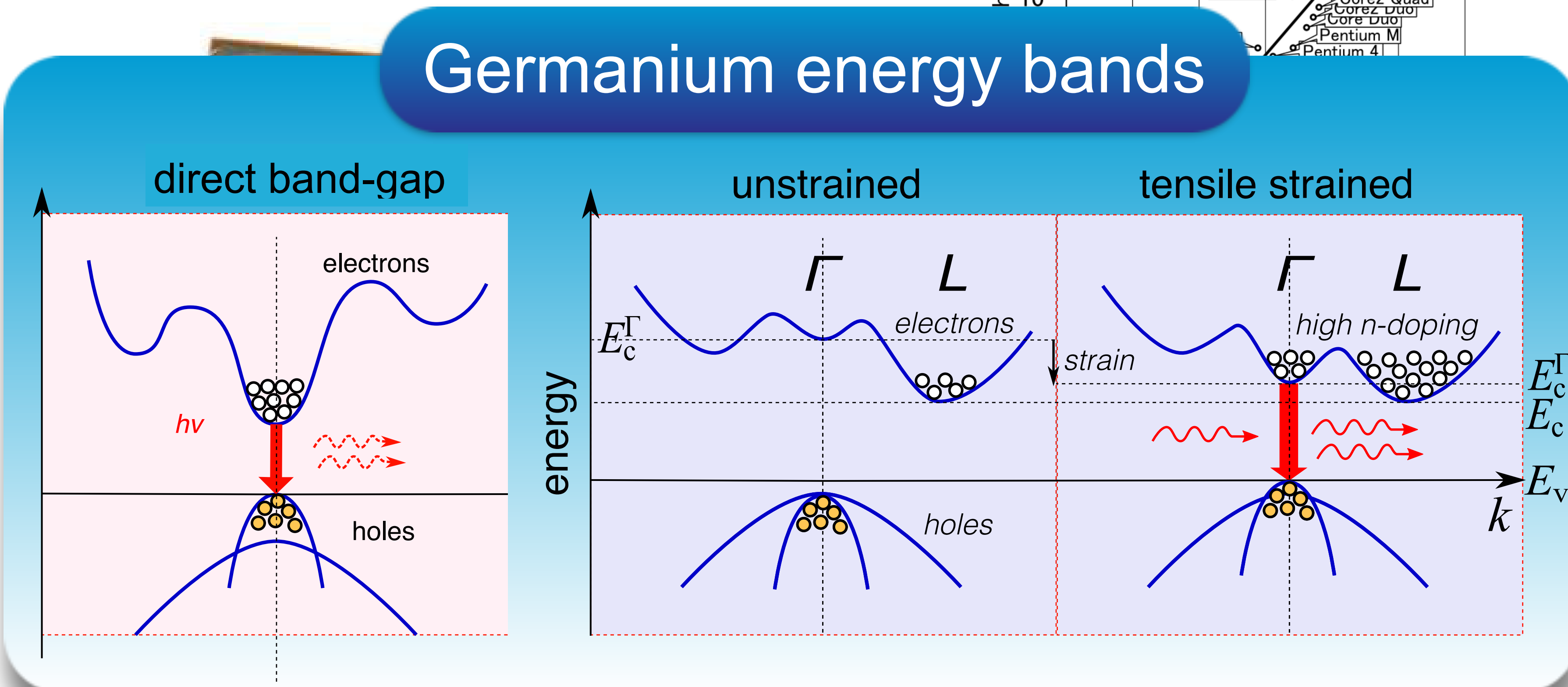
#transistors doubles every 2 years

… which is why we want More than Moore, i.e., provide added value functionalities on Si-chip.

Our goal: Monolithically integrated photonics
Problem: Bulk Si and Ge do not emit light!

Moore’s law comes to an end …





Problem: Bulk Si and Ge do not emit light!

Motivation - germanium based approaches

2012

An electrically pumped germanium laser

Rodolfo E. Camacho-Aguilera,[1] Yan Cai,[1] Neil Patel,[1] Jonathan T. Bessette,[1] Marco Romagnoli,[1,2] Lionel C. Kimerling,[1] and Jurgen Michel[1,*]

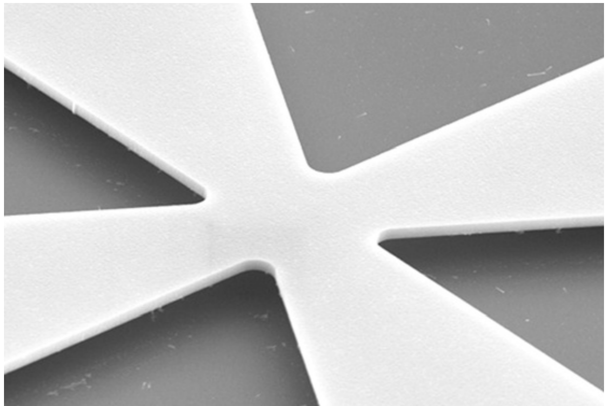
[1]*Massachusetts Institute of Technology, 77 Massachusetts Ave., Cambridge, MA 02139, USA*
[2]*PhotonIC Corporation, 5800 Uplander Way, Los Angeles, CA 90230, USA*
**jmichel@mit.edu*

Abstract: Electrically pumped lasing from Germanium-on-Silicon pnn heterojunction diode structures is demonstrated. Room temperature multimode laser with 1mW output power is measured. Phosphorous doping in Germanium at a concentration over $4\text{x}10^{19}\text{cm}^{-3}$ is achieved. A Germanium gain spectrum of nearly 200nm is observed.

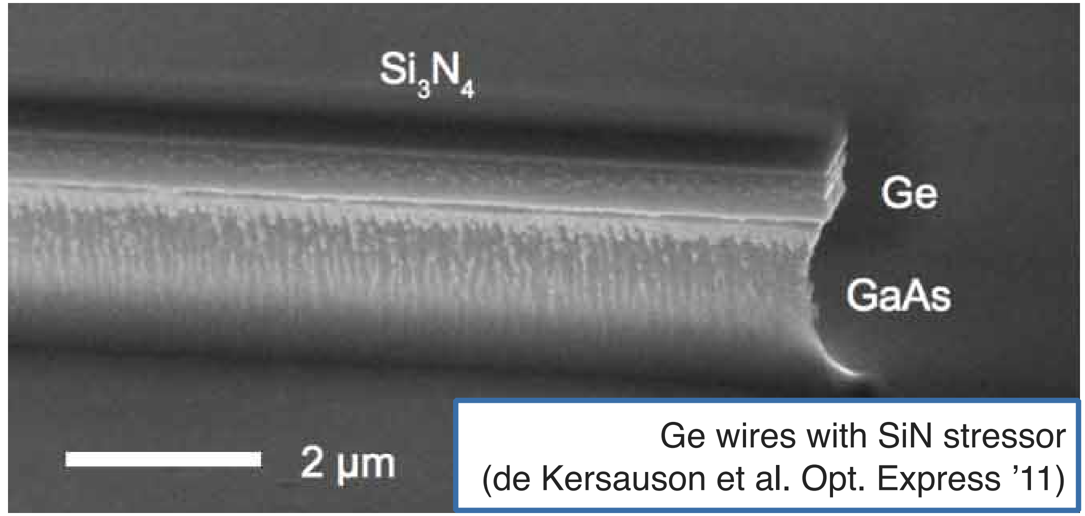
OCIS codes: (140.2020) Diode lasers; (140.3380) Laser materials; (140.5960) Semiconductor lasers; (160.3130) Integrated optics materials.

short integration times to assure wide spectrum analyses. Measurement time for these large laser devices is ultimately limited by metal contact breakdown due to the high current flow. Figure 2(a) shows no spectral features above the noise floor. When the injection current

