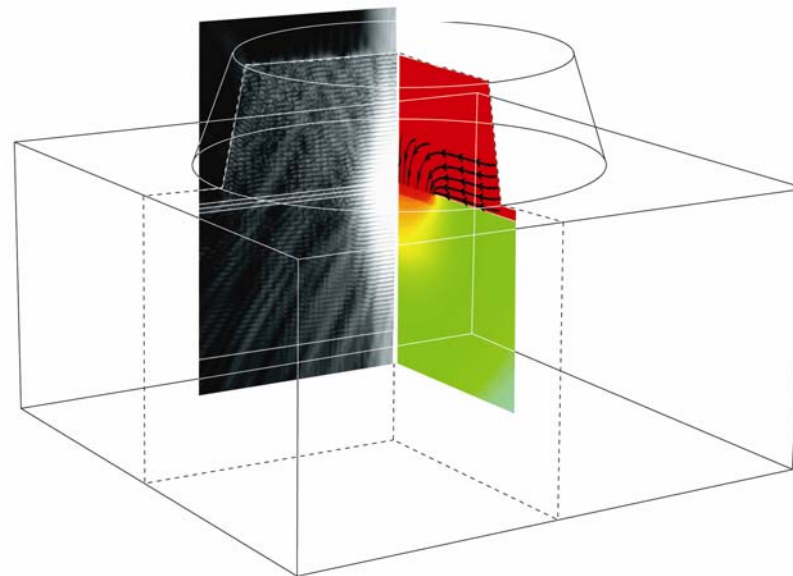


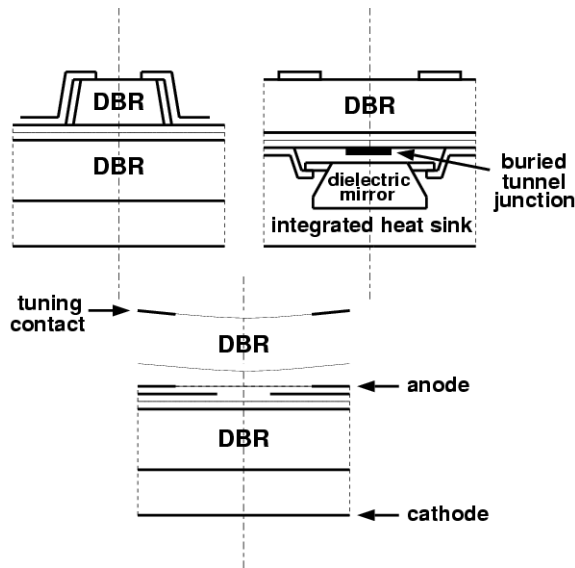
Microscopic Opto-Electro-Thermal VCSEL Device Simulation

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NUSOD'04, UCSB, 25 August 2004, 1.00pm

Device Structures



Interdependent Design Tasks

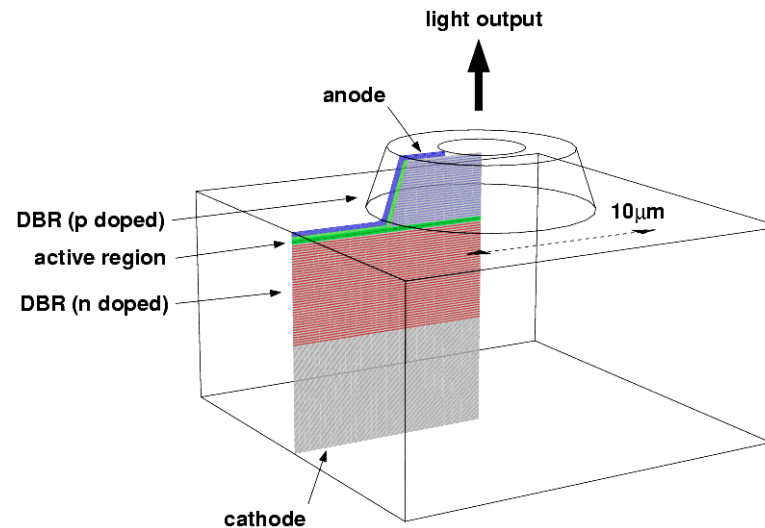
- (single) mode control
- output power
- thermal design
- cavity / gain peak alignment
- modulation / transient response
- current / mode confinement
- farfield control

Physics

- Optics:
large (optical length), complex structure, gain and loss (material and radiation)
- Electronics:
bulk, heterojunction, and QW carrier transport, self-heating

Material Systems

- AlGaAs/GaAs (750-1050nm)
InGaAlAs/InP, InGaAsP/InP,
InGaNaAs/GaAs (1300,1550nm)
- with given electronic, thermal, optical properties



Coupled Problem

- optical, electronic, and thermal problems are coupled!
- problems have different length scales and solutions have different behaviour (wave propagation & diffusive)

The Coupled Electro-Thermo-Optical Simulator:

- Microcavity Optical Problem
- Electro-Thermal Transport
- Self-Consistent Solution of Coupled System of Equations

Applications:

- Optimisation of Optical Microcavity
- Coupled Electro-Thermo-Optical VCSEL Analysis
- Calibration and Numerical Performance of VCSEL Model

Conclusions

Acknowledgements

Semi-classical Approach: Classical Maxwell and QM Polarization

$$\nabla \times \mu_r^{-1}(\mathbf{r}) \cdot [\nabla \times \mathbf{E}(\mathbf{r}, t)] + \frac{1}{c_0^2} \frac{\partial^2}{\partial t^2} [\varepsilon_r(\mathbf{r}, t, \tau) * \mathbf{E}(\mathbf{r}, t - \tau)] = \mathbf{F}(\mathbf{r}, t)$$

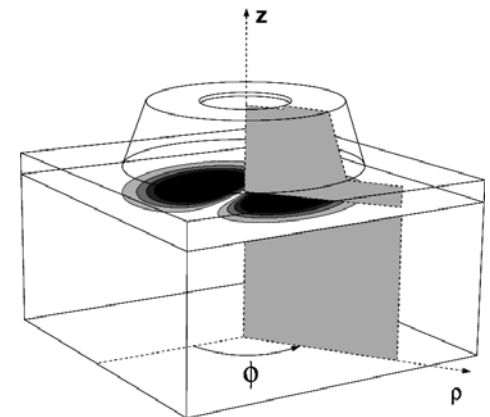
Expansion in Eigenfrequencies, Slowly Varying Amplitude Approximation, and Adiabatic Dielectrics Yields:

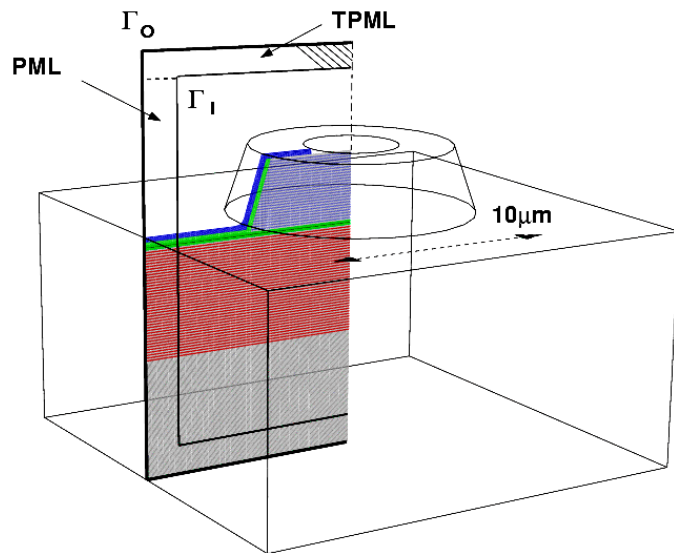
Complex Helmholtz Equation (3D!):
$$\nabla \times \mu_r^{-1}(\mathbf{r}) \cdot [\nabla \times \underline{\mathbf{E}}_k(\mathbf{r}, t)] = \frac{\omega_k^2(t)}{c_0^2} \varepsilon_r(\mathbf{r}, t, \omega_k) \cdot \underline{\mathbf{E}}_k(\mathbf{r}, t)$$

Photon Rate Equation:
$$\frac{d}{dt} S_k(t) = -2\omega_k''(t) S_k(t) + R_k^{sp}(t)$$

Body of Revolution transforms 3D Helmholtz to set of 2D Solutions:

$$\begin{aligned} \underline{\mathbf{E}}_s(\rho, \phi, z) &= \underline{\mathbf{E}}_{T,0}(\rho, z) \\ &+ \sum_{m=1}^{\infty} [\underline{\mathbf{E}}_{T,m}(\rho, z) \cos m\phi + E_{\phi,m}(\rho, z) \mathbf{e}_{\phi} \sin m\phi] \\ \underline{\mathbf{E}}_a(\rho, \phi, z) &= E_{\phi,0}(\rho, z) \mathbf{e}_{\phi} \\ &+ \sum_{m=1}^{\infty} [\underline{\mathbf{E}}_{T,-m}(\rho, z) \sin m\phi + E_{\phi,-m}(\rho, z) \mathbf{e}_{\phi} \cos m\phi] \end{aligned}$$





EM Radiation Effects pertinent for mode control:

Perfectly Matched Layers (PML) as “Free-Space” boundary conditions

Introduce anisotropic magnetic Permeability:

$$\Lambda(\mathbf{r}) = \begin{bmatrix} \Lambda_x(\mathbf{r}) & 0 & 0 \\ 0 & \Lambda_y(\mathbf{r}) & 0 \\ 0 & 0 & \Lambda_z(\mathbf{r}) \end{bmatrix}$$

$$\varepsilon_r(\mathbf{r}, \omega) = \varepsilon'_r(\mathbf{r}, \omega) + i\varepsilon''_r(\mathbf{r}, \omega)$$

Helmholtz Equation:

$$\nabla \times \Lambda^{-1}(\mathbf{r}) \cdot (\nabla \times \underline{\mathbf{E}}(\mathbf{r})) = \frac{\omega^2}{c_0^2} \Lambda(\mathbf{r}) \varepsilon_r(\mathbf{r}) \cdot \underline{\mathbf{E}}(\mathbf{r})$$

Output Power and Energy Transfer Rate through Top Aperture:

$$P_{out} = \iiint_{TPML} \langle \nabla \cdot \mathbf{S}(\mathbf{r}) \rangle dV \quad L_{out,k} = \frac{\iiint_{TPML} \langle \nabla \cdot \mathbf{S}_k(\mathbf{r}) \rangle dV}{\iiint_O \langle w_k(\mathbf{r}) \rangle dV}$$

Variational Functional of modified Helmholtz Equation:

$$F(\underline{\mathbf{E}}) = \frac{1}{2} \int_0^{2\pi} \int_0^{\rho} \int_0^z \left[(\nabla \times \underline{\mathbf{E}}) \cdot \Lambda^{-1} \cdot (\nabla \times \underline{\mathbf{E}}) - \frac{\omega^2}{c_0^2} \underline{\mathbf{E}} \cdot \varepsilon_r \Lambda \cdot \underline{\mathbf{E}} \right] \rho d\phi d\rho dz$$

Rayleigh-Ritz: insert Edge Node Finite Element Basis:

$$\underline{\mathbf{E}}_{T,m}(\rho, z) = \sum_{i=1}^{3,4} \varphi_{Ti}^e \mathbf{N}_i^e(\rho, z) \quad E_{\phi,m}(\rho, z) = \sum_{i=1}^{3,4} \varphi_{\phi i}^e N_i^e(\rho, z)$$

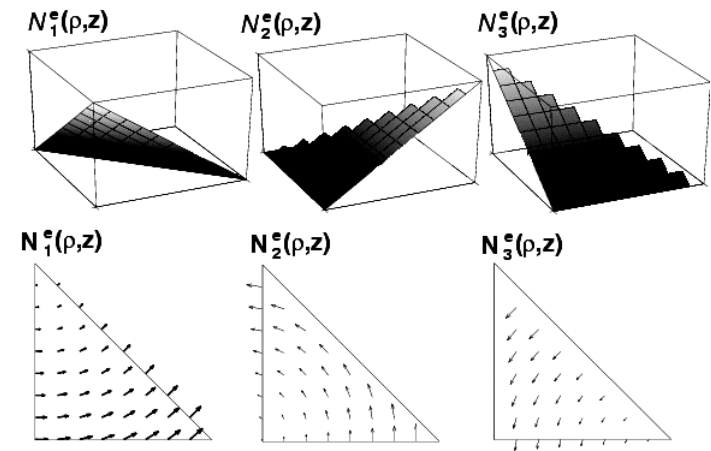
Build Variational: $\frac{\delta F}{\delta \underline{\mathbf{E}}} = 0$

Sparse Matrix Eigenproblem:

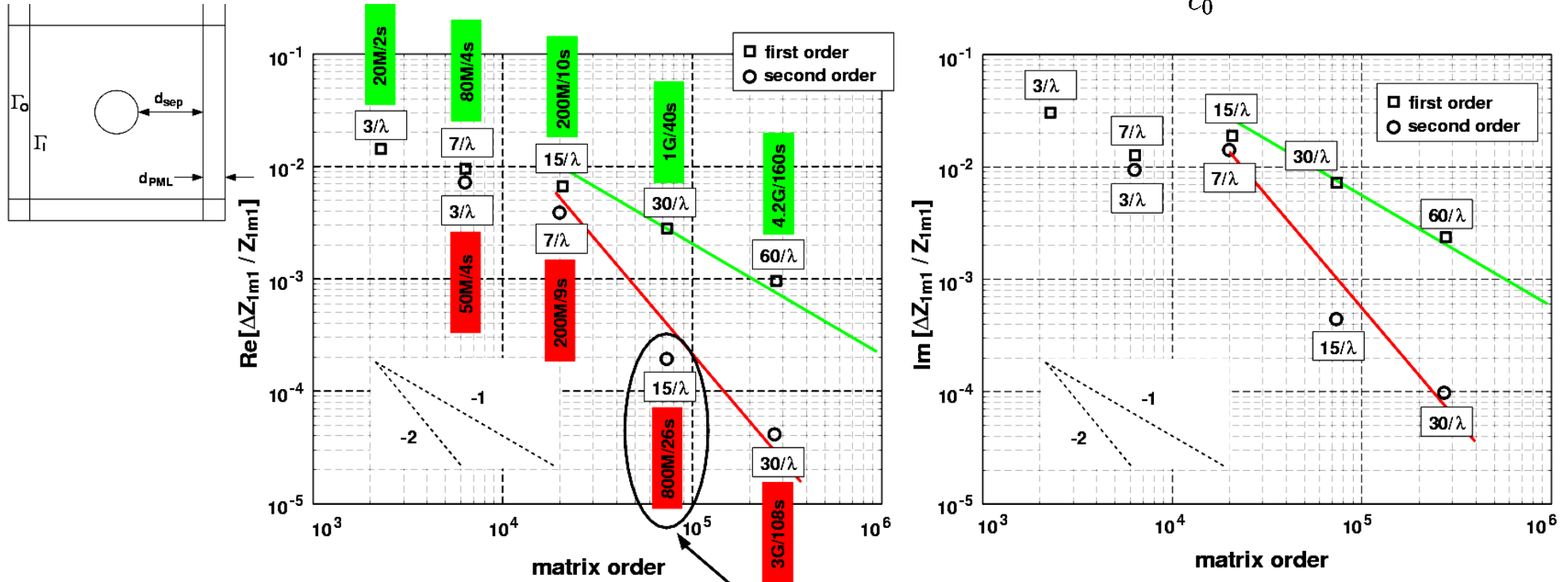
$$\begin{bmatrix} A_{TT,m} & A_{T\phi,m} \\ A_{\phi T,m} & A_{\phi\phi,m} \end{bmatrix} \cdot \begin{Bmatrix} \varphi_{T,m,k} \\ \varphi_{\phi,m,k} \end{Bmatrix} = \frac{\omega_k^2}{c_0^2} \begin{bmatrix} B_{TT,m} & B_{T\phi,m} \\ B_{\phi T,m} & B_{\phi\phi,m} \end{bmatrix} \cdot \begin{Bmatrix} \varphi_{T,m,k} \\ \varphi_{\phi,m,k} \end{Bmatrix}$$

Optical modes: Inner Eigenpairs of large sparse generalised complex symmetric Eigenproblem.

Complex Frequency $\omega_k = \omega'_k - i\omega''_k$ Re: Resonance Freq. Im: Field Decay Rate



Free dielectric sphere (radiation boundary condition), with eigenvalue: $Z_{nmr} = \frac{\sqrt{\epsilon_r \mu_r}}{c_0} r_0 (\omega'_{nmr} - i\omega''_{nmr})$



Bulk Carrier and Heat Transport:

- Thermodynamic model

Poisson $\nabla \cdot (\varepsilon \nabla \phi) = -e (p - n + N_D^+ - N_A^-)$

Continuity
$$\begin{aligned} \nabla \cdot \mathbf{j}_n &= e \left(R + \frac{\partial}{\partial t} n \right) \\ -\nabla \cdot \mathbf{j}_p &= e \left(R + \frac{\partial}{\partial t} p \right) \\ -\nabla \cdot \mathbf{S} &= H + c_{th} \frac{\partial}{\partial t} T \end{aligned}$$

Current
$$\begin{aligned} \mathbf{j}_n &= -en\mu_n (\nabla \phi_n + P_n \nabla T) \\ \mathbf{j}_p &= -ep\mu_p (\nabla \phi_p + P_p \nabla T) \\ \mathbf{S} &= -\kappa_{th} \nabla T \end{aligned}$$

Carrier Transport at Heterojunctions:

- single junctions: thermionic emission model
- DBR stacks: artificial material with effective carrier and heat conductivity

Carrier Transport at Quantum Wells:

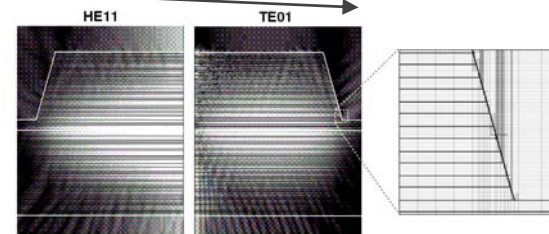
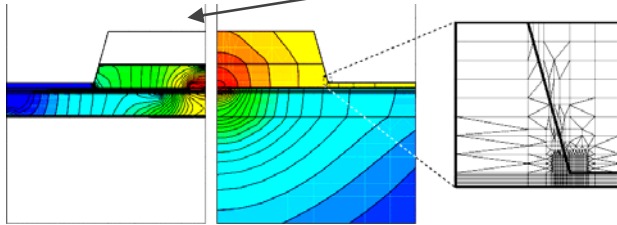
- treatment as scattering center (normal to QW), carrier capture and escape rate equation, equilib. distribution for continuum and bound carriers
- thermodynamic model (in QW plane)
- $H = \text{Joule heat} + \text{Thomson/Peltier heat} + \text{recombination heat}$

- Drift-diffusion + self-heating, carriers and lattice in local thermal equilibrium.
- Rate equations for quantum transport.
- Box Method formulation of discretised equations.

Assume $\tau_{\text{mod}} \gg \tau_{\text{ph}} \Rightarrow$ slowly varying amplitude approximation, using frequency domain ansatz:

$$\nabla \times \mu_r^{-1}(\mathbf{r}) \cdot [\nabla \times \mathbf{E}(\mathbf{r}, t)] + \frac{1}{c_0^2} \frac{\partial^2}{\partial t^2} [\varepsilon_r(\mathbf{r}, t, \tau) * \mathbf{E}(\mathbf{r}, t - \tau)] = \mathbf{F}(\mathbf{r}, t)$$

electro-
thermal
domain



optical
domain

Photon Rate Equation (lumped circuit equation)

