

*Crosslight Software Overview,
New Features
& Updates*

Dr. Peter Mensz

Device Simulators

- Lastip/Pics3d
 - Laser diode FEM models in 2D/3D
- Apsys 2D and 3D
 - Any other compound semiconductors device FEM models, excluding stimulated emission.
 - E.g. photodetectors, LEDs, HEMTs.
- APSYS Quantum-MOS 2D and 3D
 - All APSYS features For small $L_{ch} \sim < 0.1\mu m$ MOSFET with ultra thin oxides (can include selfconsistent Poisson and Schroedinger Eqs. Solver tunneling, Many Body corrections)

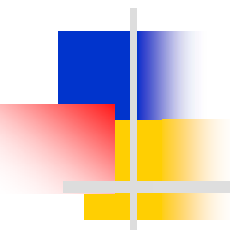
Optional Modules and Advanced Features: 3

- Quantum Tunneling Option
- Complex MQW Option
- Selfconsistent MQW Model
- VCSEL Option
- Vectorial Wave Function
- PML/EEIM Option and Radiative Mode
- Waveguide Modes of Passive Devices
- 3D Flow Option ;3D Optical+ 3D flow(Elect.+Therm.)
- Semiconductor Optical Amplifier Option
- Light Emitting Diode Option
- LED Ray Tracing Option
- FIBER-Grating/External Cavity Option
- Travel Wave Optical Amplifier (for high speed SOA)
- Second Order Grating Option
- Beam Propagation Method Option
- Fiber/External-Cavity
- Optically Pumped Laser Option
- Many Body and Exciton Option
- 8x8 k.p Model
- Photon-Absorbing Waveguide Option
(3D-Simulation for SOA, EAM, WPD)

Semiconductor Physical Process Simulators

- PROCOM- 3D Chemical and Fluid Dynamic MOCVD Process Simulator
 - Chemical species distributions in reactor.
 - Gas flow pattern.
 - Temperature distribution.
 - Film deposition rates and composition.
 - Common impurity incorporation.
- CSUPREM- 3D Semiconductor Processing Simulator
 - physical models for ion implantation, deposition, etching, diffusion, and oxidation.
 - Export doping profiles needed in device simulations.
 - Based on technology licensed from Stanford University (Prof. Robert Dutton's group).

Quantum Drift-Diffusion Model



In Crosslight Device Simulators

Introduction: Device evolution

- **Optoelectronic devices:**

- Laser diode: from double heterostructure laser to quantum well laser.
- LED: from bulk to multiple quantum wells.

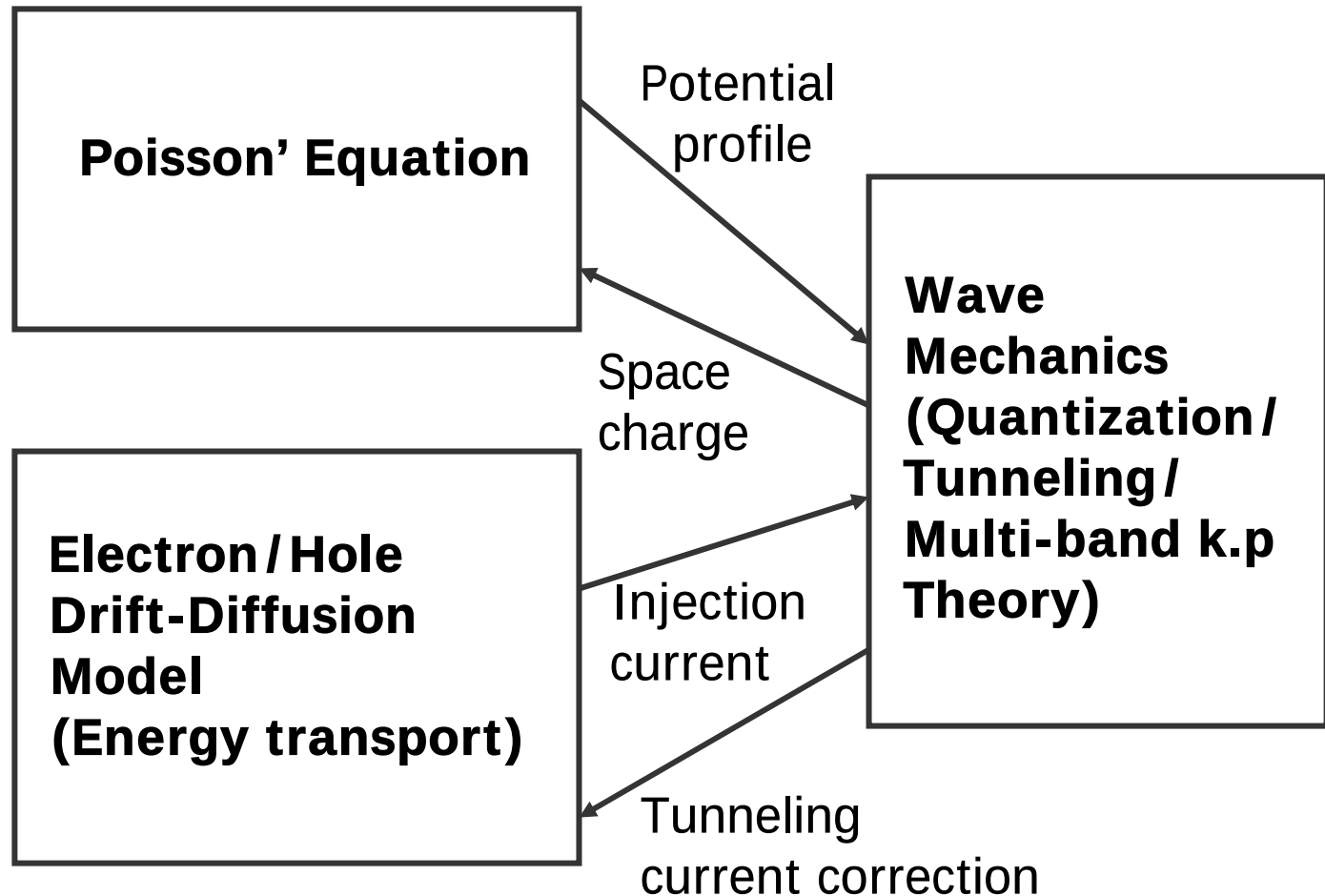
- **Silicon IC:**

- CMOS gate length from several microns down to deep submicrons.
- Semiconductor from pure Si to strained Si on SiGe.