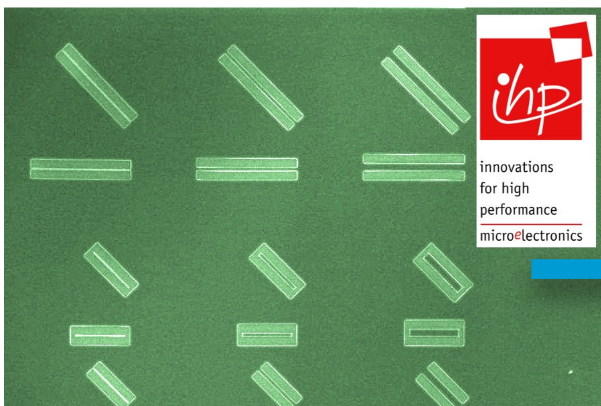
Motivation - germanium based approaches



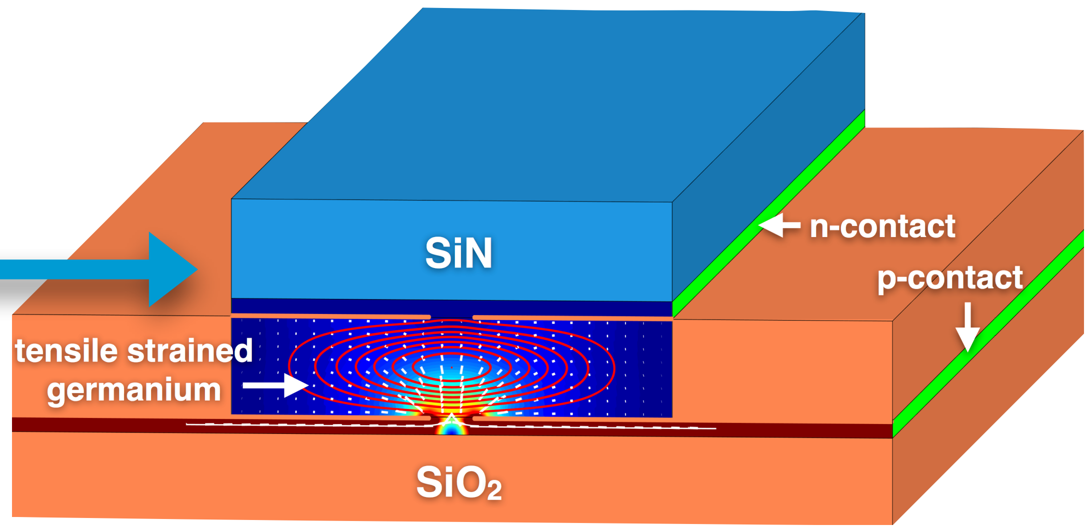
suspended Ge structures
(from Gassenq et al. APL ’15)



Ge wires with SiN stressor
(de Kersauson et al. Opt. Express ’11)



CMOS fabricated Ge microstrip
(from Capellini et al. Opt. Express ’14)



MATHEON D-OT1
www.wias-berlin.de/projects/ECMath-OT1

2. Heuristic Improvement

Heuristic Improvement

Topology Optimization

Optimize material distribution to maximize gain via band gaps

Elasticity

$$\mathrm{div}\Big(\mathbb{C} : (e(u) - e_0) + \sigma_0\Big) = 0 \quad \text{(E)}$$

Doping Optimization

optimize doping to maximize gain / minimize threshold currents

band edges: $E_\mathrm{c}(e), E_\mathrm{v}(e)$ **Upscaling** optical gain: $g(\xi;\omega,e)$

Optoelectronic PDE Model

van Roosbroeck

$$\begin{aligned} -\nabla\cdot\varepsilon\nabla\psi &= q(C+p-n) \\ -\nabla\cdot\mu_n n\nabla\phi_n &= +R \\ -\nabla\cdot\mu_p p\nabla\phi_p &= -R \end{aligned} \quad \text{(vR)}$$

Helmholtz Equation

$$\left[\nabla^2 + \frac{\omega^2}{c^2}\varepsilon_r(\xi;\omega,e)\right]\Theta = \beta^2\Theta \quad \text{(H)}$$

Photon Number Equation

$$\dot{S} = v_\mathrm{g}(2\mathrm{Im}\beta - \alpha_\mathrm{c})S + \dot{S}_\mathrm{sp} \quad \text{(Ph)}$$

Recombination & equations of state in (vR)

$$R = v_\mathrm{g} g(\xi;\omega,e)|\Theta|^2 S + \widetilde{R}$$

$$n = n_c\mathcal{F}\left(\frac{q(\psi-\phi_n)-E_c(e)}{k_BT}\right)$$

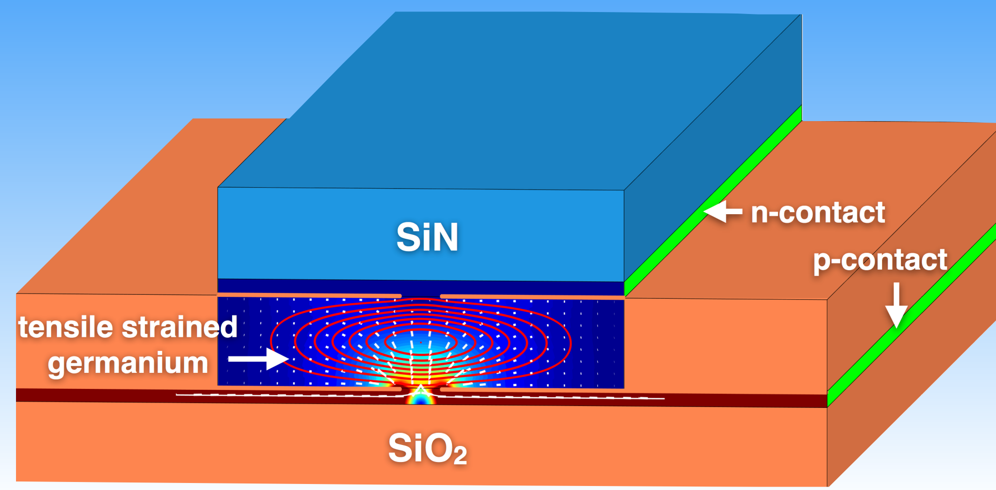
$$p = n_v\mathcal{F}\left(\frac{q(\phi_p-\psi)+E_v(e)}{k_BT}\right)$$

Permittivity in (H)

$$\varepsilon_r = \left(n_r + i\frac{c}{2\omega}\left[g - \ell\right]\right)^2$$

Unknowns

(vR)	(H)	(Ph)	(E)
$\xi = (\psi,\phi_n,\phi_p)$	(Θ,β)	S	u



Heuristic Improvement

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Upscaling

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optical gain: $g(\xi; \omega, e)$

