**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 Optoelectronic Devices: Introduction to Physics and Simulation_  

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

Optoelectronic Device Modeling

Electronic Model

Gain/Absorption Model

Thermal Model

Optical Model
Electron Energy Bands

- based on Schrödinger Equation $H\Psi=E\Psi$
  - $\Psi$ - 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
  - $k_x, k_y, k_z$ = momentum in space

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Energy Bands

- Fermi Energy Position

- Conduction and Valence Bands: $E(k)$
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

\[ \nabla e \nabla \phi = -e(n - p + C) \]
\[ \nabla J_n = e(R - G) \]
\[ \nabla J_p = -e(R - G) \]
\[ j_n = -en\mu_n \nabla \phi + eD_n \nabla n \]
\[ j_p = -ep\mu_p \nabla \phi - eD_p \nabla p \]
\[ R = R_{HH} + R_{Auger} + R_{impact} + R_{diffusion} \]
\[ G = G_{bulk}(\alpha, \vec{E}) \]

\( \phi_{bi} = \frac{q}{2} \left( n + p \right) \)

\( n \) and \( p \) are electron and hole carrier densities, \( \alpha(T, E) \) and \( \beta(T, E) \) are electron and hole current densities, \( R(T) \) and \( G(T) \) are recombination and generation rates, \( \phi(T) \) is the electrostatic potential, \( \vec{E}(T) \) is the optical field strength, \( \alpha(T) \) and \( \beta(T) \) are optical gain and absorption coefficients, \( \epsilon(T) \) is the dielectric constant, \( \mu(T) \) and \( \mu(T) \) are carrier mobilities.

\[ D = \frac{\mu_n(n) \mu_p(p)}{\mu_n(n) + \mu_p(p)} \]

\( p-n \)-Junction

Doping \( (10^{18} \text{cm}^{-3}) \)

Voltage \( (V) \)

Field \( (kV/cm) \)

Potential \( (V) \)

Bands \( (eV) \)

0.4 0.5 0.6

Vertical Distance \( (\mu m) \)
Mobility of Electrons and Holes

\[ \mu(T) = \mu_0 \left( \frac{T}{300} \right)^{a} \]

\[ \mu(N_{dop}) = \mu_{dop} + \frac{\mu_0 - \mu_{dop}}{1 + (N_{dop}/N_{ref})} \]

Recombination Mechanisms

Spontaneous emission: \( R_{\text{spont}} = B (n p - n_0 p_0) \)

Auger recombination: \( R_{\text{Aug}} = (n C_n + p C_p) (n p - n_0 p_0) \)

Recombination Parameters

Multi-Quantum Well Active Region
Semiconductor Heterojunctions

<table>
<thead>
<tr>
<th>Semiconductor A</th>
<th>Semiconductor B</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_0^A$</td>
<td>$E_0^B$</td>
</tr>
<tr>
<td>affinity $\chi_0^A$</td>
<td>$\chi_0^B$</td>
</tr>
<tr>
<td>$E_c^A$</td>
<td>$E_c^B$</td>
</tr>
<tr>
<td>band gap $E_g^A$</td>
<td>$E_g^B$</td>
</tr>
<tr>
<td>$E_v^A$</td>
<td>$E_v^B$</td>
</tr>
<tr>
<td>split-off $\Delta^A / 3$</td>
<td>$\Delta^B / 3$</td>
</tr>
<tr>
<td>$\Delta E_c$</td>
<td>$E_{v,av}^B$</td>
</tr>
</tbody>
</table>

Energy Band Gap vs. Composition for III-V Compounds

Example: VCSEL

Energy Band Diagram

Defects at fused InP/GaAs interface
**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

\[
\begin{align*}
\frac{\partial}{\partial r} \kappa_r \frac{\partial T}{\partial r} + \frac{1}{r} \kappa_r \frac{\partial T}{\partial r} + \frac{\partial}{\partial z} \kappa_z \frac{\partial T}{\partial z} &= \frac{\partial P}{\partial V}(r,z) \\
\end{align*}
\]

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

with anisotropic thermal conductivity in bottom DBR

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

\( (\kappa_1, \kappa_2) \) - bulk material thermal conductivities

\( d_1, d_2 \) - DBR layer thicknesses > phonon mean free path.
InP Alloy Thermal Conductivity