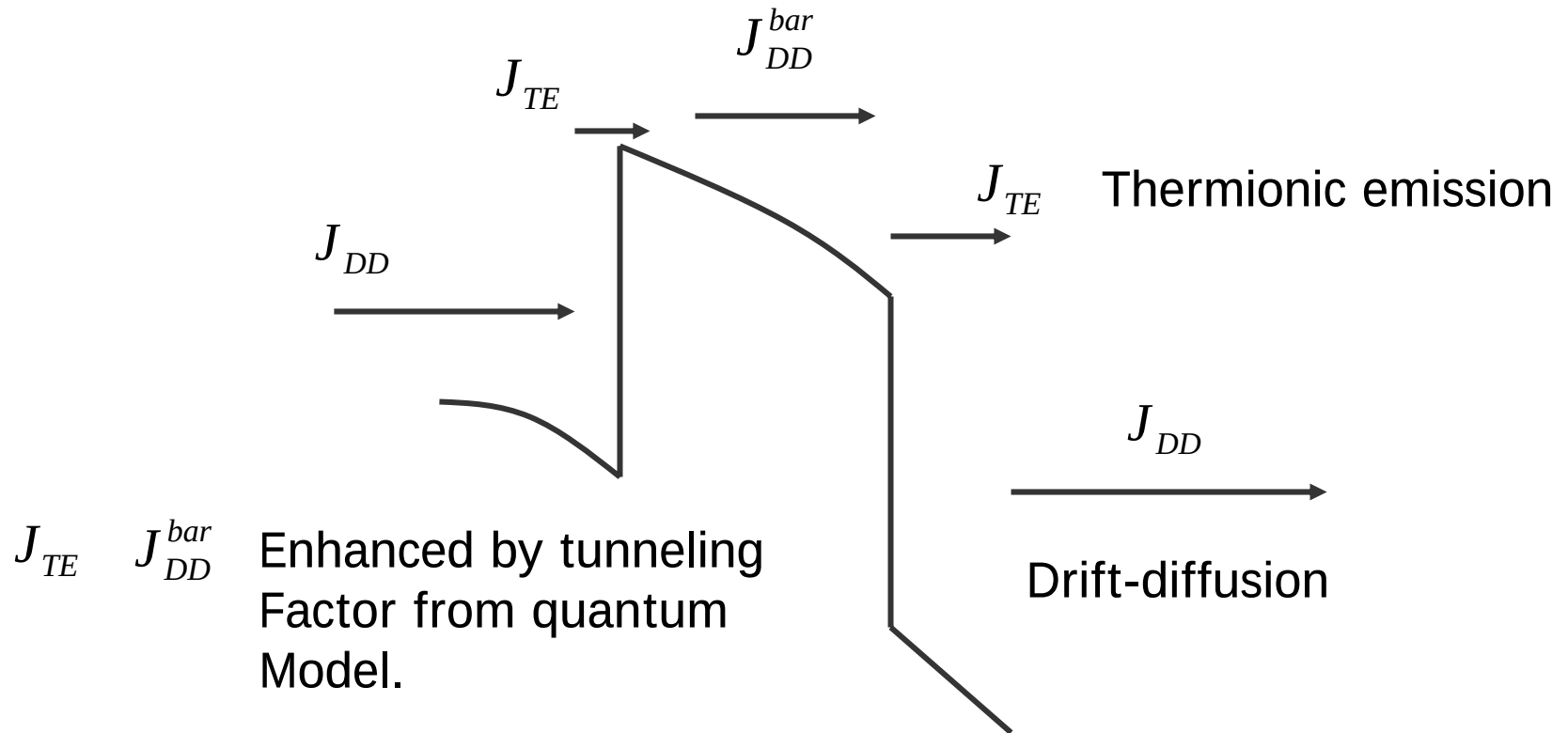
- **Generalized quantum effect:**

- Size effect: quantum confinement;
 - QUNTUM WELLS,
 - QUANTUM DOTS,
 - QUANTUM WIRES
- Quantum tunneling (intraband and interband).
- Band structure engineering: strain dependent valley splitting, density of state design, mobility enhancement and optical transition selection.

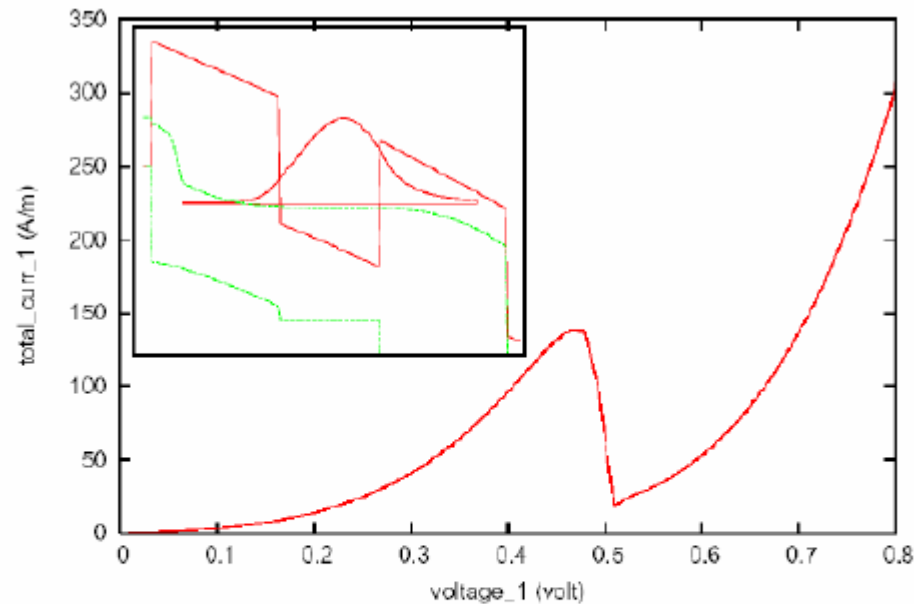
Integrated Quantum-Drift-Diffusion Model