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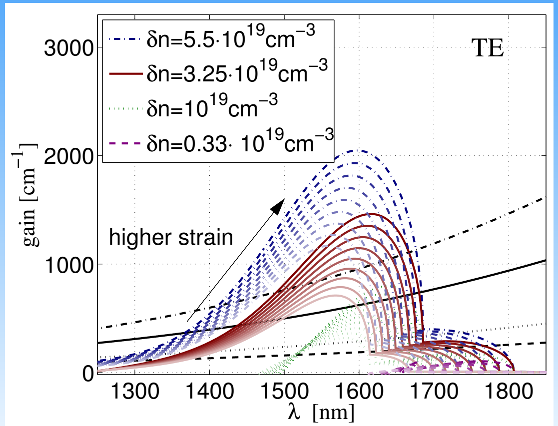
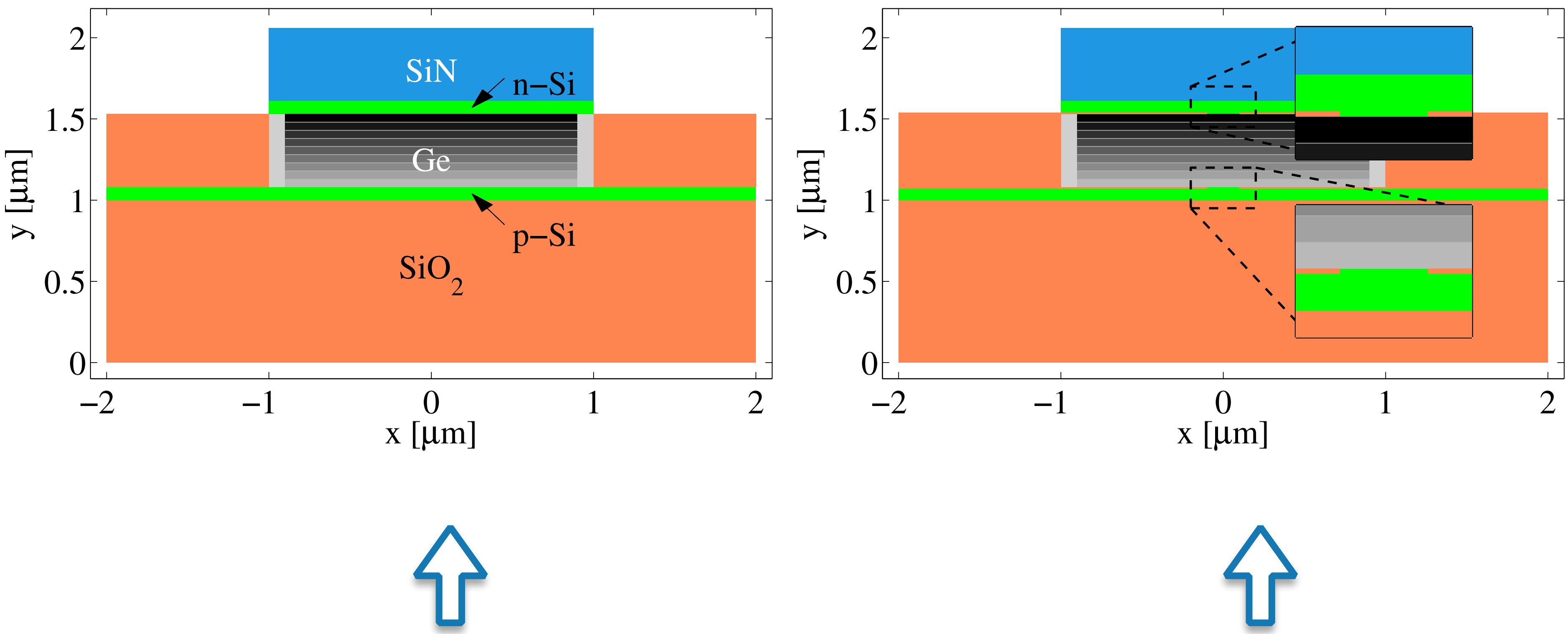


