NUSOD 2005 Tutorial MA1

Introduction to Optoelectronic Device Simulation

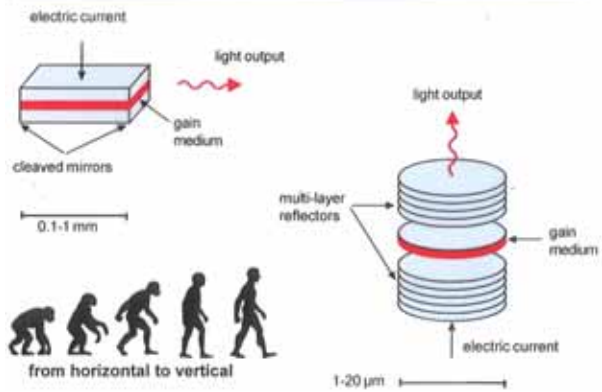
by Joachim Piprek

Outline:

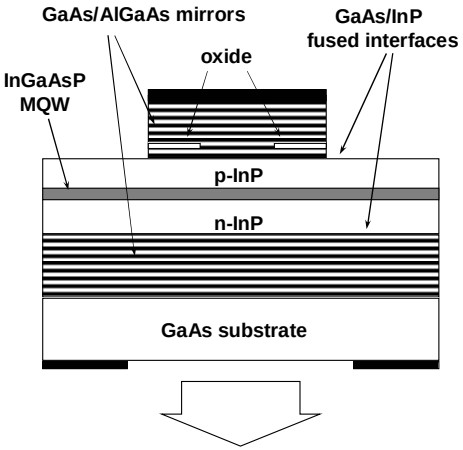
1. Introduction: VCSEL Example
2. Electron Energy Bands
3. Drift-Diffusion Model
4. Thermal Model
5. Gain/Absorption Model
6. Optical Model

Main source:
Semiconductor Optoelectonic Devices: Introduction to Physics and Simulation
by J. Piprek, Academic Press, San Diego, 2003

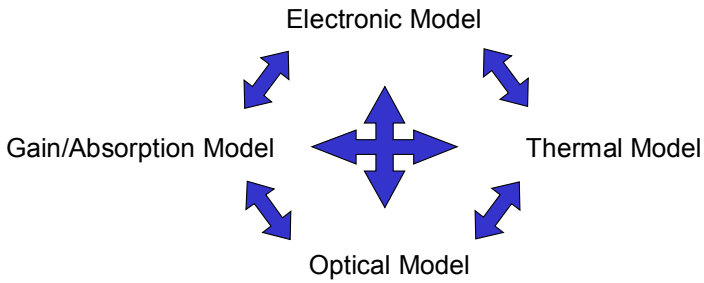
Horizontal and Vertical Cavitiy Lasers



Example: 1.55µm Vertical-Cavity Surface-Emitting Laser (VCSEL)



Optoelectronic Device Modeling



Electron Energy Bands

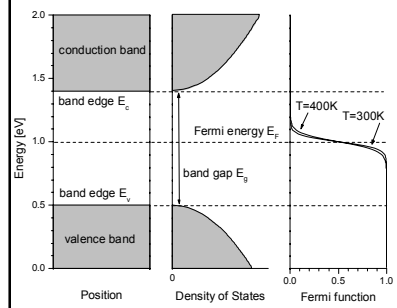
- based on Schrödinger Equation $H\Psi=E\Psi$

  Ψ - electron wave function
  H – Hamiltonian
  E – electron energy

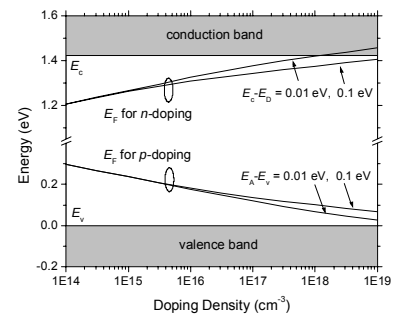
- material parameters:
  lattice constants
  electron effective mass
  Luttinger parameters
  energy gaps, offsets
  elastic stiffness constants
  deformation potentials

- output: $E(x,y,z, k_x,k_y,k_z)$
  x,y,z = position in space
  k_x,k_y,k_z $\propto$ momentum in space