$$\frac{d}{dt} S_k(t) = -2\omega_k''(t) S_k(t) + R_k^{sp}(t)$$

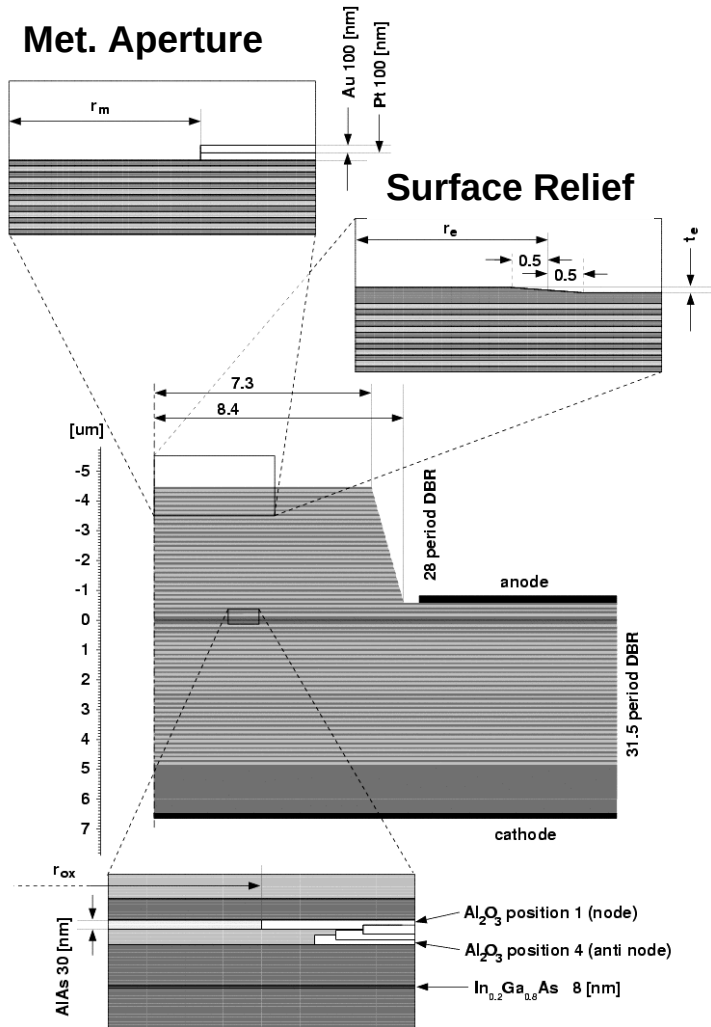
+ Electro-Thermal Equations (device equations)

- “Slow” time scale (ns).
- Inhomogeneous mesh density.
- Solve coupled System of Equations on electro-thermal mesh by Newton-Raphson scheme.

Vectorial Helmholtz Equation

$$\nabla \times \mu_r^{-1}(\mathbf{r}) \cdot [\nabla \times \mathbf{E}_k(\mathbf{r}, t)] = \frac{\omega_k^2(t)}{c_0^2} \varepsilon_r(\mathbf{r}, t, \omega_k) \cdot \mathbf{E}_k(\mathbf{r}, t)$$

- Normalised mode patterns.
- “Fast” time scale (fs) in frequency domain.
- More homogeneous mesh density.
- Solve using JDOZ with preconditioner $\mathbf{M} = (\mathbf{A} - \lambda \mathbf{B})^{-1}$ and guess λ .



Device:

- AlGaAs/GaAs,
top 28 / bottom 31.5 DBR pairs
- Lasing Wavelength 980 nm

Simulation (approx.):

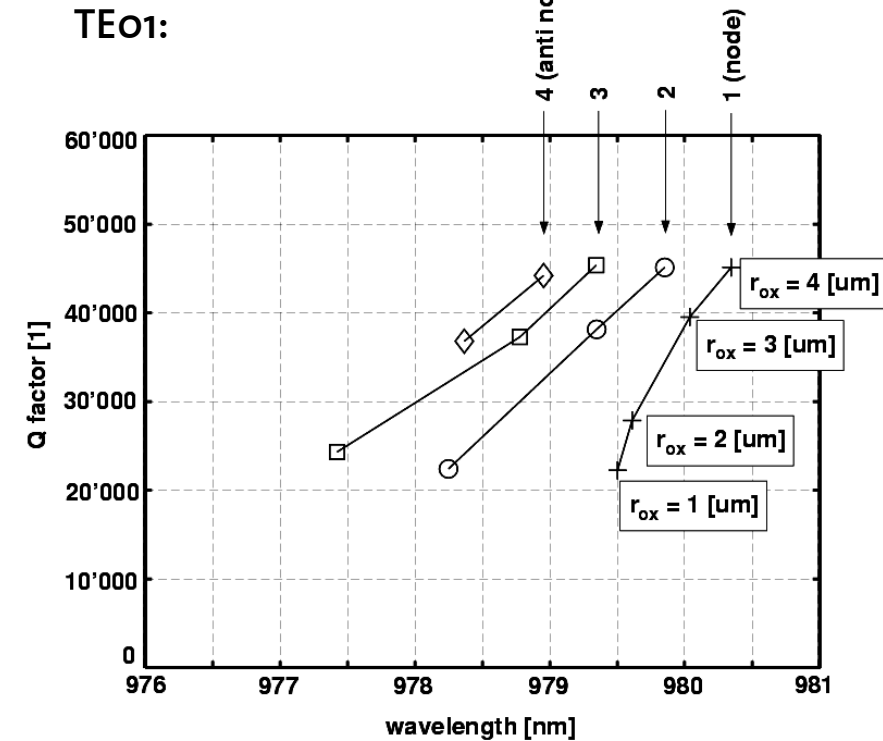
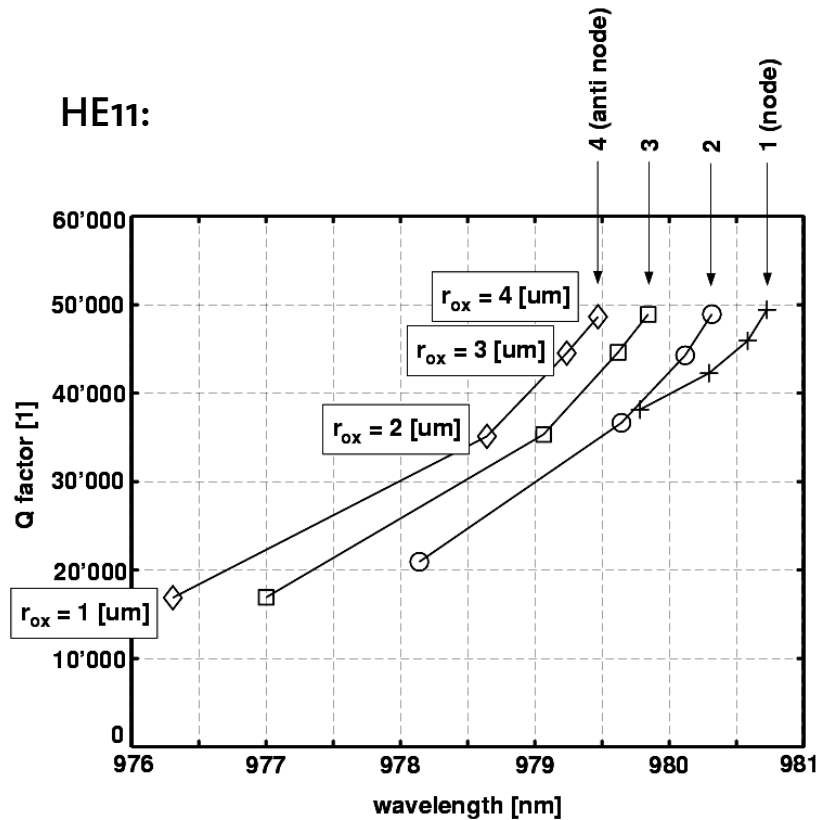
- Only Optical Simulation
- 160'000 FE (2nd order), 30/ λ resolution
- order 2M, 15 GBytes, 12 min.