tight binding calculations: M. Virgilio

WIAS TeSCA

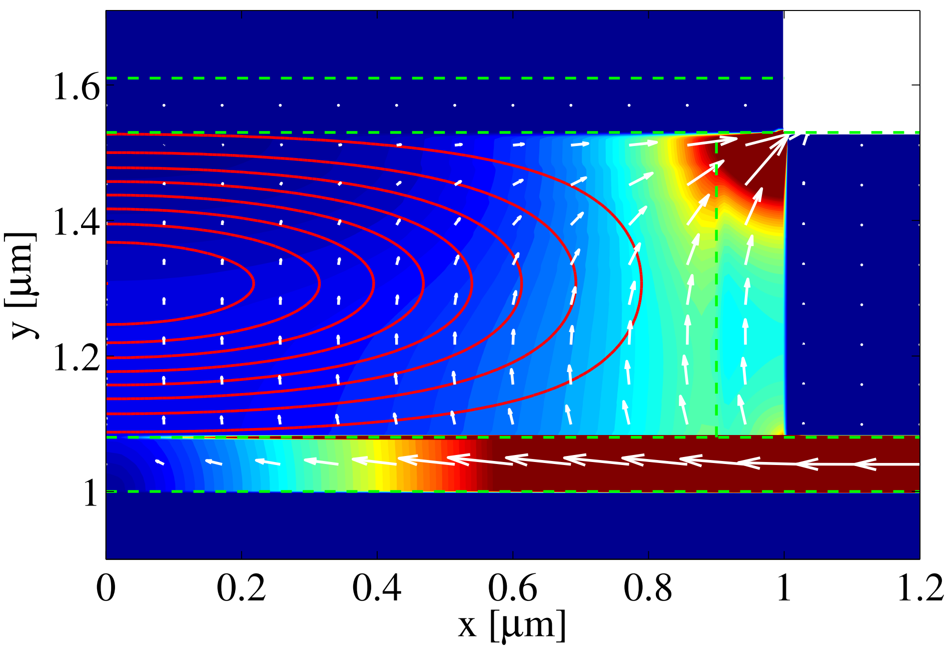


standard design

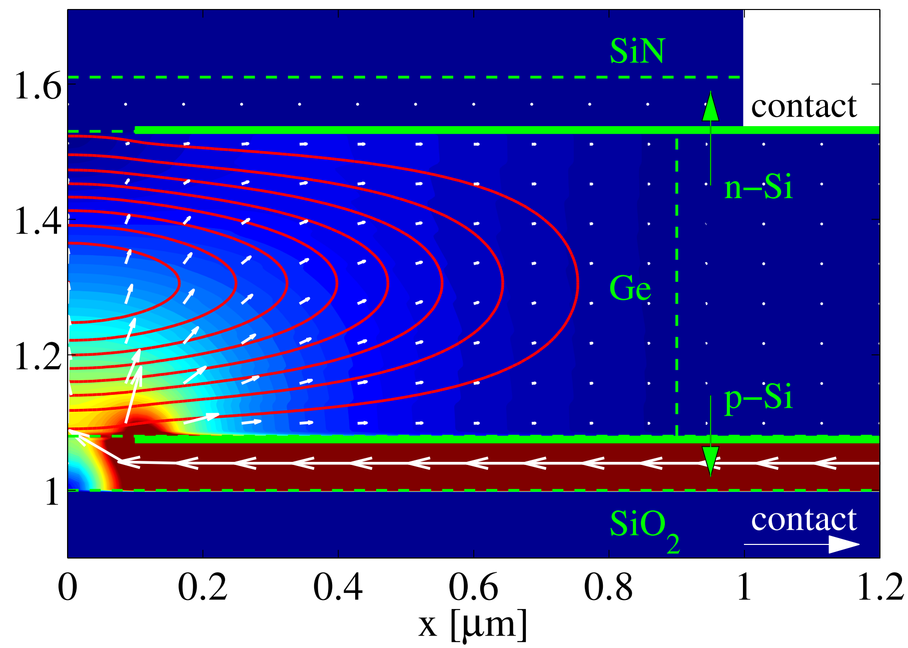
aperture design

Heuristic Improvement

WIAS TeSCA



standard design



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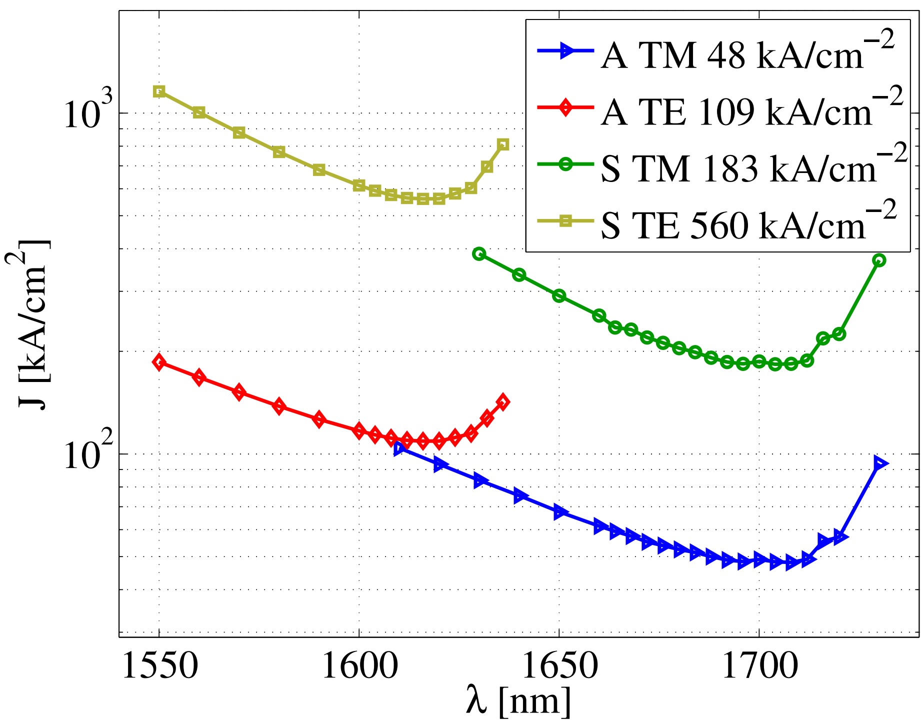
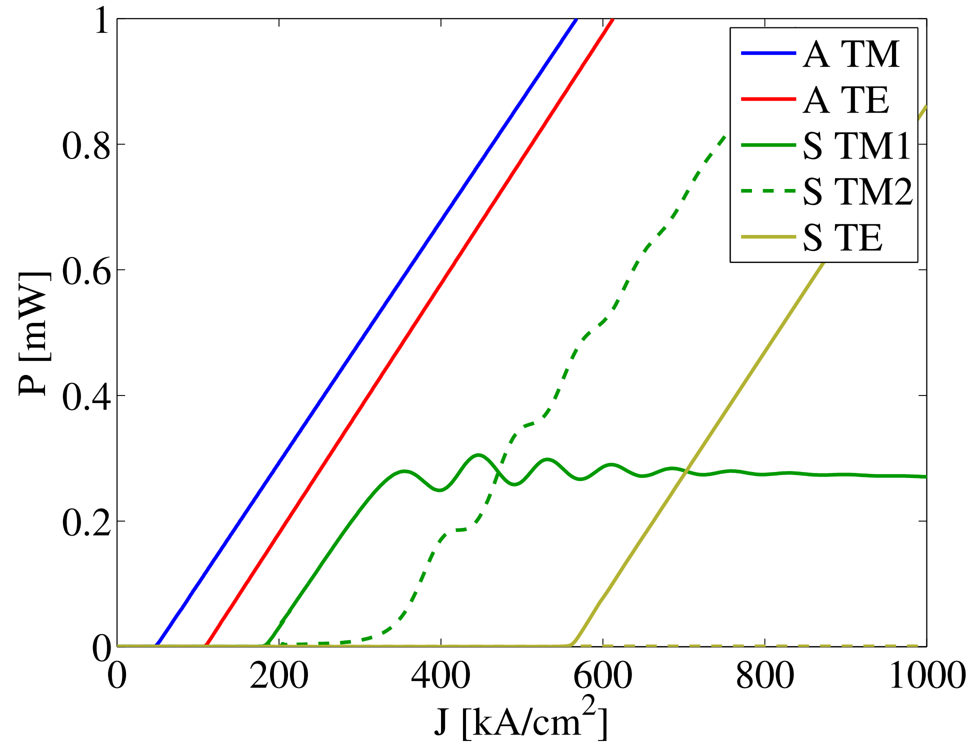
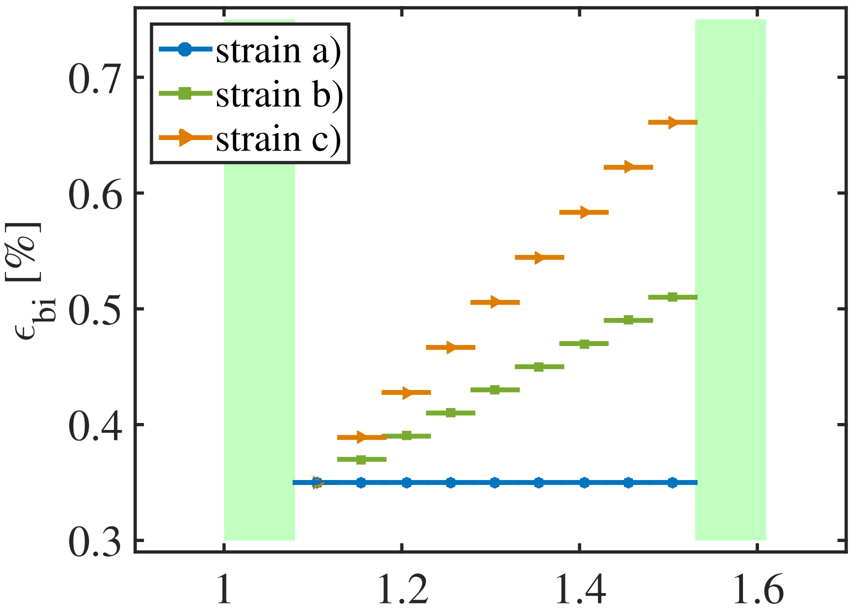
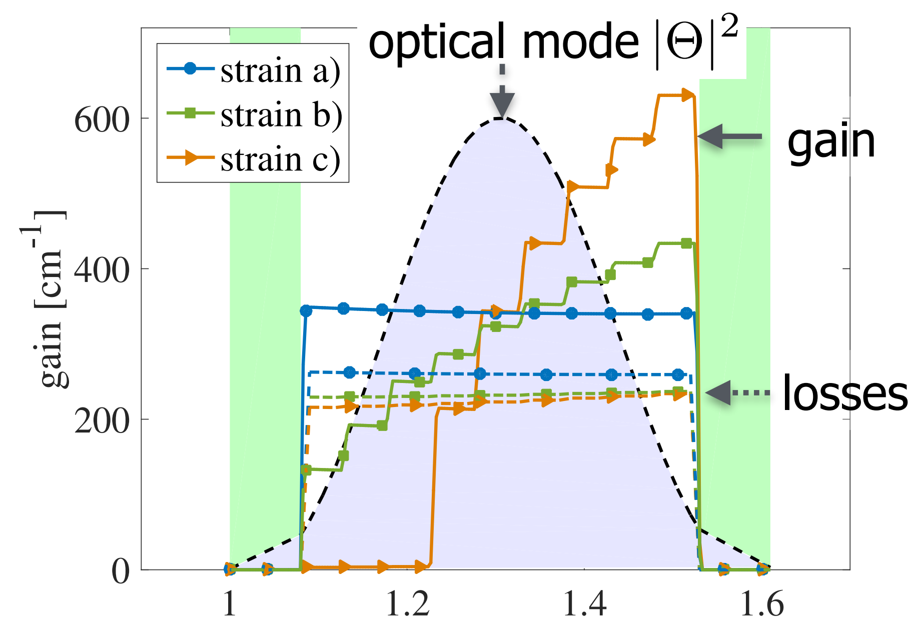




4x lower threshold current with aperture design

Heuristic Improvement





What has been learned?

$$\text{maximize} \int_{\Omega} |\Theta|^2 (\text{gain} - \text{losses})\, \mathrm{d}x$$

P, Thomas, Koprucki, Glitzky, Capellini, Guha, Schröder, Virgilio, Gärtner, Nürnberg; IEEE Photonics Journal 2015
——; IEEE Proceedings Int. Conf. Opt. Devices (NUSOD) 2015
——; Optical and Quantum Electronics 2016
——; Proceedings of „Advanced Solid State Lasers 2015"

3. Doping Optimization

References (non-extensive)

- Selberherr *„Analysis and Simulation of Semiconductor devices“*
- Markowich *„The stationary semiconductor device equations“*
- Burger & Pinnau *„Fast optimal design of semiconductor devices“*
- Hinze & Pinnau *„Second-order approach to optimal semiconductor design“, ….*
- Naumann & Wolff *„A uniqueness theorem for weak solutions of the stationary semiconductor equations“*
- *…*

Doping Optimization

Doping optimization

$$\min_{X \times \mathbf{C}} \left\{ -Q_1(\xi) + \frac{\gamma}{2} \|C - \bar{C}\|^2_{\mathbf{C}} \right\}$$

s.t. $\xi \in X$ solves (vR)

maximize gain regularize doping

$$Q_1 = \int |\Theta|^2 (g - \ell)\, \mathrm{d}x$$

Existence of sol. of (vR)