Quantum tunneling correction

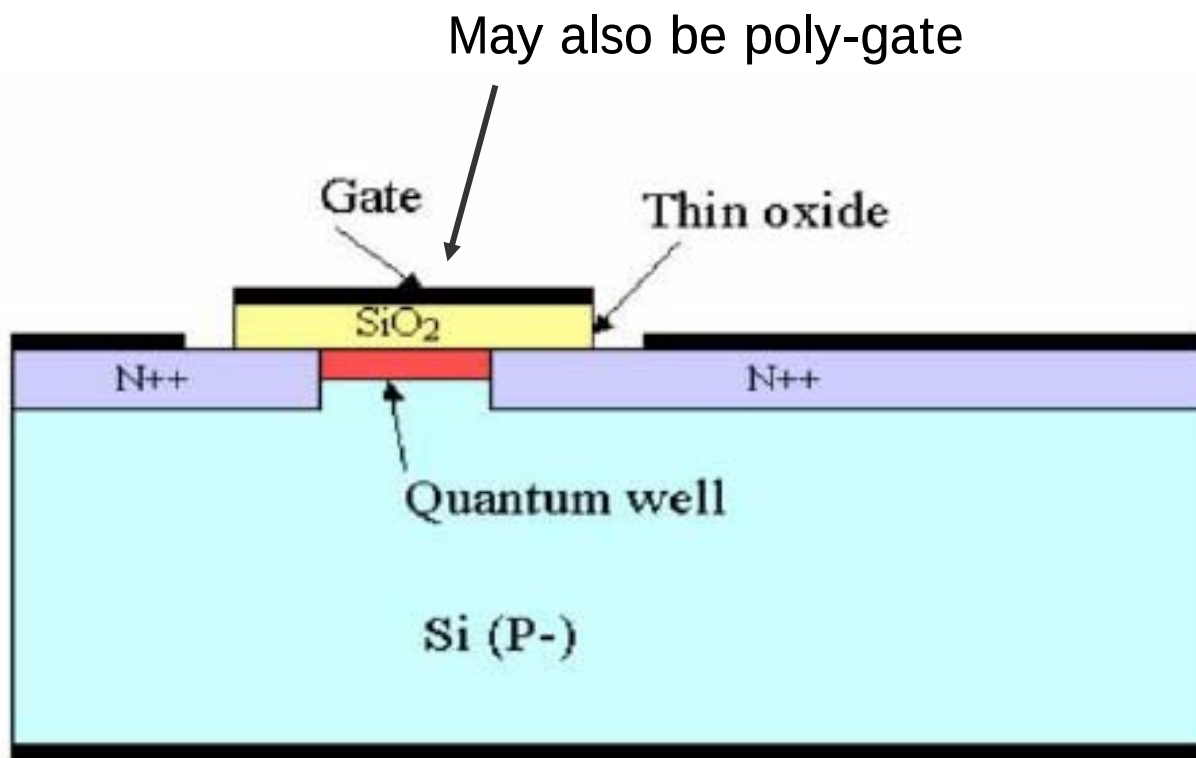


Demonstration: RTD simulation

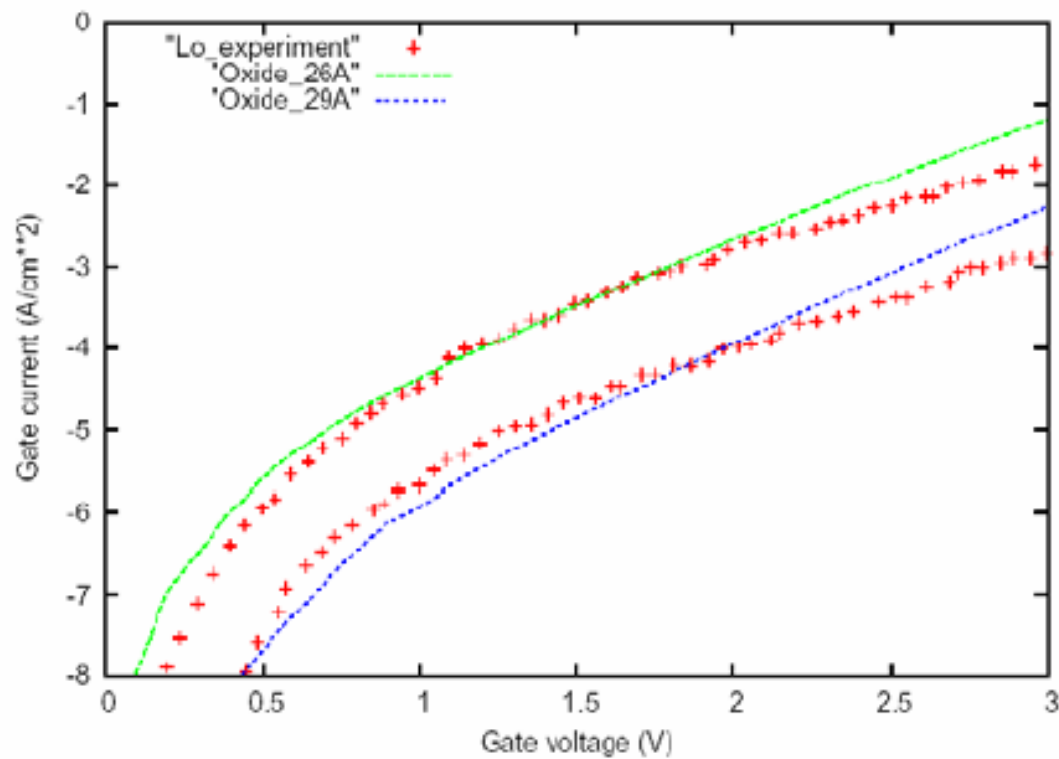


Band diagram, the confined wave function and the resonant I-V characteristics indicating injection carriers are energetically resonating with the confined energy level at a certain bias.

Quantum / classical regions in a MOSFET



Quantum-DD model works!



Use of direct tunneling model with restricted 2D carrier distribution in continuity equation.

Material Properties As Commands

- **Ease of management:**

- Input commands and material parameters completely define a simulation.
- Material parameters are isolated from numerical calculation.

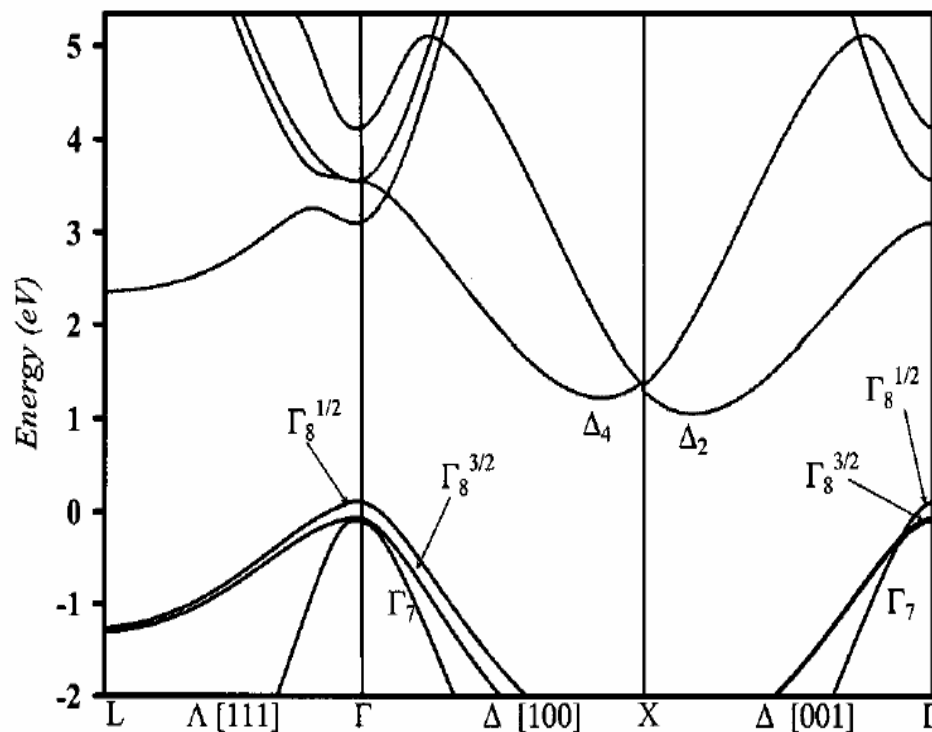
- **Flexible:**

- Nearly any kind of parameter dependence (temperature, doping, composition) may be implemented or modified by user.
- Fortran/C syntax and logical control.
- Numerical tables may also be included in macro.

Types of material macros

- **Basic bulk material macro.**
- **Strained/unstrained symmetric zincblende quantum well.**
- **Strained wurtzite symmetric quantum well.**
- **OLED**
- **Complex quantum wells (coupled, non-symmetric, type-II, etc.)**
- **Complex MOS quantum well.**
- **General complex strained QW (strained silicon QW).**

Strained Silicon



Complete first principle band Structure model too difficult To be included in 3D drift-Diffusion solver. Use Composition parameterization Instead.