3 Design Features:

- Oxide Placement (node -> antinode)
- Metallic Top Aperture (absorber)
- Surface Relief (anti-resonant structure)

- Typical VCSEL design task inaccessible to scalar solvers, can be handled by mode solver.
- High accuracy requires increased but tolerable computational resources.

plain cavity



- Anti node oxide produces strongest effect (blue shift and diffraction losses) upon reducing radius of oxide aperture; node oxide the weakest effect.
- For strong optical confinements cavity becomes single mode (TE₀₁ is cut off).

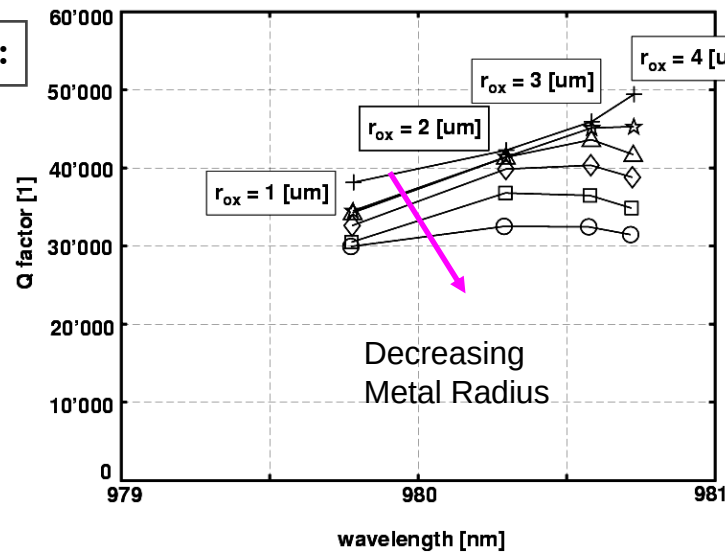
Design Case: Metal Aperture and Surface Relief

12/19

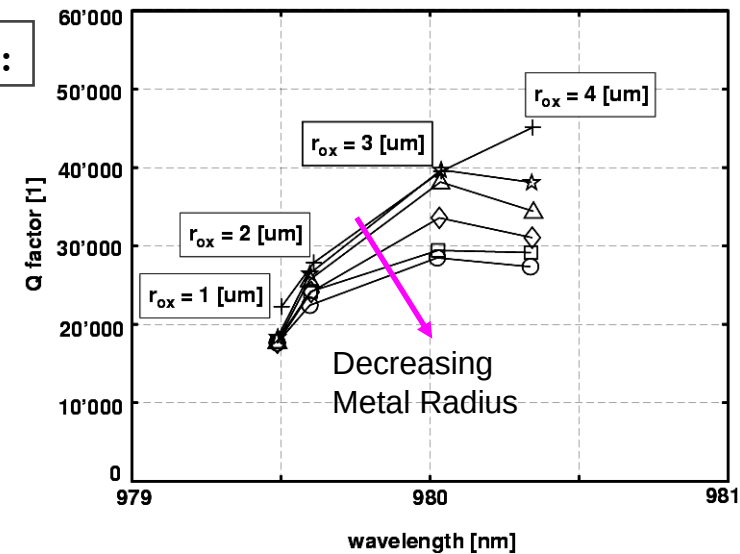
Metal

node oxide,
plus: no absorber,
r: 3.5 μm (star)
... 1.5 μm (circle)

HE11:



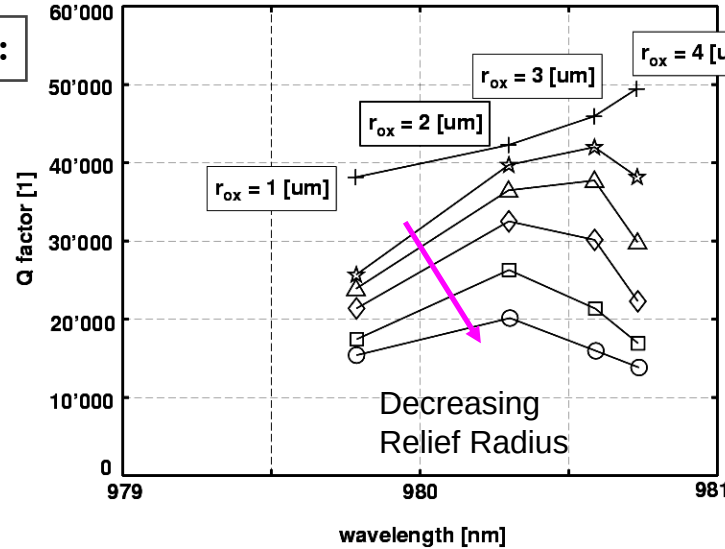
TE01:



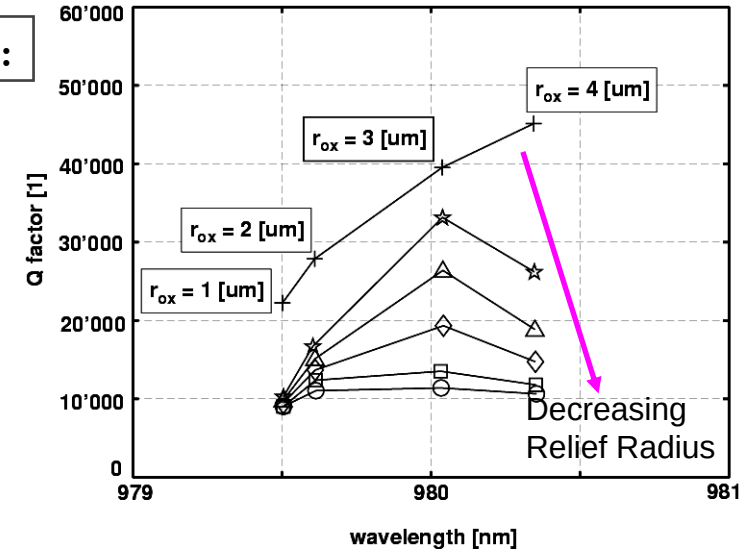
Surface Relief

node oxide,
plus: no relief,
r: 3.5 μm (star)
... 1.5 μm (circle)