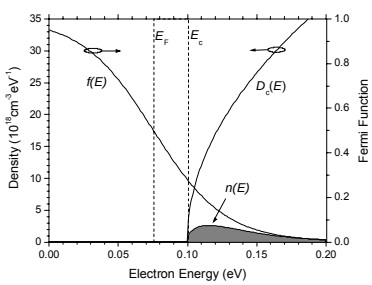
Energy Bands



Fermi Energy Position

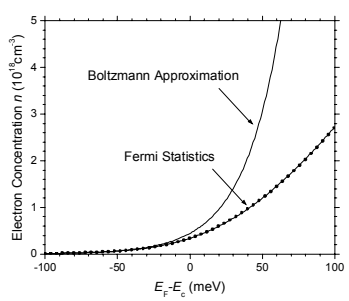


Electron Distribution n(E)

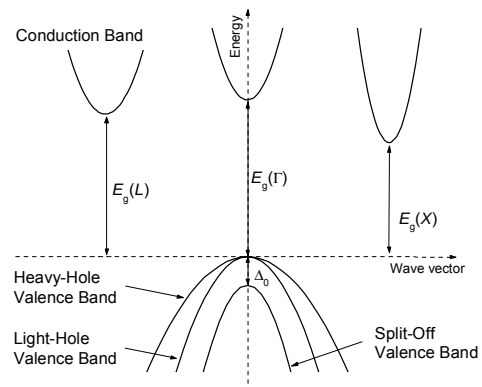


$$f(E) = \frac{1}{1 + \exp\left[\frac{E - E_F}{k_B T}\right]}$$

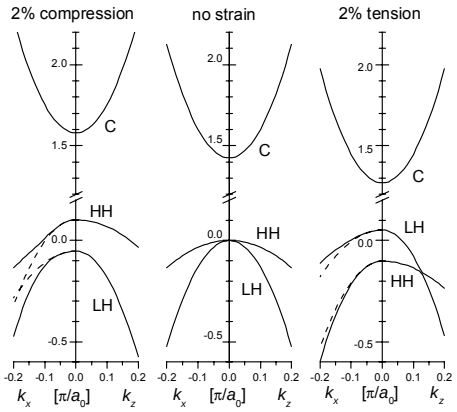
Fermi vs. Boltzmann



Conduction and Valence Bands: E(k)



Influence of Strain (GaAs)



Drift-Diffusion Model

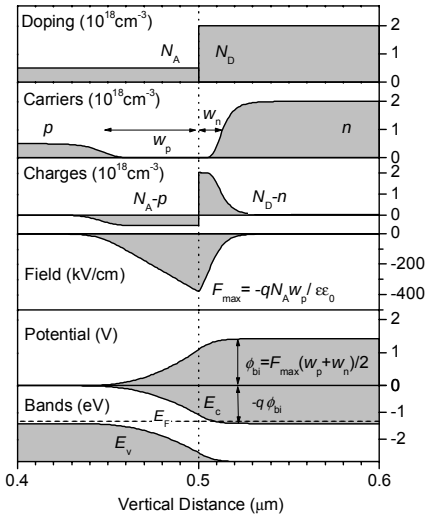
- based on Semiconductor Transport Equations
- input: geometry, materials, doping
- material parameters:
  - carrier mobility
  - carrier generation & recombination
  - dielectric constant
  - energy band offsets
- output: density of electrons (n) and holes (p)
  - current density distribution (j)
  - current vs. voltage (IV)

Drift-Diffusion Equations

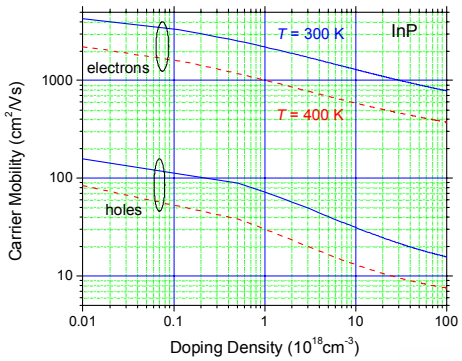
$$
\begin{aligned}
\nabla \varepsilon \nabla \phi &= -e(n - p + C) \\
\nabla \vec{J}_n &= e(R - G) \\
\nabla \vec{J}_p &= -e(R - G) \\
\vec{j}_n &= -en\mu_n \nabla \phi + eD_n \nabla n \\
\vec{j}_p &= -en\mu_p \nabla \phi - eD_p \nabla p \\
R &= R_{SRH} + R_{Auger} + R_{spont} + R_{stim}(g, \vec{E}) \\
G &= G_{abs}(\alpha, \vec{E})
\end{aligned}
$$