Macro needs for all composition range:

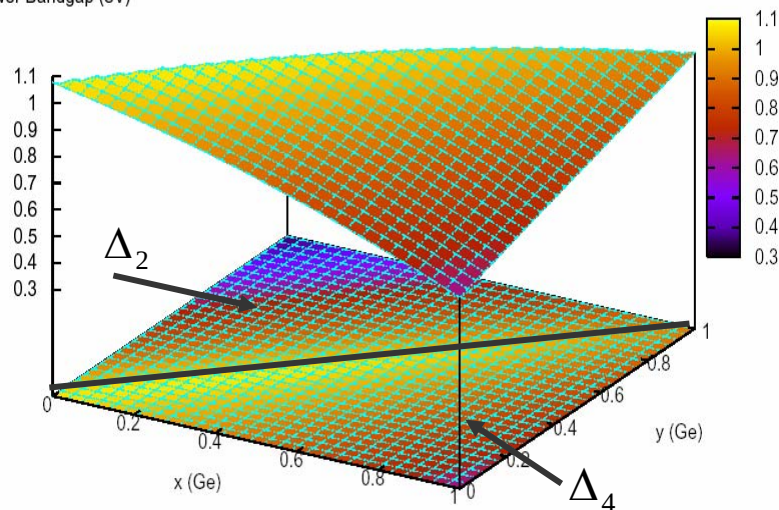
- ☐ Strained bandgap for different valleys.
- ☐ DOS masses for each valley, for both perpendicular and parallel directions.
- ☐ Bandgap discontinuity

Strained Si on SiGe (Richard et. Al. J. Appl. Phys. Vol. 94,1795)

Parameterization of Strained Silicon Band Structure

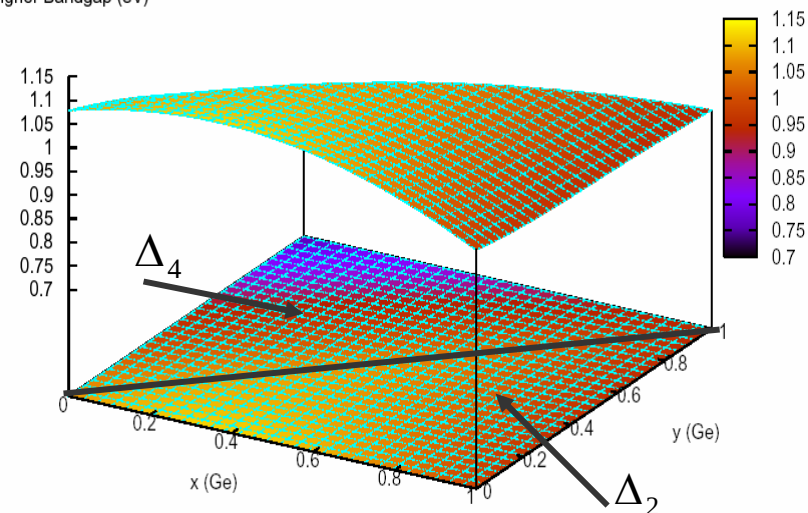
Strained Si(1-x)Ge(x)/Unstrained Si(1-y)Ge(y)

Lower Bandgap (eV)



Strained Si(1-x)Ge(x)/Unstrained Si(1-y)Ge(y)

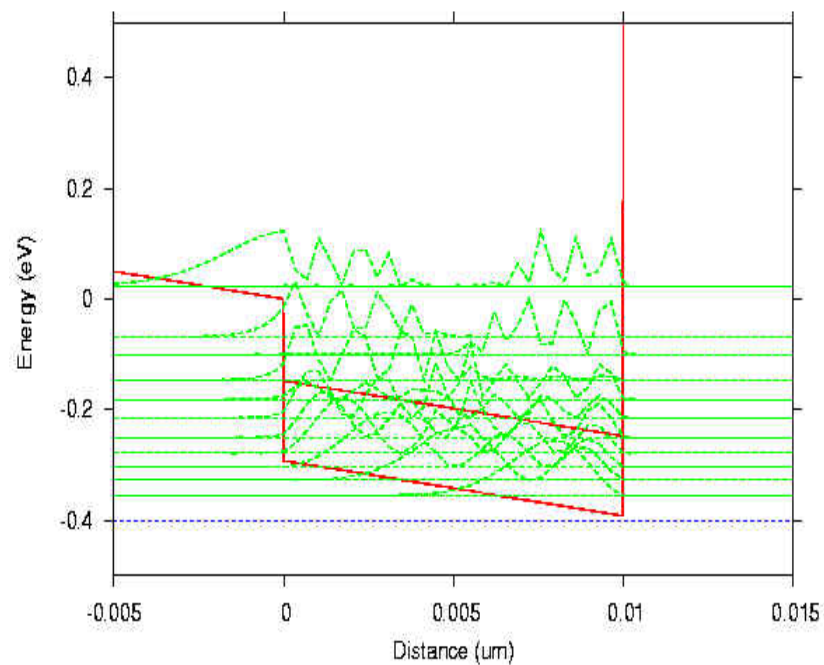
Higher Bandgap (eV)



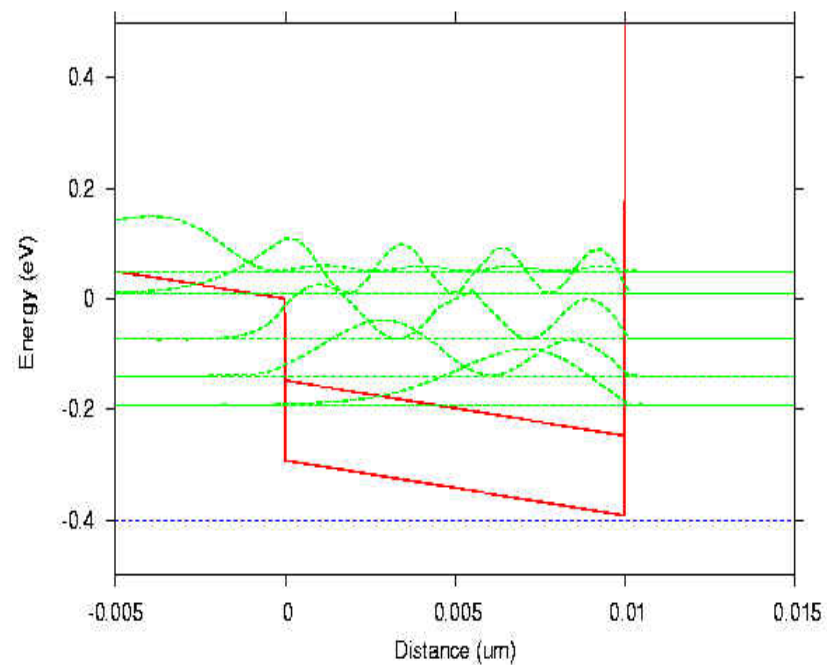
Implemented in Crosslight material macro library

Strained Si(1-x)Ge(x) on relaxed Si(1-y)Ge(y) (Rieger&Vogl, Phys. Rev B48, 14276)

Strained Si on Relaxed SiGe

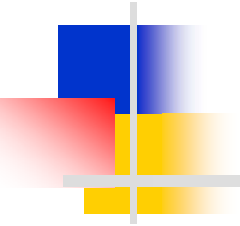


**Lower valley: smaller parallel mass
but larger perpendicular mass.**



**Higher valley: larger parallel mass
but smaller perpendicular mass.**

Complex LD / VCSEL Simulation and Advanced Quantum Well Models.