HE11:



TE01:



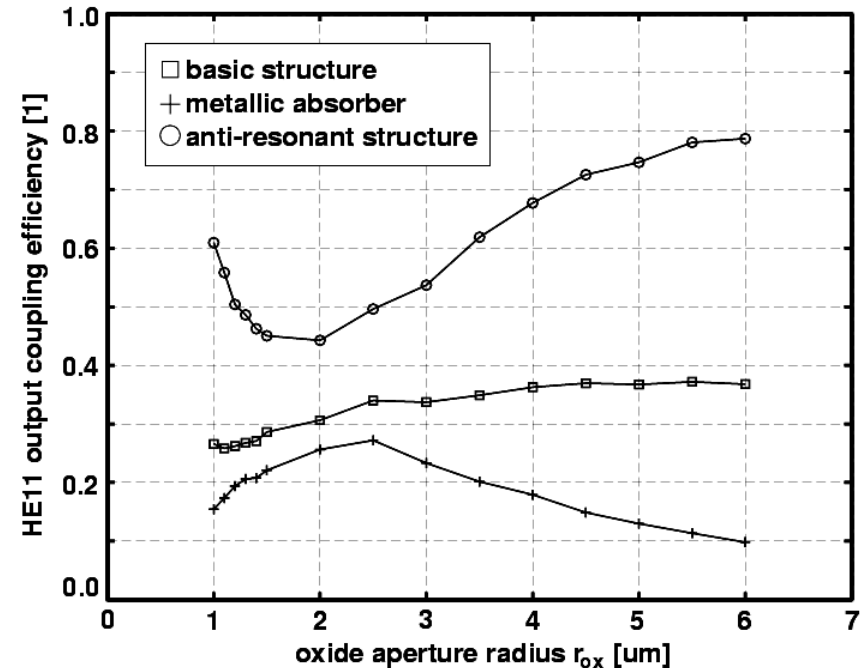
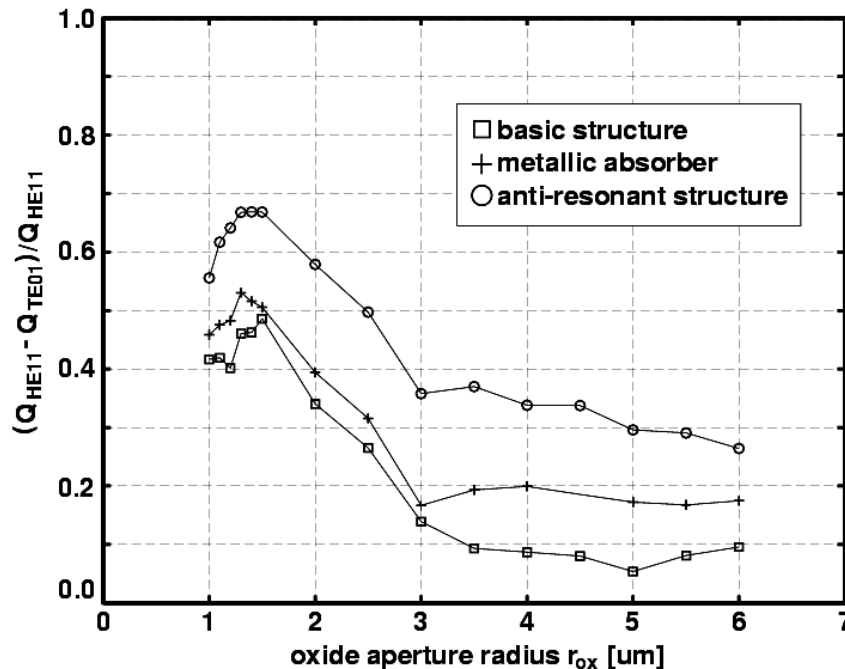
metal: $r = 2.5 \text{ } \mu\text{m}$