electron and hole carrier densities $n(\vec{r}), p(\vec{r})$
electron and hole current densities $\vec{j}_n(\vec{r}), \vec{j}_p(\vec{r})$
recombination and generation rates $R(\vec{r}), G(\vec{r})$
electrostatic potential $\phi(\vec{r})$
optical field strength $\vec{E}(\vec{r})$
optical gain and absorption $g(\vec{r}), \alpha(\vec{r})$
electron charge e
doping density $C(\vec{r})$
dielectric constant $\varepsilon(\vec{r})$
carrier mobilities $\mu_n(\vec{r}), \mu_n(\vec{r})$ $\quad (D = \frac{kT}{e}\mu)$

p-n-Junction



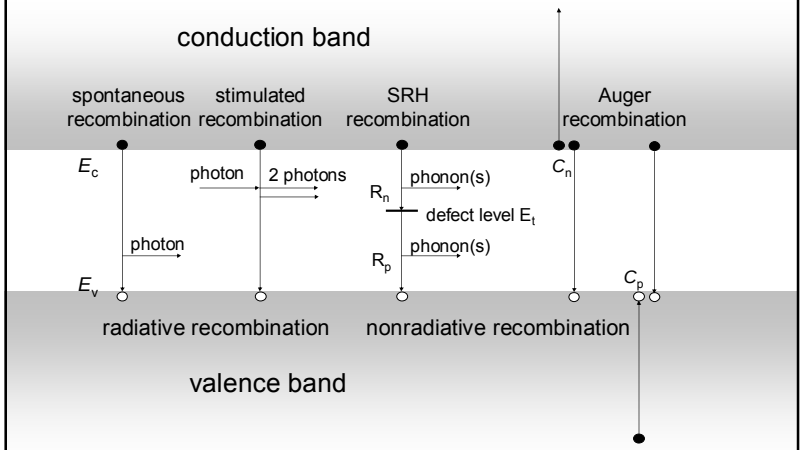
Mobility of Electrons and Holes



$$\mu(T) = \mu_o \left(\frac{T}{300\ \mathrm{K}}\right)^a$$

$$\mu(N_{dop}) = \mu_{dop} + \frac{\mu_o - \mu_{dop}}{1 + (N_{dop}/N_{ref})}$$

Recombination Mechanisms



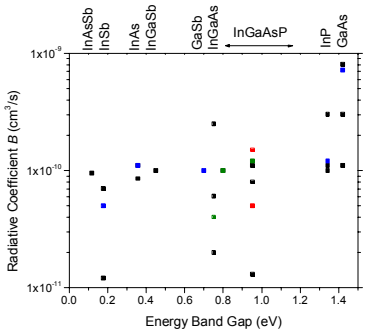
Recombination Parameters