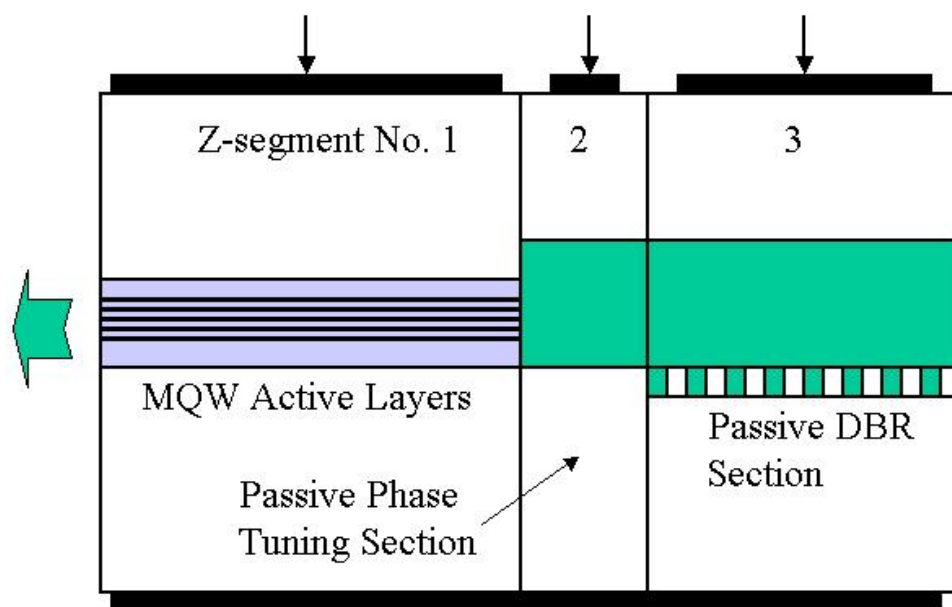




Contents

- **Multiple section tunable DFB / DBR laser.**
- **Fiber / external-cavity lasers**
- Multiple lateral / longitudinal mode simulation.
- Lateral mode competition in VCSEL.
- Different k.p theories.

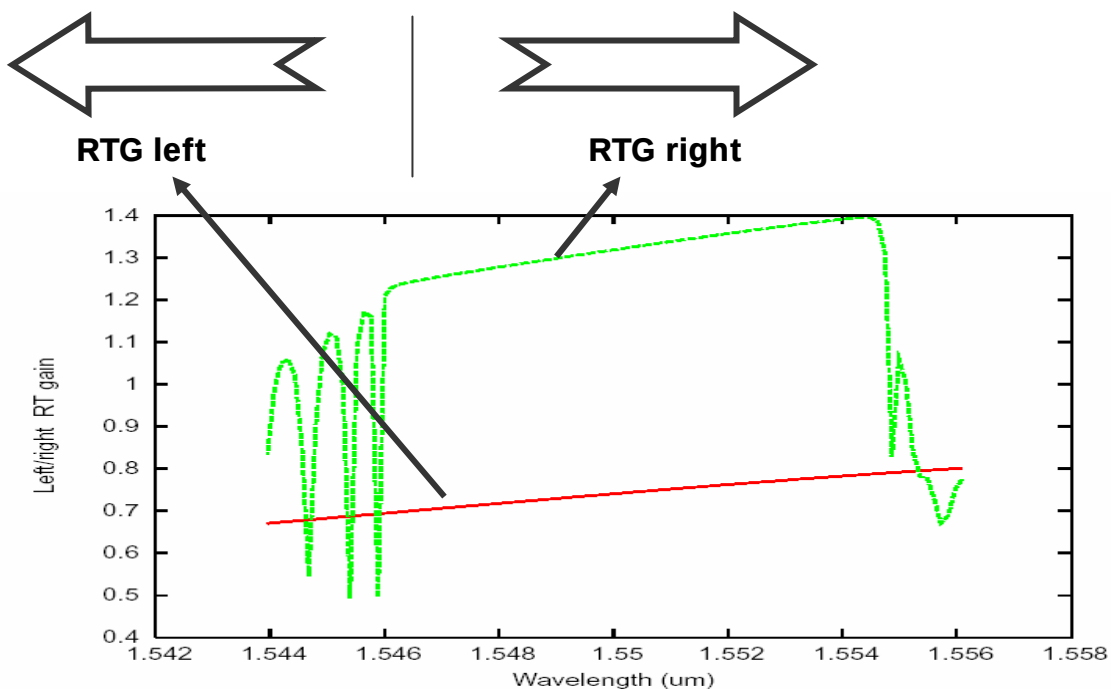
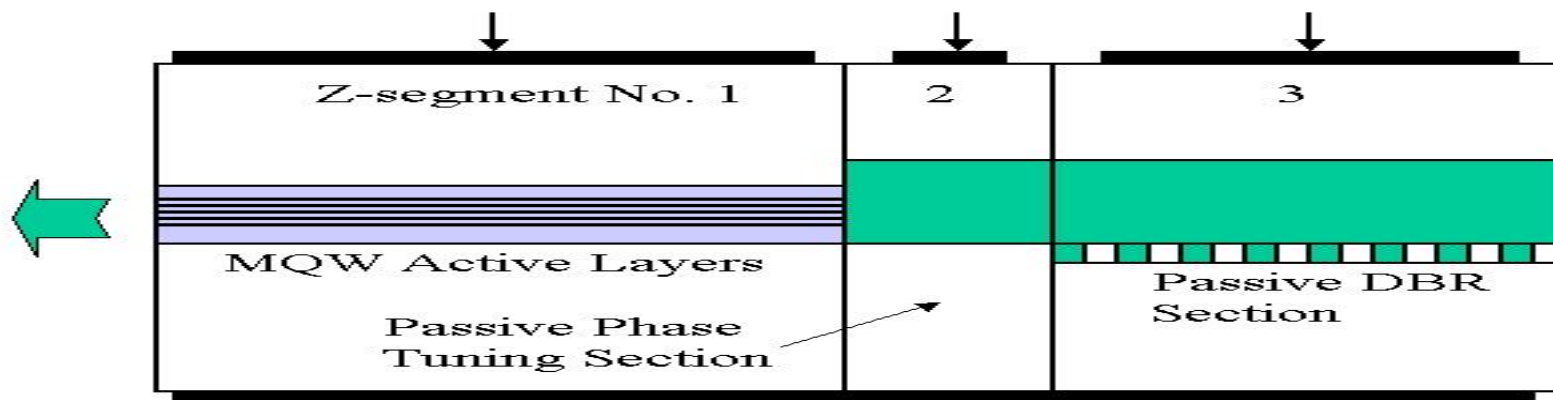
3-section DBR laser