anti-resonant structure: $r = 2.5 \text{ } \mu\text{m}$, $d = 72 \text{ nm}$

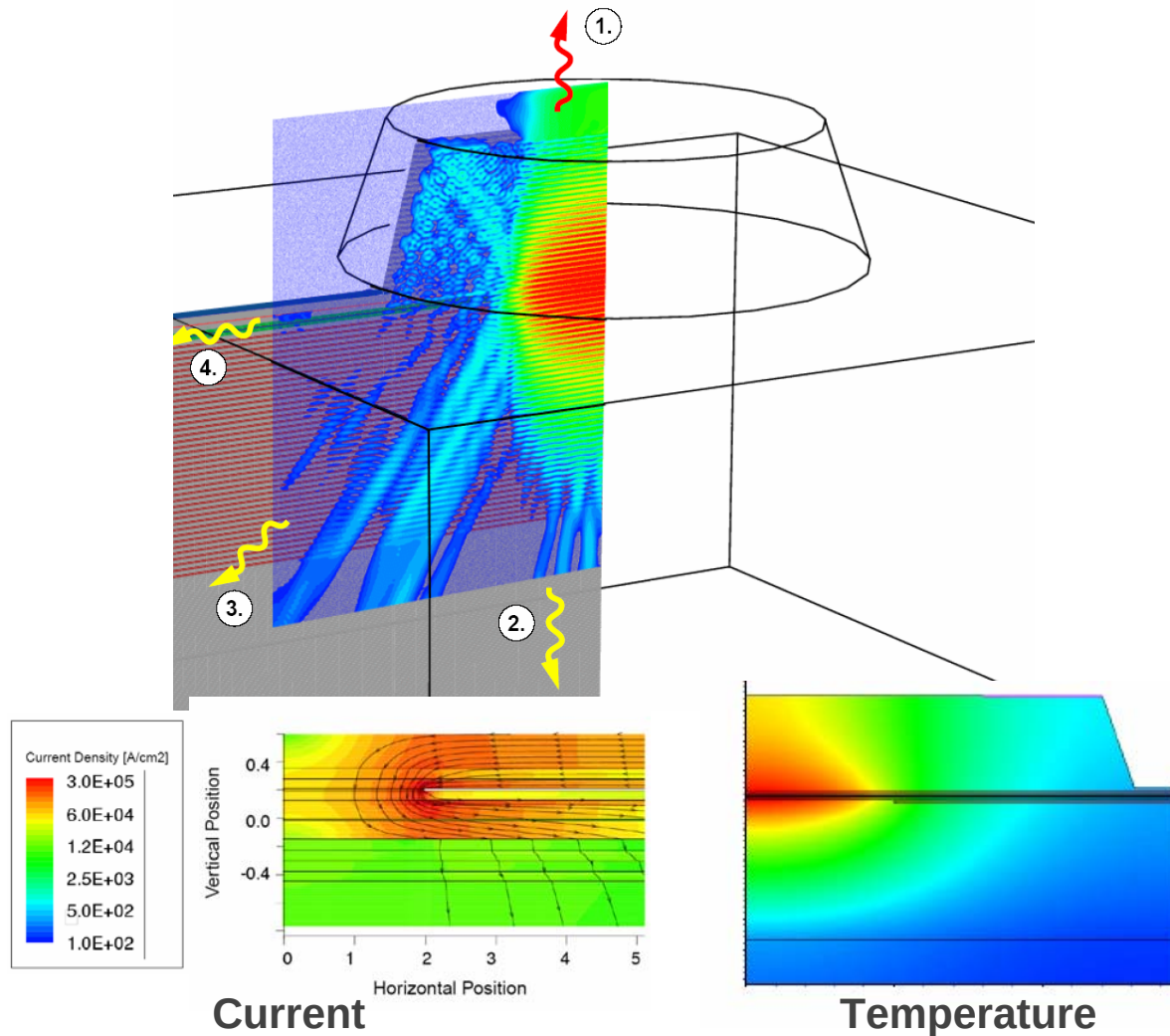
mode discrimination

node oxide

output coupling



- Mode discrimination: anti-resonant structure wins, metal aperture gives only marginal improvement.
- Anti-resonant structure: additional diffracted radiation is coupled back to output by anti-reflex zone for narrow oxides. Metal aperture: shadowing effects for large oxides.



Key Results:

- Optical Losses in 2 Dimensions
- Thermal Lensing (2% increase in refr. Index at Temp, Maximum)
- Diffraction by Oxide Confinement
- Current Crowding

Standing Waves:

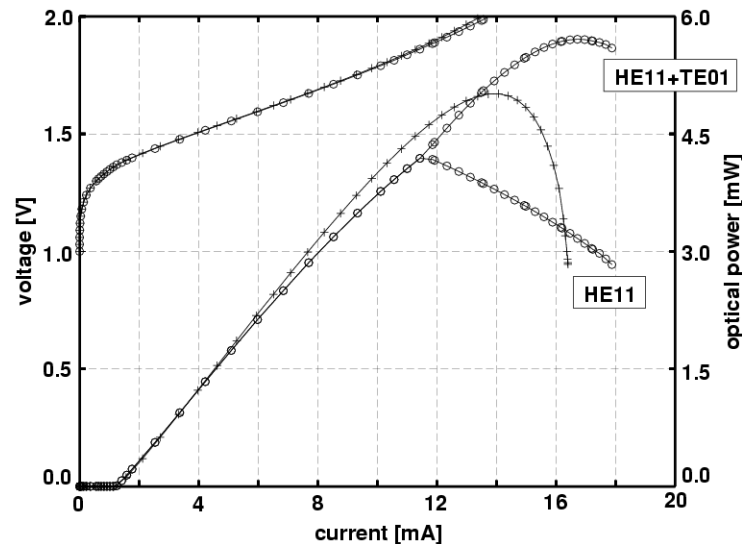
High Field Intensity in Cavity Center

Traveling Waves:

1. Laser Output
2. Bragg Losses
3. Radiating Waves
4. Guided Surface Waves

Device

- AlGaAs/InGaAs(qw)/GaAs, top 28 / bottom 31.5 DBR pairs
- node oxide aperture $r = 3 \text{ } \mu\text{m}$, surface relief $r = 2.5 \text{ } \mu\text{m}$
- 980 nm

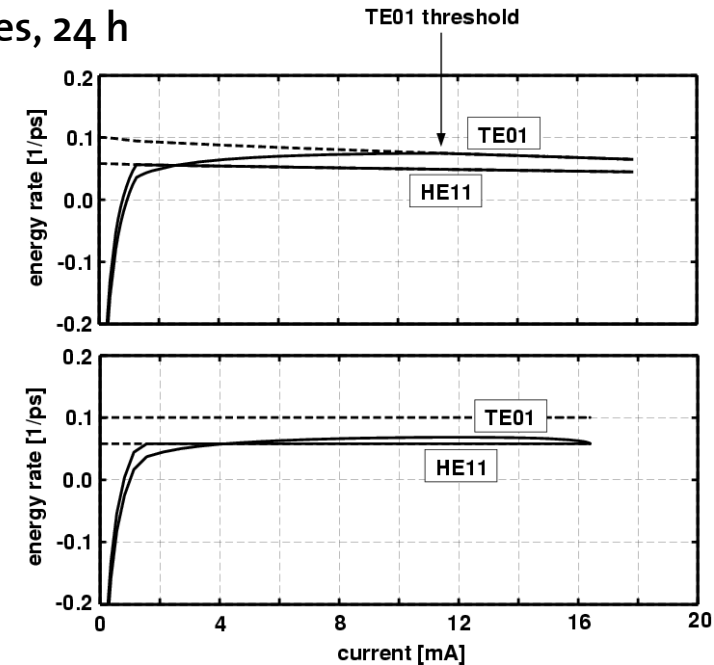


Simulation (approx. data):

- optical: 160'000 FE (1st order), $30/\lambda$ resolution
- electro-thermal: 10'000 FE
- 8 GBytes, 24 h

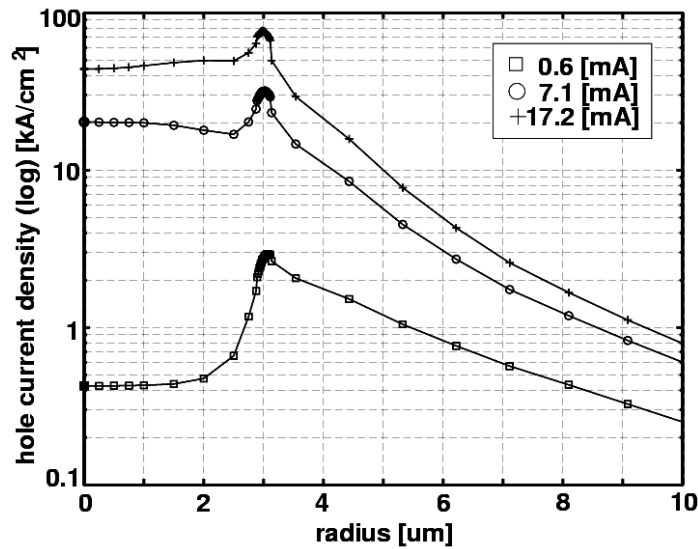
self-consistent

non-self-consistent

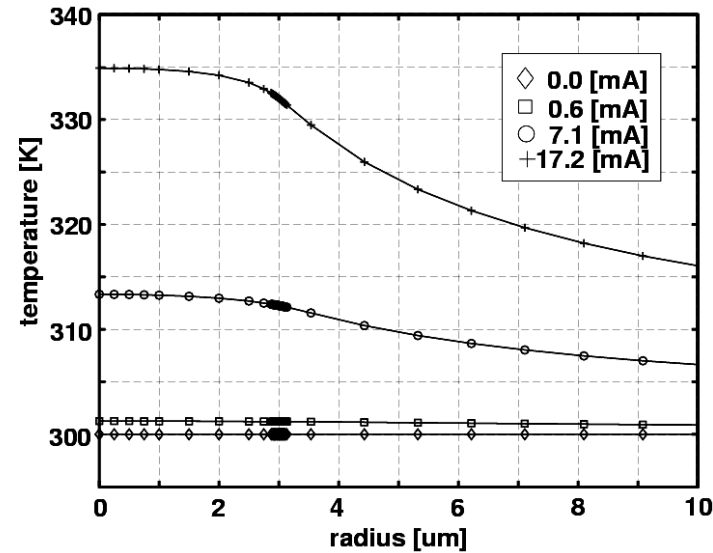


- Solution with and without self-consistent solution of Helmholtz equation.
- Heating reduces diffraction losses (smoothes dielectric profile), increases confinement factor and reduces metal loss (thermal lensing).