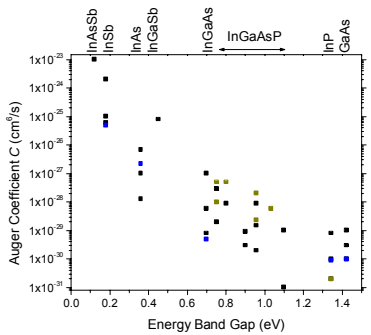
spontaneous emission

$R_{spon}=B\ (np-n_0p_0)$

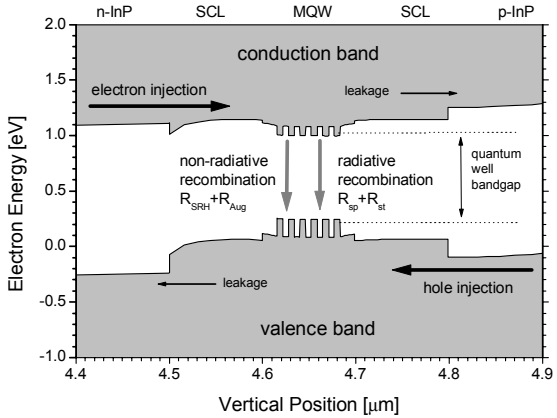
Auger recombination

$R_{Aug}=(nC_n+pC_p)(np-n_0p_0)$

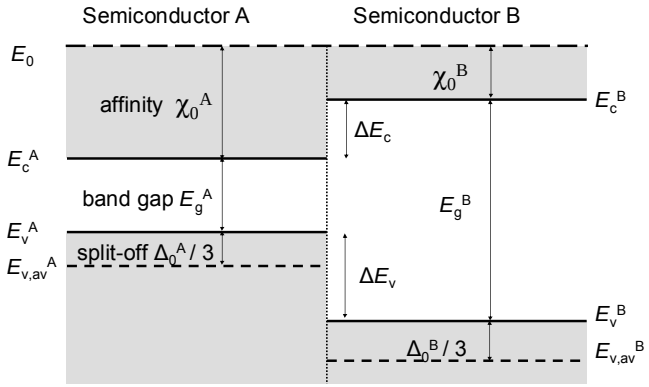




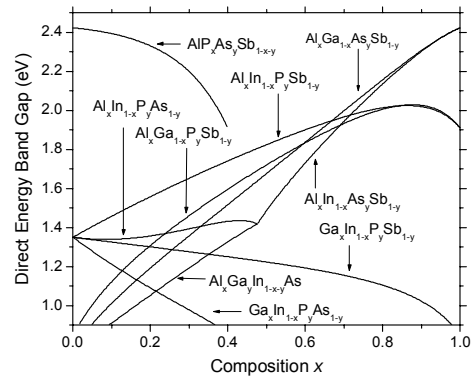
Multi-Quantum Well Active Region



Semiconductor Heterojunctions

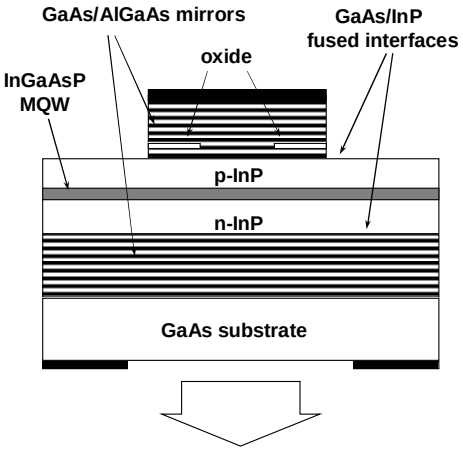


Energy Band Gap vs. Composition for III-V Compounds



lattice matched to InP

Example: VCSEL



Defects at fused InP/GaAs interface

Energy Band Diagram

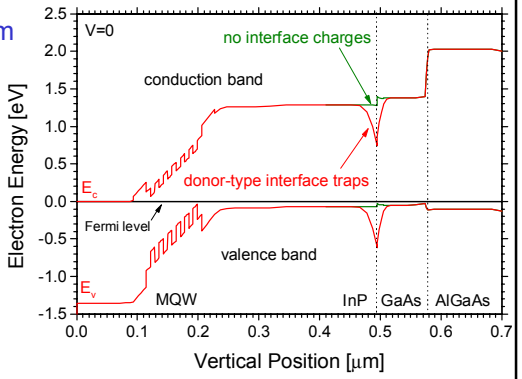
InP/GaAs band offset

ΔE_c=0.12eV

ΔE_v=0.05eV

donor-type interface traps

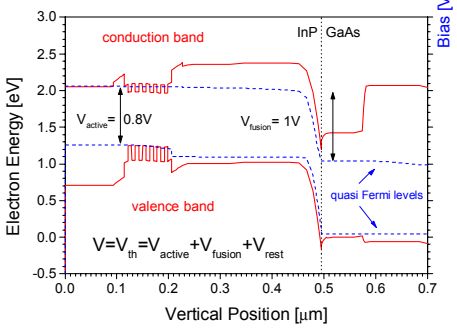
density	10^{13}cm^{-2}
energy	0.7eV + E_v
cross section	10^{-17}cm^2

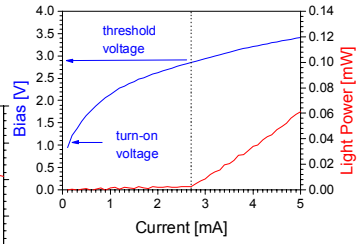


npnp Shockley diode switch (thyristor)