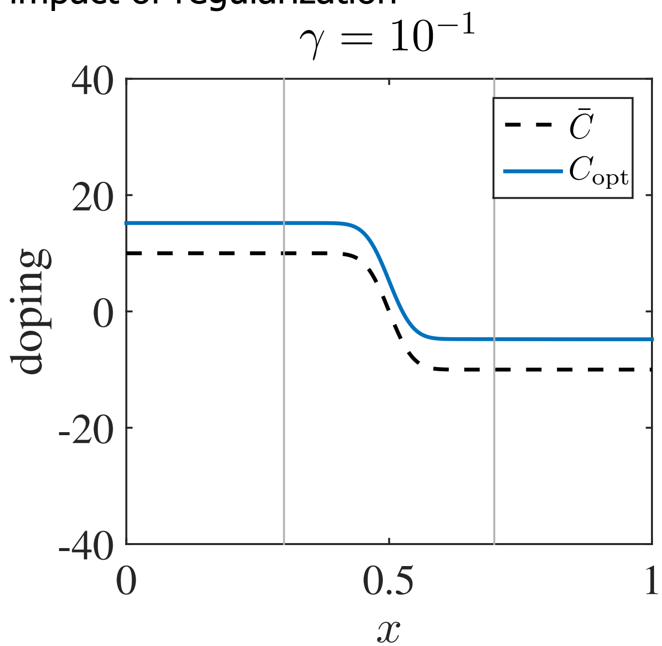
Existence of min. of **DO**

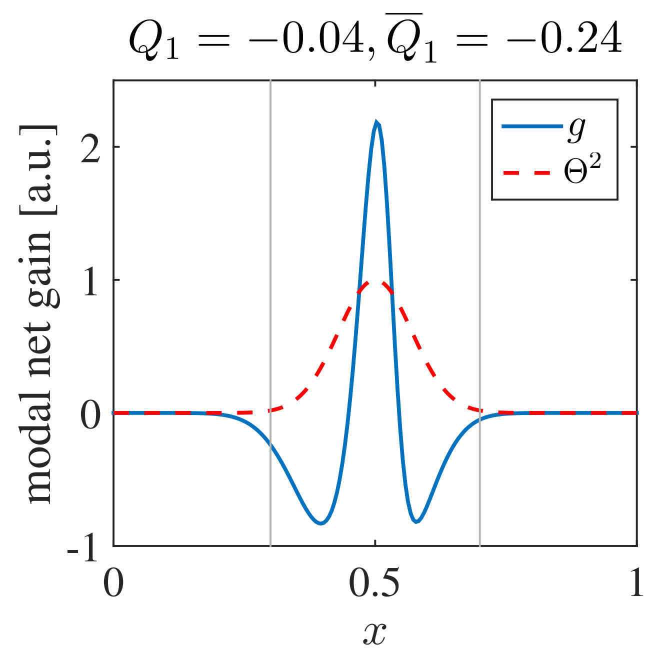
$$\mathbf{C} \in \{L^2, H^1, H^1_0\}$$

Numerics
1D FD with chem. potentials
fully coupled Newton
2nd order optimization

Rotundo, Thomas, P.
ICTT Proc. 2015
(MATHEON preprint)

impact of regularization





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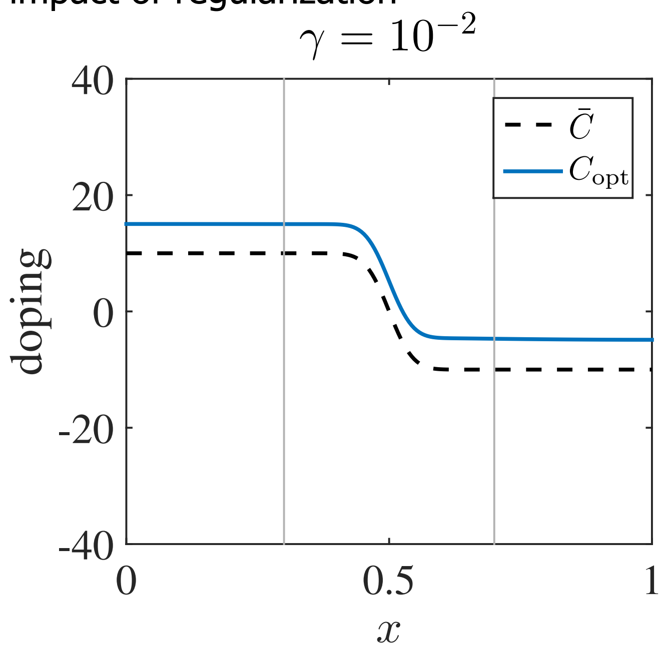

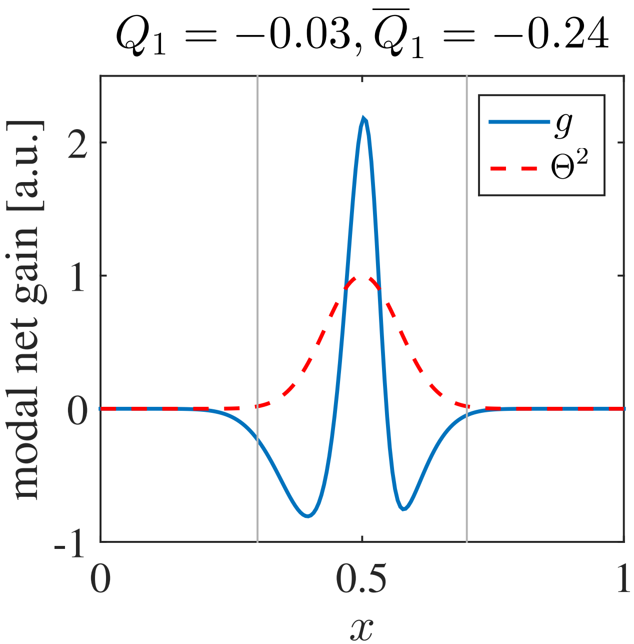

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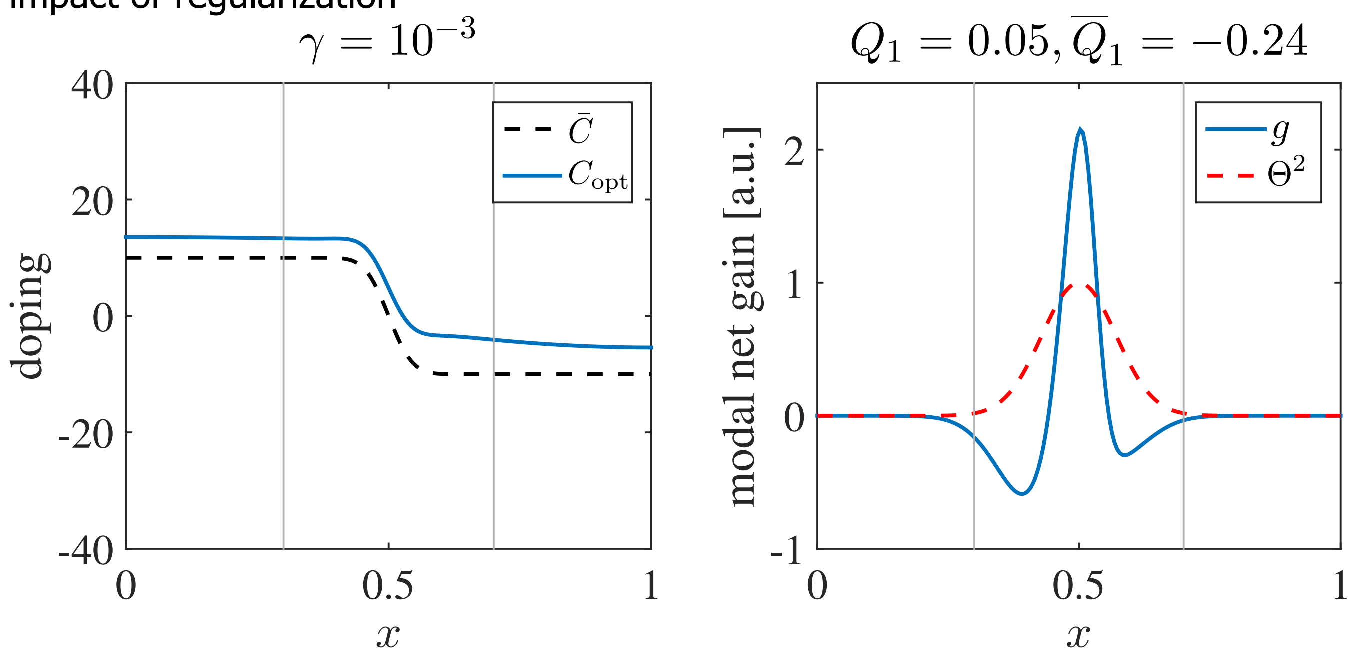