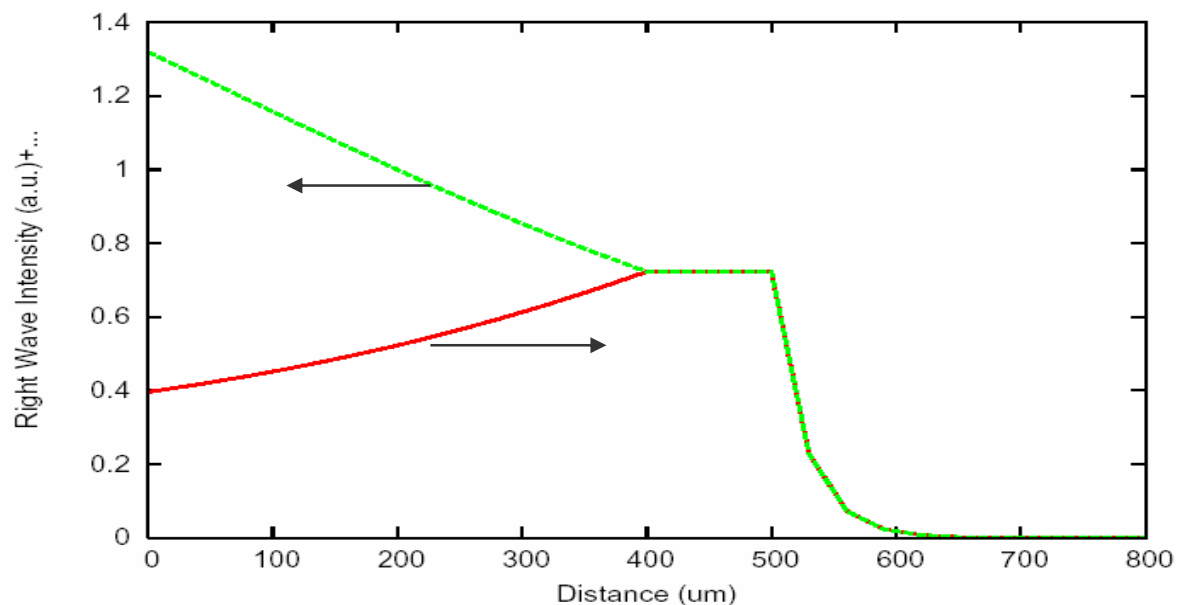
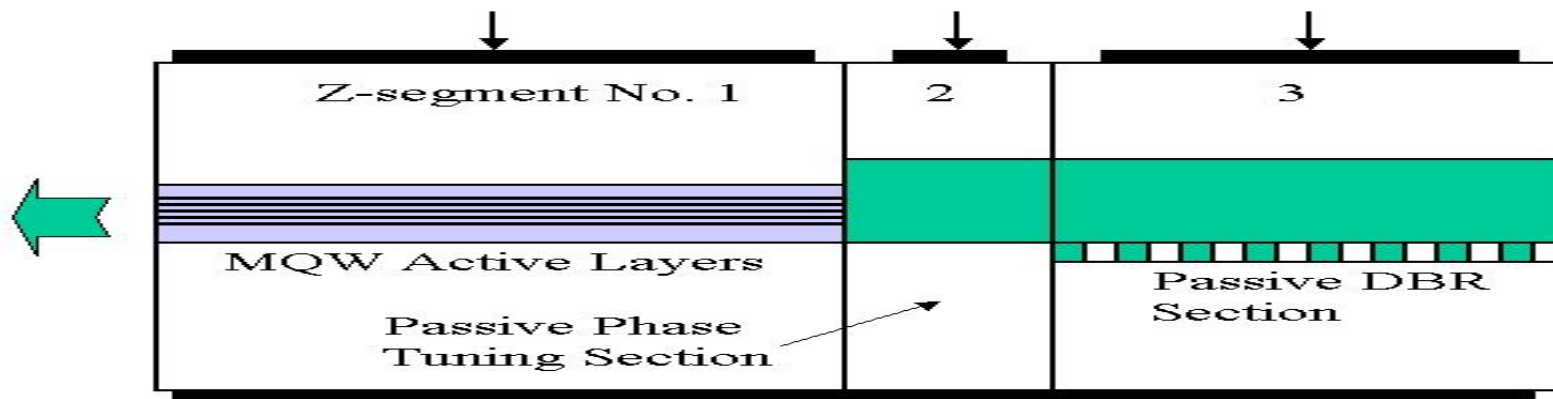
Physical model required:

- Current injection (drift-diffusion model) for all segments.
- MQW gain model in segment 1.
- Index change model in segment 2 & 3.
- DBR grating model in segment 3 (coupled mode theory).
- Lateral optical mode solver for all segments.
- Longitudinal mode model (Green's function theory) for all segments.

Round trip gain (RTG)



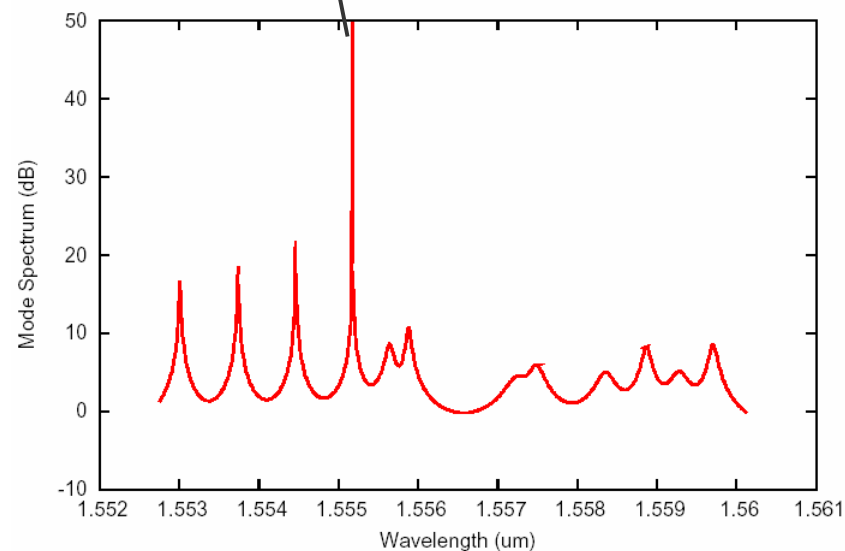
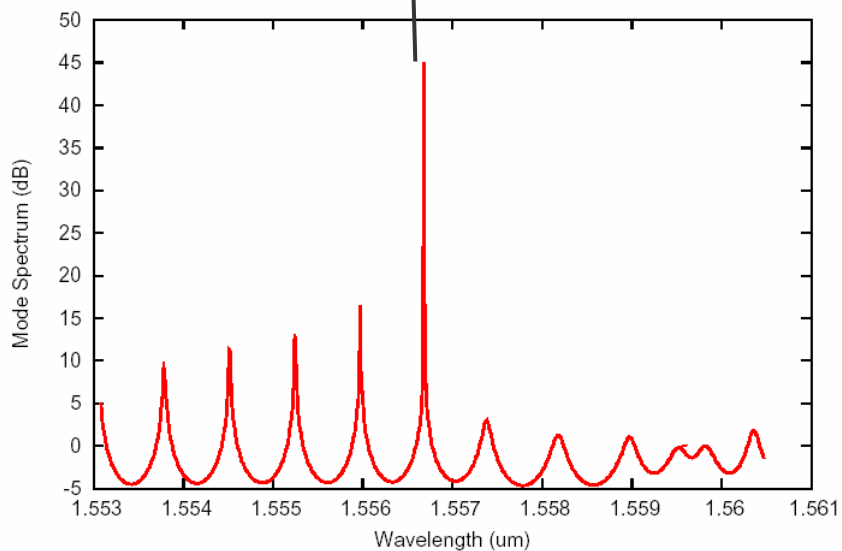
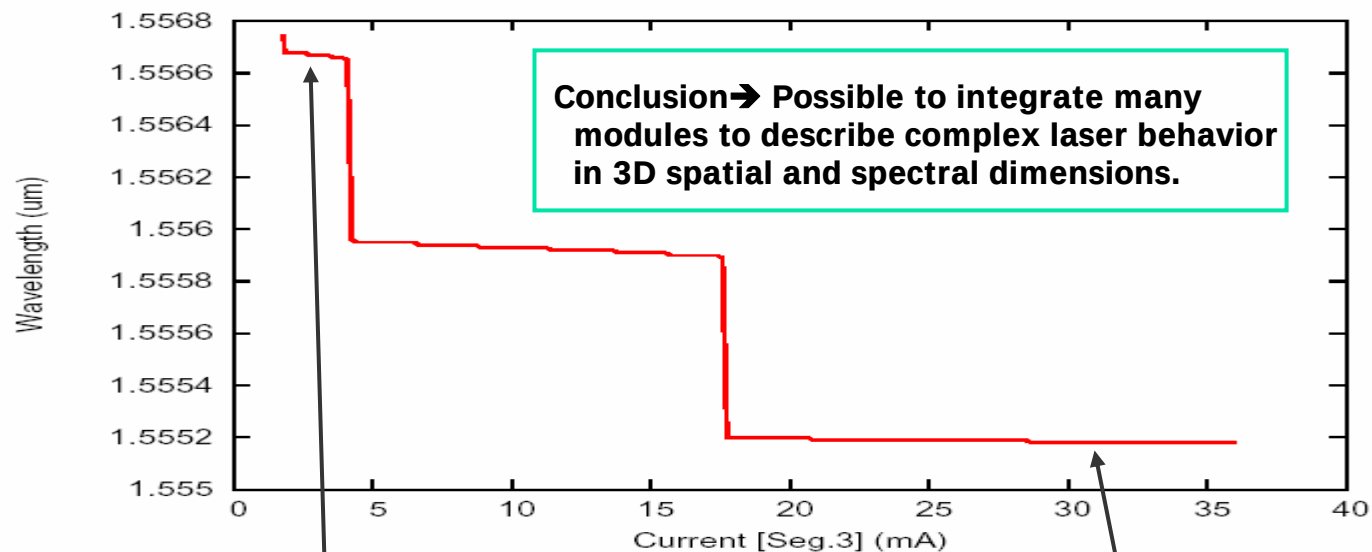
Longitudinal mode distribution