VCSEL Threshold Voltage

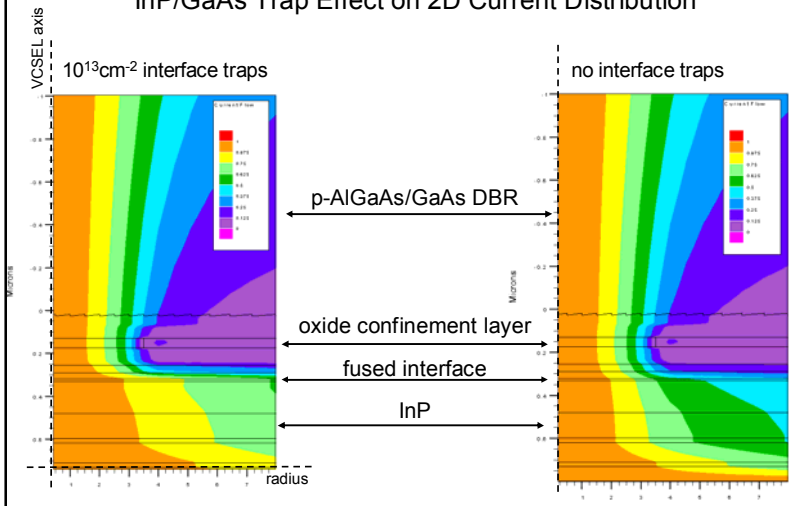
$V_{th}=V_{active}+V_{fusion}+V_{rest}$





donor-type defects create high interface resistance

InP/GaAs Trap Effect on 2D Current Distribution



Thermal Model

- based on Heat Flux Equation
- input: geometry, materials
  heat source distribution P(r,z)
  - Joule heat
  - nonradiative recombination
  - absorption etc.
- material parameters (steady state)
  thermal conductivity k(T,r,z)
- output: temperature distribution T(r,z)
  thermal resistance

Heat Flux Equation (r,z)

$$\frac{\partial}{\partial r}\kappa_r\frac{\partial T}{\partial r}+\frac{1}{r}\kappa_r\frac{\partial T}{\partial r}+\frac{\partial}{\partial z}\kappa_z\frac{\partial T}{\partial z}=-\frac{\partial P}{\partial V}(r,z)$$

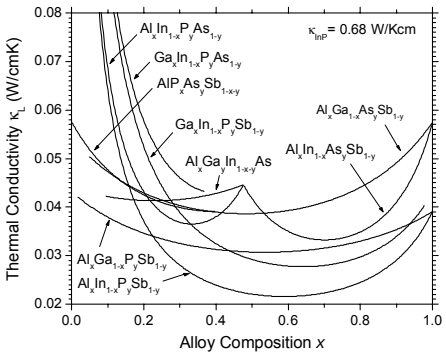
(T - temperature , $\partial P/\partial V$ - heat power density)

with anisotropic thermal conductivity in bottom DBR

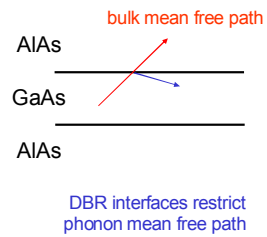
$$\kappa_r=\frac{d_1\,\kappa_1+d_2\,\kappa_2}{d_1+d_2}\quad\text{and}\quad\kappa_z=\frac{d_1+d_2}{d_1/\kappa_1+d_2/\kappa_2}$$

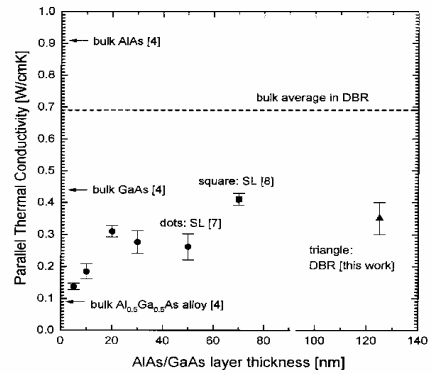
(κ_1,κ_2 - bulk material thermal conductivities
d_1, d_2 - DBR layer thicknesses > phonon mean free path).