<table>
<thead>
<tr>
<th>Alloy Composition</th>
<th>Thermal Conductivity $\kappa$ (W/cmK)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{Al}<em>{x}\text{In}</em>{1-x}\text{P}<em>{y}\text{As}</em>{1-y}$</td>
<td>$0.02$</td>
</tr>
<tr>
<td>$\text{Ga}<em>{x}\text{In}</em>{1-x}\text{P}<em>{y}\text{As}</em>{1-y}$</td>
<td>$0.04$</td>
</tr>
<tr>
<td>$\text{Al}<em>{x}\text{Ga}</em>{1-x}\text{P}<em>{y}\text{As}</em>{1-y}$</td>
<td>$0.06$</td>
</tr>
<tr>
<td>$\text{Al}<em>{x}\text{In}</em>{1-x}\text{As}<em>{y}\text{Sb}</em>{1-y}$</td>
<td>$0.08$</td>
</tr>
<tr>
<td>$\text{Ga}<em>{x}\text{In}</em>{1-x}\text{As}<em>{y}\text{Sb}</em>{1-y}$</td>
<td>$0.10$</td>
</tr>
</tbody>
</table>

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Thin Layer Thermal Conductivity

- AlAs
- GaAs
- AlAs

DBR interfaces restrict phonon mean free path

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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)

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VCSEL Heat Flux

Geometry                      Temperature             Heat Flux

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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 \( g(T, \lambda, N) \)

basic gain calculation

\[
g = C_g \, M^2 \, D_r \, (f_c-f_v) \]

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

spontaneous emission

\[
\text{rsp} = C_{sp} \, M^2 \, D_r \, D_{opt} \, f_c(1-f_v) \]

- \( C_{sp} \): pre-factor
- \( D_{opt} \): photon density of states

Quantum Well Energy Bands

Spontaneous Emission and Gain
**Quantum Well Gain Spectrum with Energy Broadening**

![Diagram showing quantum well gain spectrum with energy broadening](image)

**Gain / Absorption vs. Carrier Density \([10^{18} \text{cm}^{-3}]\)**

![Diagram showing gain vs. absorption vs. carrier density](image)

**Temperature Effects on VCSEL Gain**

- emission wavelength, \(N=3\times10^{18}\text{cm}^{-3}\)

![Diagram showing temperature effects on VCSEL gain](image)

\(=>\) 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 \(\alpha(T,z)\)
- 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

\[ \varepsilon = \varepsilon_1 + i \varepsilon_2 \]

\[ \varepsilon_1 = n^2 - k^2 \]

\[ \varepsilon_2 = 2 n k \]

\[ k = \frac{\lambda \alpha}{4\pi} \]

\[ n - \text{refractive index} \]

\[ \alpha - \text{absorption const.} \]

\[ \lambda - \text{wavelength} \]

Helmholtz Equations

Within uniform, isotropic, and passive layers

\[ \nabla^2 \vec{E} + k_o^2 \varepsilon \vec{E} = 0 \]

\[ \nabla^2 \vec{H} + k_o^2 \varepsilon \vec{H} = 0 \]

Reduced scalar waveguide equations for harmonic wave in z-direction

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

\( k - \text{wave vector} \)

\( \beta - \text{propagation constant} \)

VCSEL: Effective Index Method

Scalar wave equation:

\[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial W}{\partial r} \right) - \frac{1}{r^2} \frac{\partial^2 W}{\partial \phi^2} + k^2 W = 0 \]

Solution:

\[ W = W_c(r) \exp(-jkz) \]

\[ W_c(r) \text{ from Bessel equation of order } m: \]

\[ \frac{d^2 W_c}{dr^2} + \left( k^2 - k_0^2 - \frac{n_j^2}{r^2} \right) W_c = 0 \]
VCSEL: Transversal Optical Intensity

Bessel Functions

Near Field Measurement

VCSEL: Vertical Optical Intensity

Bessel Functions Near Field Measurement

VCSEL: 2D Mode Matching

980nm Vertical-Cavity Laser
top: GaAs/AlO (2.8µm)
bottom: GaAs/AlGaAs

VCSEL: Vertical Optical Intensity

Conclusion

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

Electronic Model

Gain/Absorption Model

Thermal Model

Optical Model

questions: piprek@ieee.org