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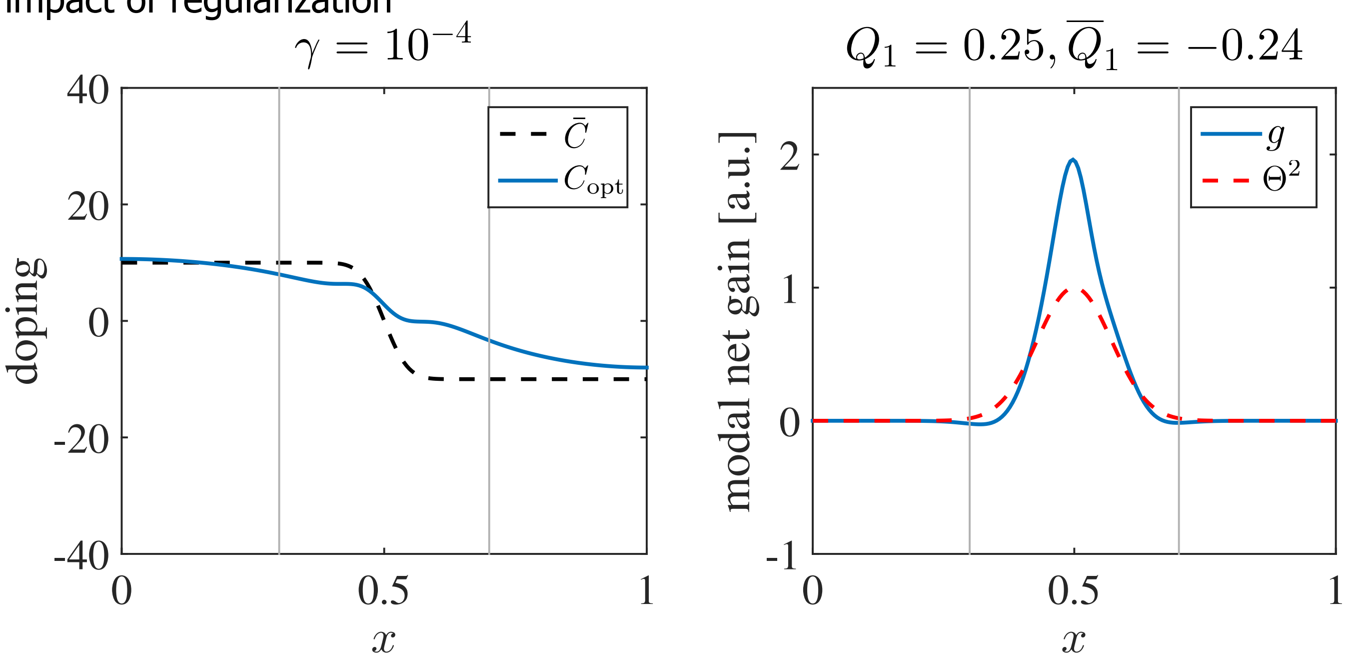

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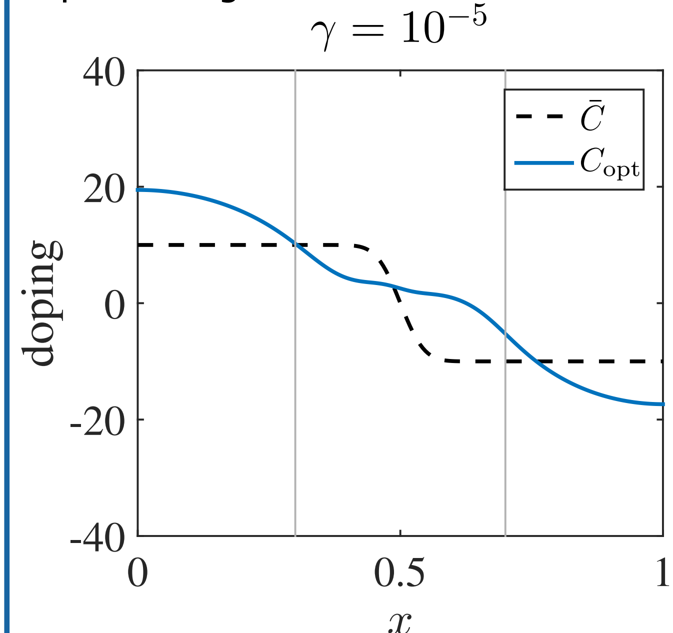

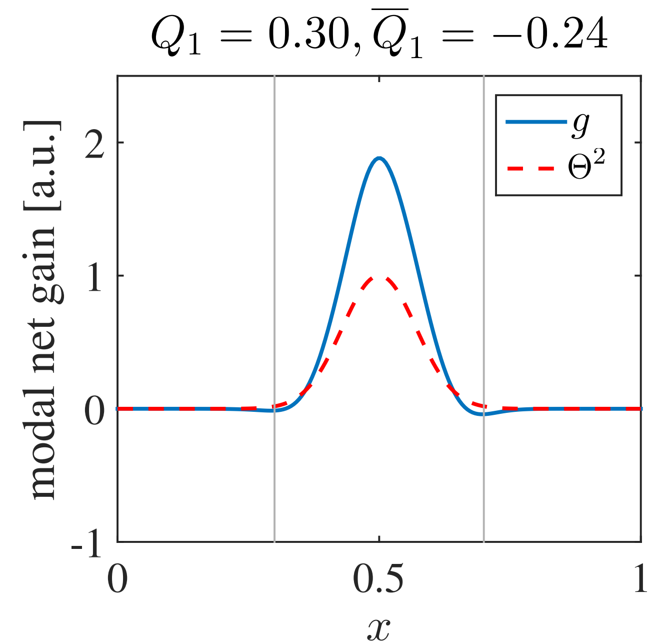

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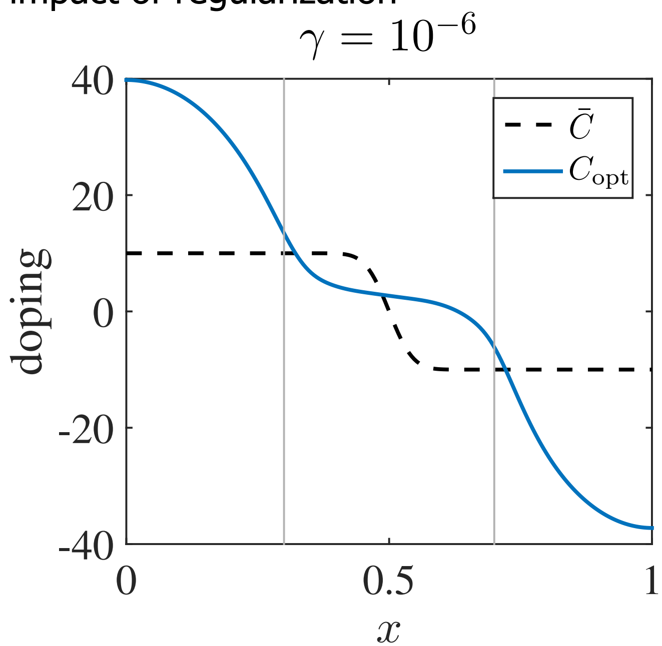