InP Alloy Thermal Conductivity



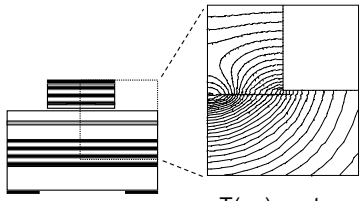
Thin Layer Thermal Conductivity



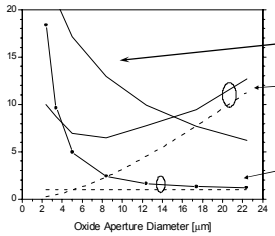


VCSEL Self-Heating

two problems:
- heat flux
- heat power



T(r,z) contours



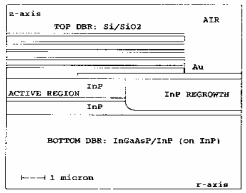
thermal resistance [100 K/W]

temperature rise [K]

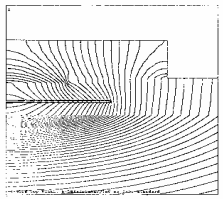
threshold current (dashed: constant)

VCSEL Heat Flux

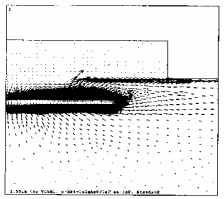
Geometry



Temperature



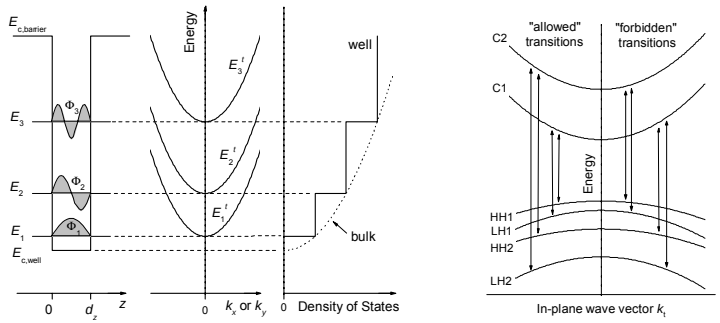
Heat Flux



Gain/Absorption Model

- based on (quantum well) energy band structure
- input: geometry, materials
- material parameters:
  - band structure parameters (incl. strain)
  - transition matrix element
  - dielectric constant
- output: band-to-band gain/absorption function g(T, λ, N)

Quantum Well Energy Bands



basic gain calculation $\boxed{g = C_g M^2 D_r (f_c - f_v)}$

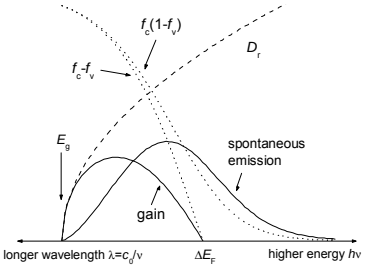
C_g	pre-factor
M	transition matrix element
D_r	reduced density of states
f_c-f_v	inversion factor
	< 0 absorption
	> 0 gain

spontaneous emission $\boxed{r_{sp} = C_{sp} M^2 D_r D_{opt} f_c(1-f_v)}$

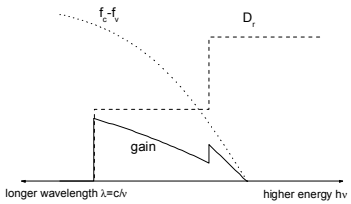
C_{sp}	pre-factor
D_{opt}	photon density of states

Spontaneous Emission and Gain

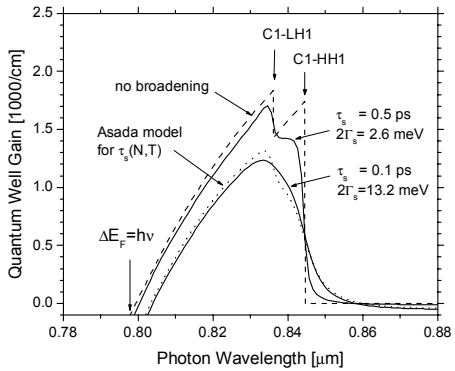
bulk semiconductor



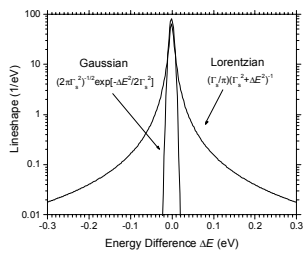
quantum well gain



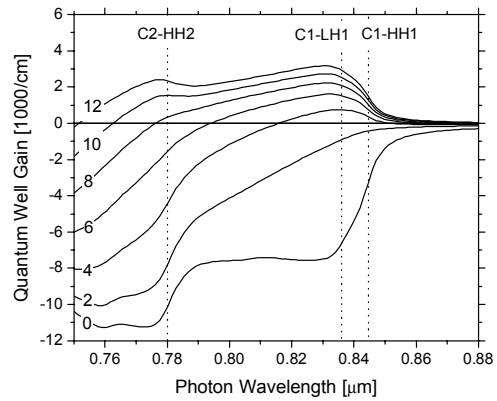
Quantum Well Gain Spectrum with Energy Broadening