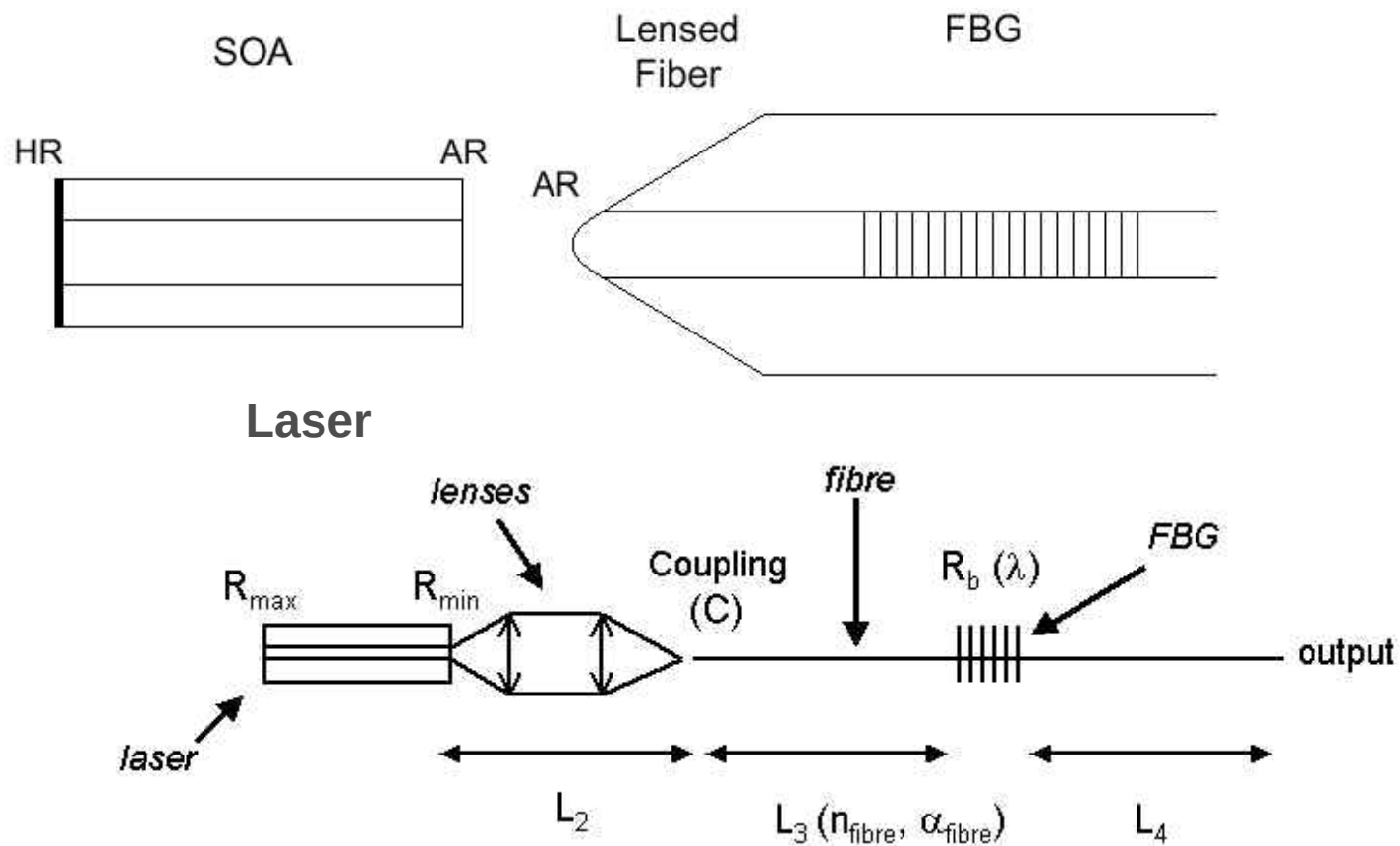
Modeling/Design Issues:

- Segments 2 & 3 should be close to but below bandgap to avoid optical loss but also to provide change of index.
- Both waveguide and DBR grating should vary with injection current.