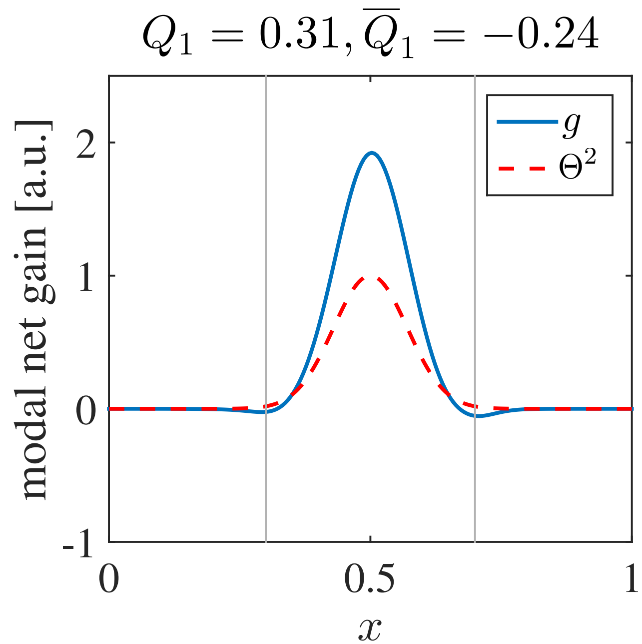

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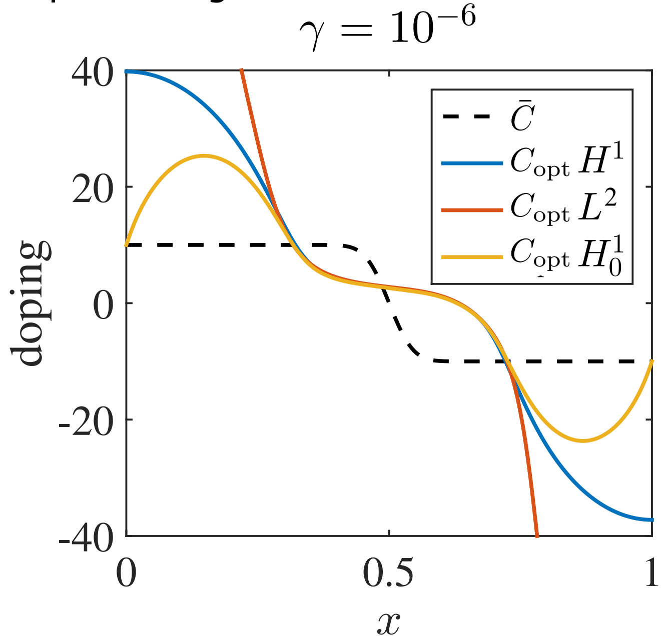

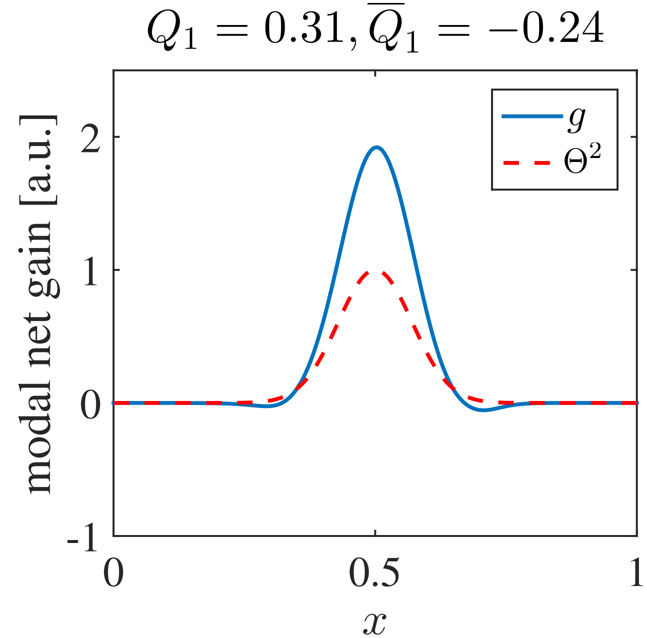

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Preliminary results
2D FEM van Roosbroeck
with no recombinations and
$\mathbf{C} = H^1_0$

Numerics
2D FEM with ch. potentials
fully coupled Newton
2nd order optimization

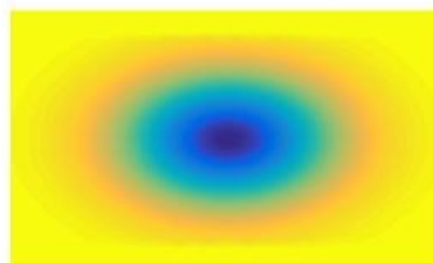
Rotundo, Thomas, P.
work in progress

impact of regularization

$\gamma = 10^0$

$Q_1 = -1.7$

$|\Theta|^2(g - \ell)$

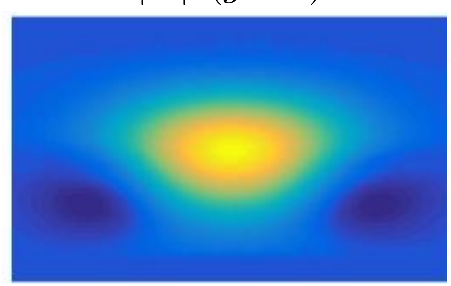


$C_{\mathrm{opt}} \approx \bar{C}$

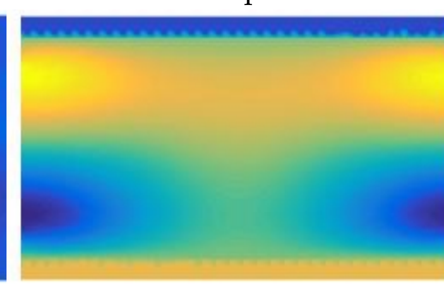
$\gamma = 10^{-4}$

$Q_1 = +0.21$

$|\Theta|^2(g - \ell)$



C_{opt}



4. Topology Optimization

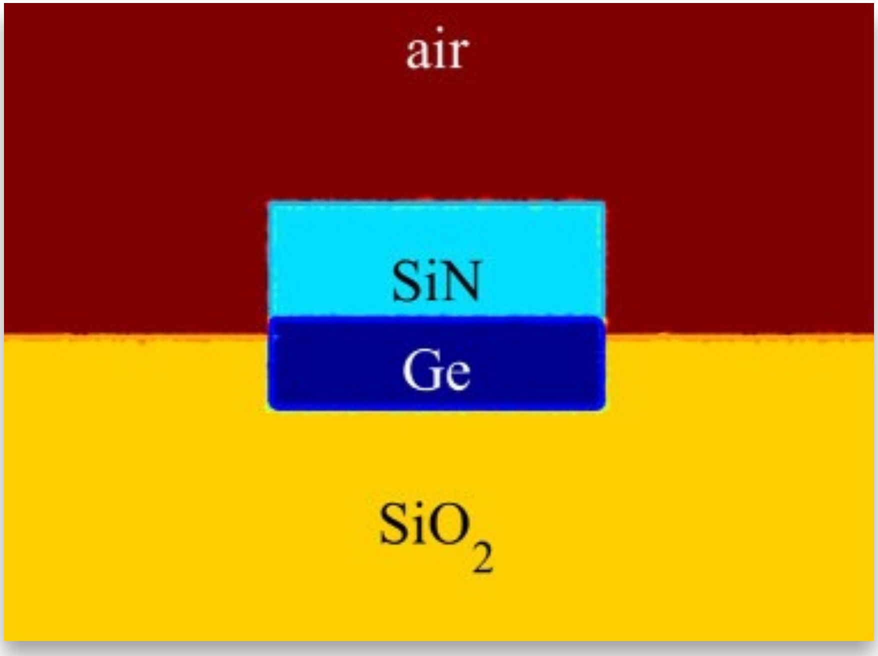
Elasticity:

$$\mathrm{div}\,(\mathbb{C} : (e(u) - e_0) + \sigma_0) = 0$$

$$\mathbb{C}(x) = \sum_{\alpha \in \{\mathrm{Ge}, \mathrm{SiN}, \mathrm{SiO_2}, \mathrm{air}\}} \mathbb{C}_\alpha \, \varphi_\alpha(x)$$

$$e_0(x) = e_0^{\mathrm{Ge}} \, \varphi_{\mathrm{Ge}}(x)$$

$$\sigma_0(x) = \sigma_0^{SiN} \, \varphi_{\mathrm{SiN}}(x)$$



Effect on band-edges:

$$F(e) = \int_D \left(\beta_1 e_{xx} + \beta_2 e_{yy}\right) \mathrm{d}x$$

Design encoded in φ

Topology optimization

$$\min_{\varphi} F\big(e(\mathbf{u})\big) + \frac{\alpha}{2}\int_{\Omega} \frac{\epsilon}{2}|\nabla\varphi|^2 + \frac{1}{2\epsilon}W(\varphi)\,\mathrm{d}x$$

s.t.