single-particle gain
with Lorentz broadening

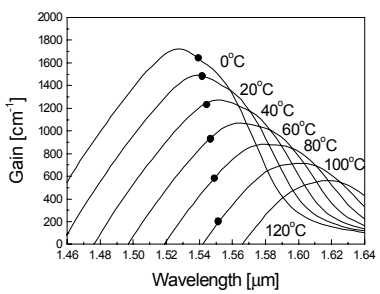


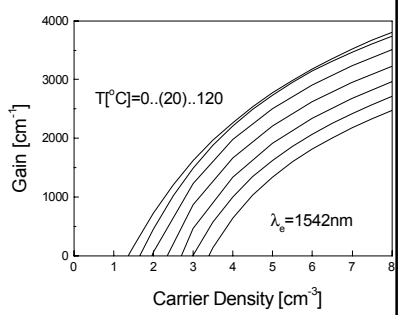
Gain / Absorption vs. Carrier Density [10^{18}cm^{-3}]



Temperature Effects on VCSEL Gain

• emission wavelength, N=3x10^{18}cm^{-3}





=> gain reduction triggers carrier density increase at higher temperatures

Optical Model

• based on Maxwell Equations

• input: geometry, materials

• material parameters:
refractive index n(T,z)
absorption coefficient α(T,z)

• output: standing wave (mode)
emission wavelength
threshold gain
optical quantum efficiency

Maxwell Equations

$$\nabla \times \vec{E} = -\mu_{opt}\frac{\partial \vec{H}}{\partial t}$$

$$\nabla \times \vec{H} = \varepsilon_{opt}\frac{\partial \vec{E}}{\partial t}$$

$$\nabla(\varepsilon_{opt}\vec{E}) = 0$$

$$\nabla(\mu_{opt}\vec{H}) = 0$$

electric fields strength $\vec{E}(\vec{r})$
magnetic fields strength $\vec{H}(\vec{r})$
dielectric constant (optical frequency) $\varepsilon_{opt}(\vec{r})$
magnetic permeability (optical frequency) $\mu_{opt}(\vec{r})$

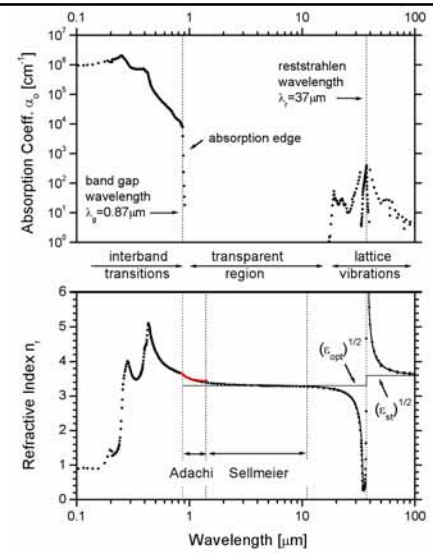
Dielectric Constant

$\varepsilon = \varepsilon_1 + i\,\varepsilon_2$

$\varepsilon_1 = n^2 - k^2$
$\varepsilon_2 = 2\,n\,k$

$k = \lambda\alpha / 4\pi$

n – refractive index
α - absorption const.
λ - wavelength



Helmholtz Equations

within uniform, isotropic, and passive layers

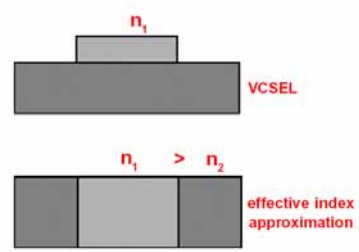
$$\nabla^2\vec{\mathrm{E}} + k_o^2\varepsilon\vec{\mathrm{E}} = 0$$
$$\nabla^2\vec{\mathrm{H}} + k_o^2\varepsilon\vec{\mathrm{H}} = 0$$

reduced scalar waveguide equations for harmonic wave in z-direction

$$\frac{\partial^2\Phi}{\partial x^2} + \frac{\partial^2\Phi}{\partial y^2} + (k^2 - \beta^2)\Phi = 0$$

k – wave vector, β – propagation constant

VCSEL: Effective Index Method



scalar wave equation:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial W}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 W}{\partial \theta^2} + \frac{\partial^2 W}{\partial z_r^2} + k^2 W = 0$$

solution:

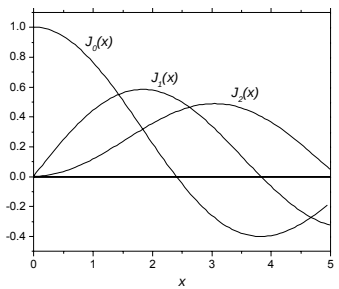
$$W = W_r(r)exp(-jk_z z_r)$$

$W_r(r)$ from Bessel equation of order m:

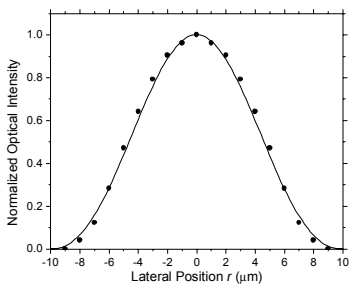
$$\frac{d^2W_r}{dr^2} + \frac{1}{r}\frac{dW_r}{dr} + \left(k^2 - k_z^2 - \frac{m^2}{r^2}\right)W_r = 0$$

VCSEL: Transversal Optical Intensity

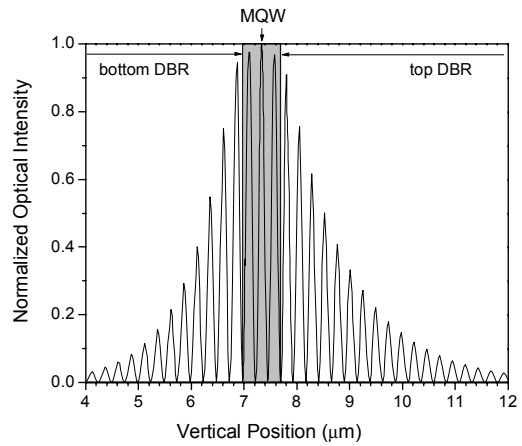
Bessel Functions



Near Field Measurement



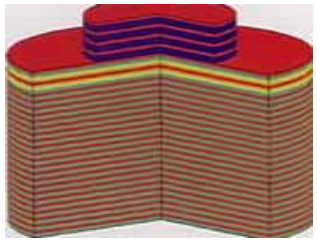
VCSEL: Vertical Optical Intensity

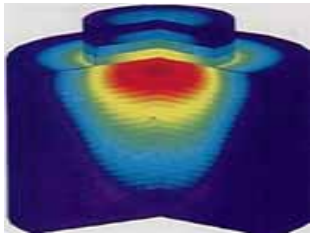


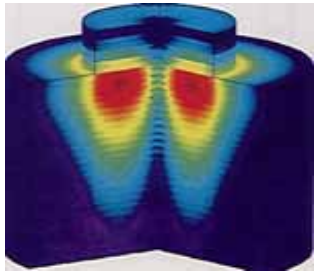
VCSEL: 2D Mode Matching

980nm Vertical-Cavity Laser

top: GaAs/Al_xO (2.8μm)
bottom: GaAs/AlGaAs



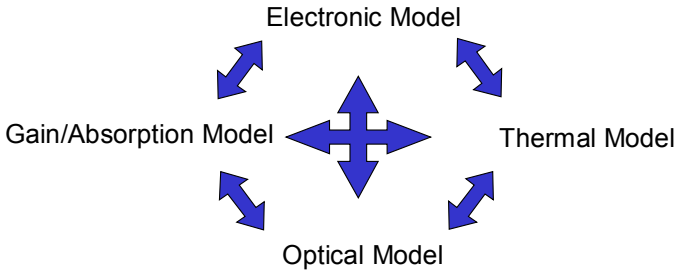




[Noble et al., IEEE J. Quantum Electronics 34, 1890 (1998)]

Conclusion

1. self-consistent combination of relevant models
2. careful adjustment of material parameters



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