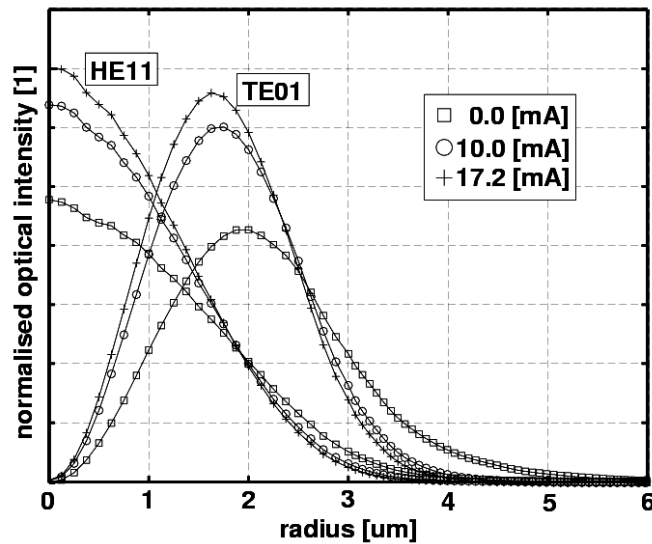
current
crowding



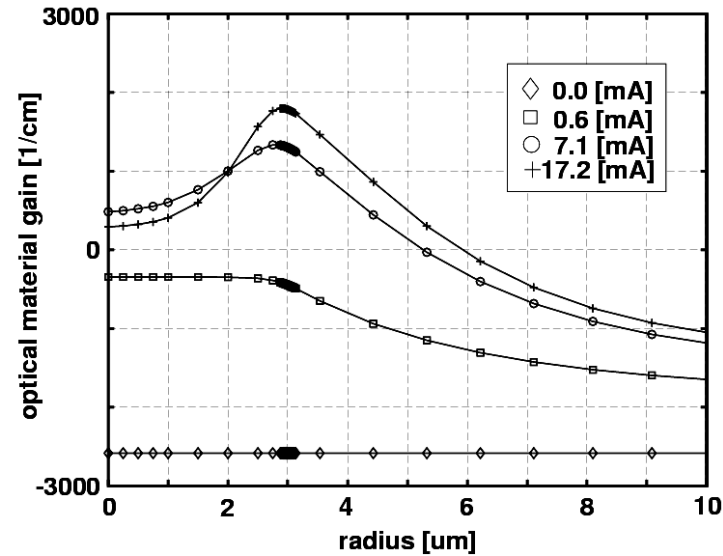
self-
heating



thermal
lensing

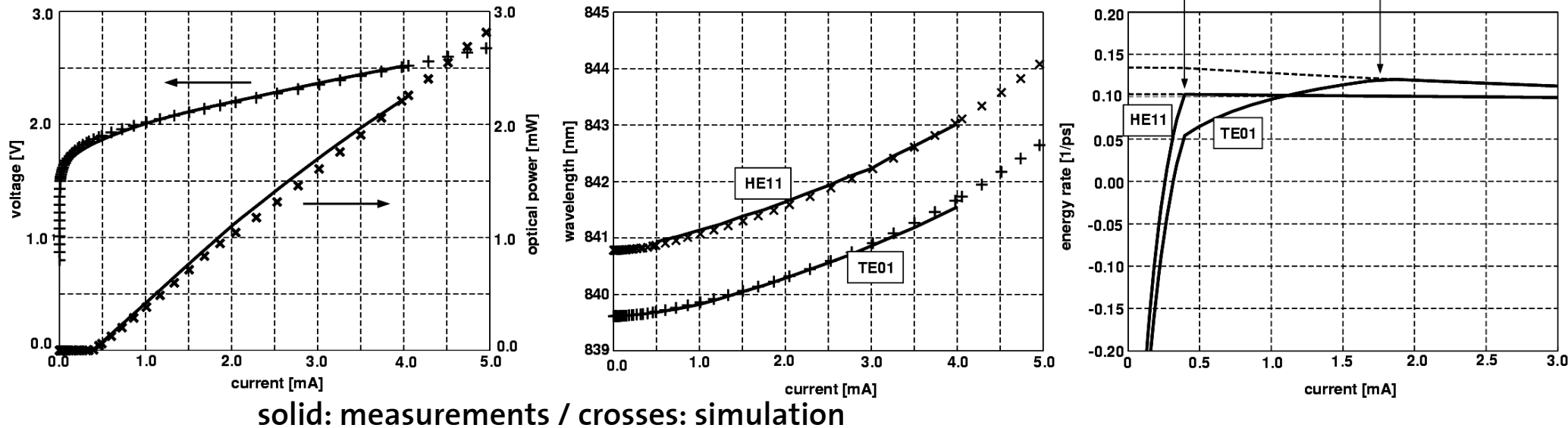


spatial hole
burning



Device

- AlGaAs/GaAs, oxide $r < 2 \mu\text{m}$, metal aperture
- 840 nm, single mode



- Good agreement of measurements and simulation.
- Experimental verification: I/V , I/P ; I/λ_1 (HE11), I/λ_2 (TE01), I_{th1} (HE11), I_{th2} (TE01) by optical spectrum.
- Experimental sanity checks: VCSEL surface temperature distribution (S_{ThM}), carrier mobility in Bragg stack (process monitor structure), I_{th} over substrate temperature.

- Comprehensive VCSEL device model was presented.
- Formulation of microcavity problem using vectorial FE is feasible (computational requirements and accuracy of result).

Important new design tasks are accessible with vectorial optics solver developed in this work.

- Self-consistent solution of coupled system of equations is mandatory for VCSEL simulations.

Gummel iteration procedure is feasible solution if optical problem is solved efficiently by a continuation scheme.

- The practical relevance of the VCSEL device model was demonstrated by benchmarks and tutorial examples.

Outlook:

- AC Analysis
- Calibration: Different Material Systems and Device Designs
- Improved Optical Solvers

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