$$\nabla\cdot\big[\mathbb{C}(\varphi):\big(e(\mathbf{u})-e_0(\varphi)\big)+\sigma_0(\varphi)\big]=0$$

$$\varphi\in\mathcal{G}=\{\varphi:\varphi\geq 0,\sum_i\varphi=1\text{ a.e.}\}$$

Goals

- maximize bi- and uniaxial strain in optical cavity D
- strain affects band edges via

$$F(e)=\int_D\big(\beta_1 e_{xx}+\beta_2 e_{yy}\big)\,\mathrm{d}x$$

Method

- phase field [Blank,Garcke,Farshbaf-Shaker,Styles]
- Why? Flexible for modelling/optimization

Properties

- non-convex & nonlinear

Topology optimization

Theoretical results

- Sensitivity of $\varphi \mapsto u$ (cont. Fréchet diff. $(H^1)^N \to (H^1_0)^2$)
- Existence of optimal topology $\bar{\varphi}$
- First-order optimality conditions (p solves adjoint equation):

$$\alpha \int \epsilon \nabla\varphi : \nabla(\hat{\varphi} - \varphi) + \frac{1}{2\epsilon}(1 - 2\varphi) : (\hat{\varphi} - \varphi)\, \mathrm{d}x$$
$$+ \int \left[\mathbb{C}'(\varphi)(\hat{\varphi} - \varphi)\right] e(\mathbf{u}) : e(p)\, \mathrm{d}x - l'_{\varphi}(\varphi, p)(\hat{\varphi} - \varphi) \geq 0 \text{ for all } \hat{\varphi} \in \mathcal{G}$$

Algorithms

- First-order methods: gradient flow, projected gradients
- Second-order methods: full Newton method, interior point

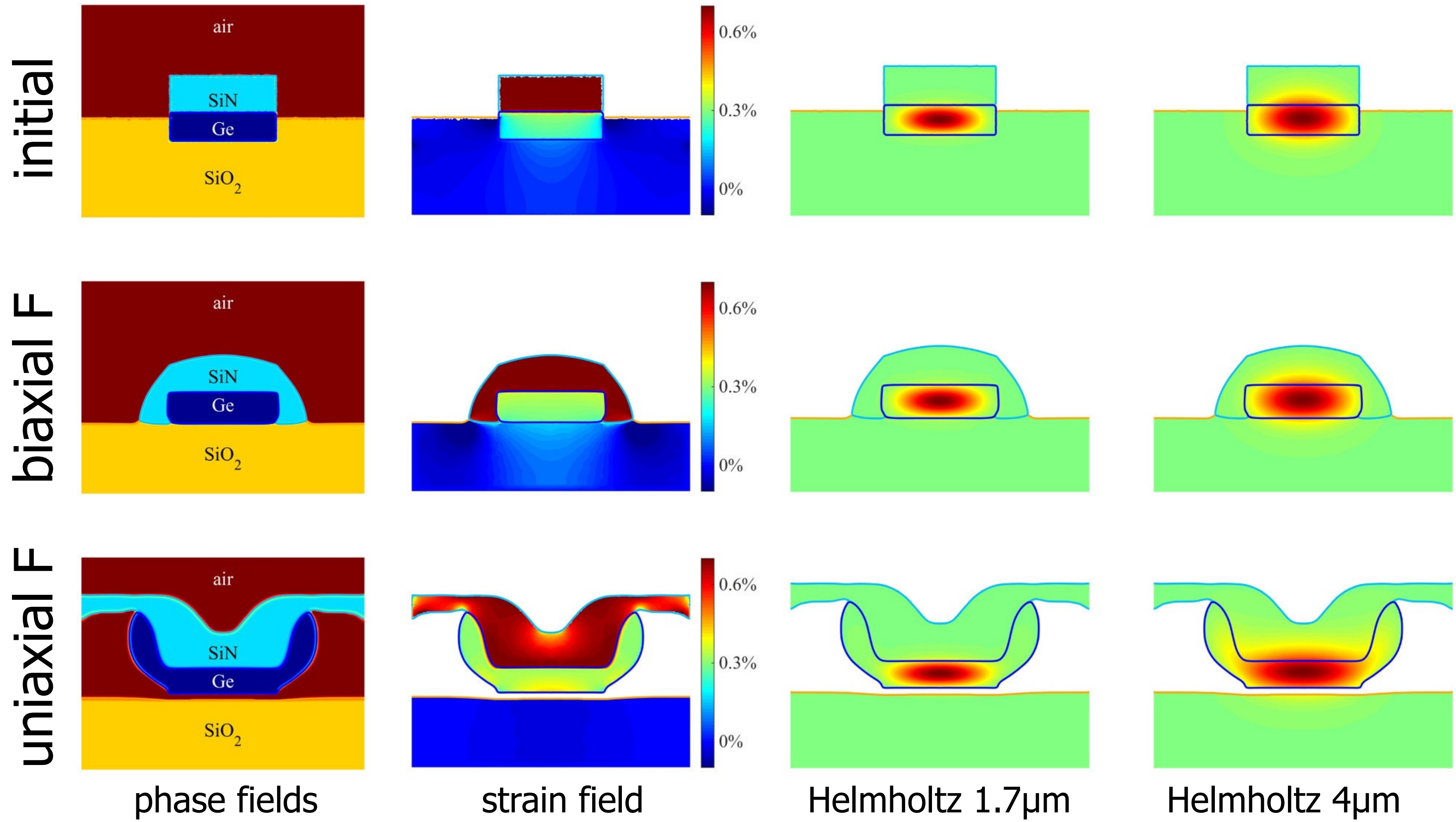
projected gradients

- fast prototype development
- transfer to IHP

interior points

- fast second order method
- tuning mesh/reg./pen. parameter

Topology optimization FEM

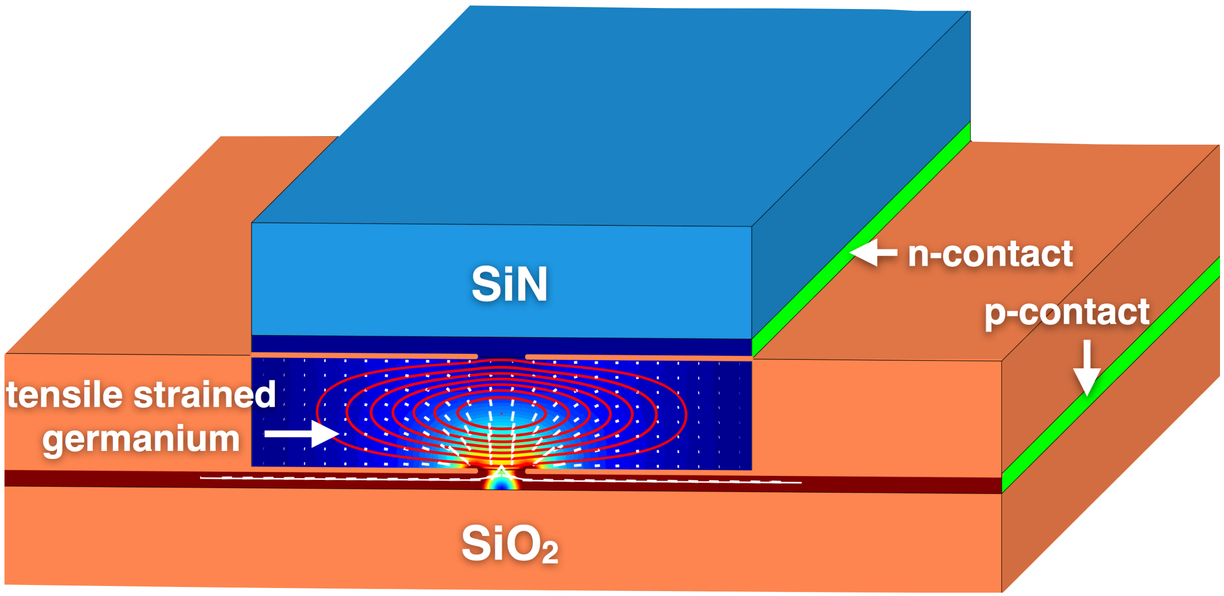


Summary

- heuristic optimization >>> overlap engineering
- doping optimization >>> dependence on regularization
- topology optimization >>> uniaxial vs biaxial

Outlook

- doping optimization (2D FEM/FVM on heterostructure with optics)
- topology optimization and optics (EVP+elasticity+phase fields)
- topology optimization and doping optimization ***in the loop***



Thank you