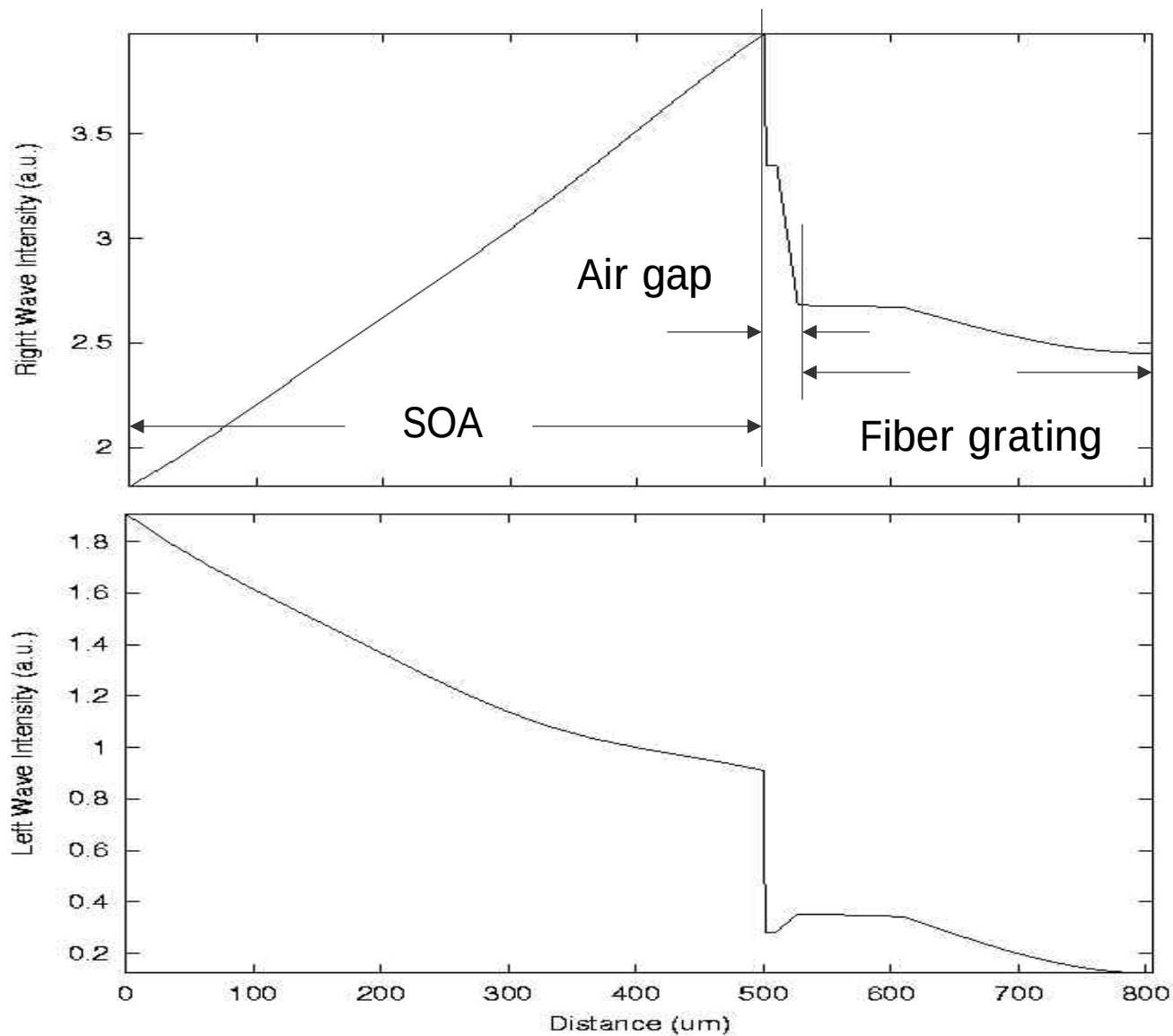
Tuning behavior



Example of fibre grating DBR laser

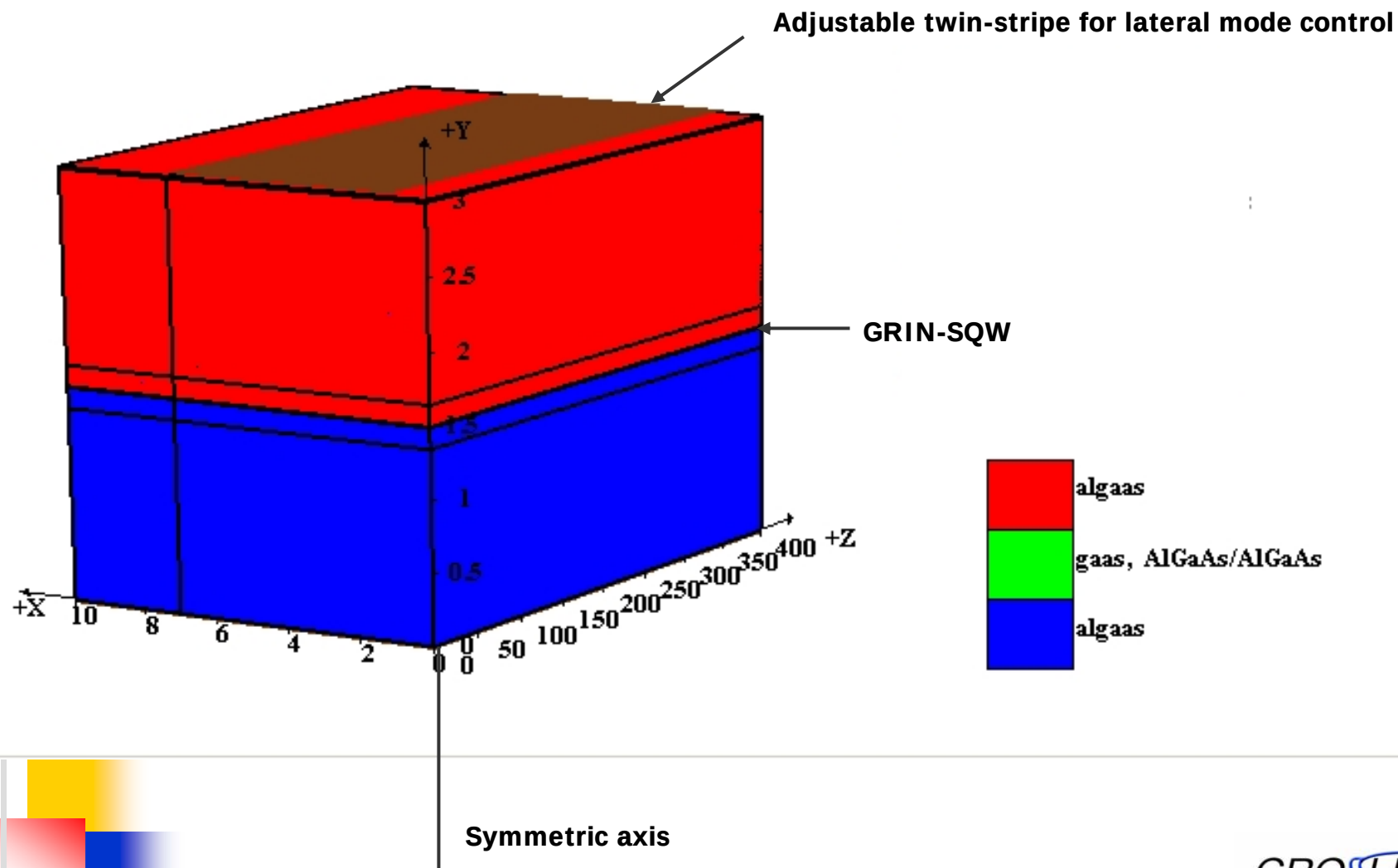


Traveling Waves:

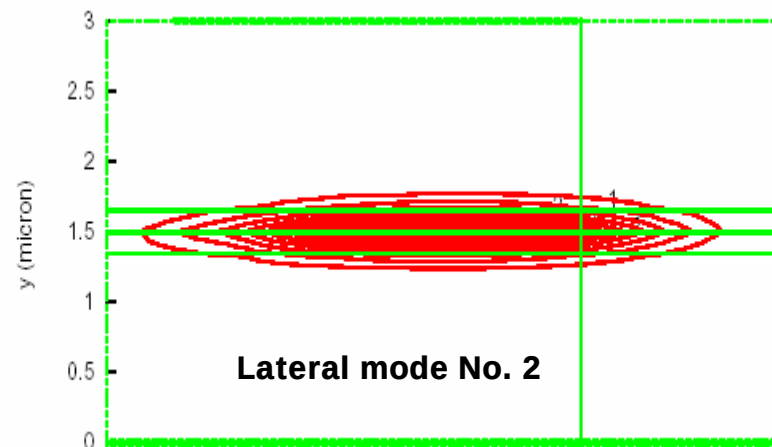
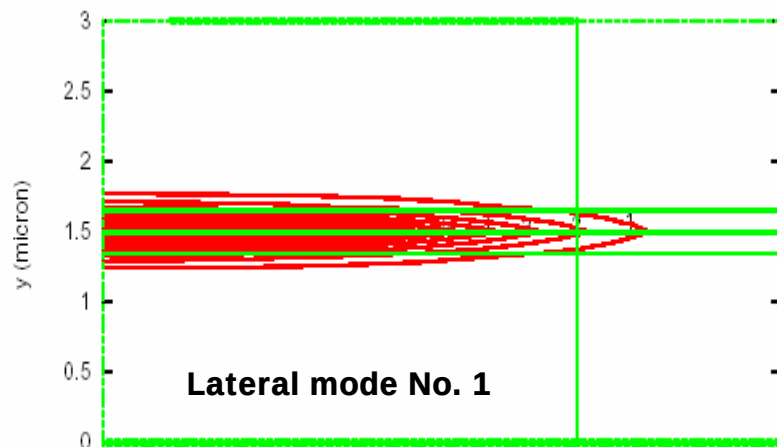
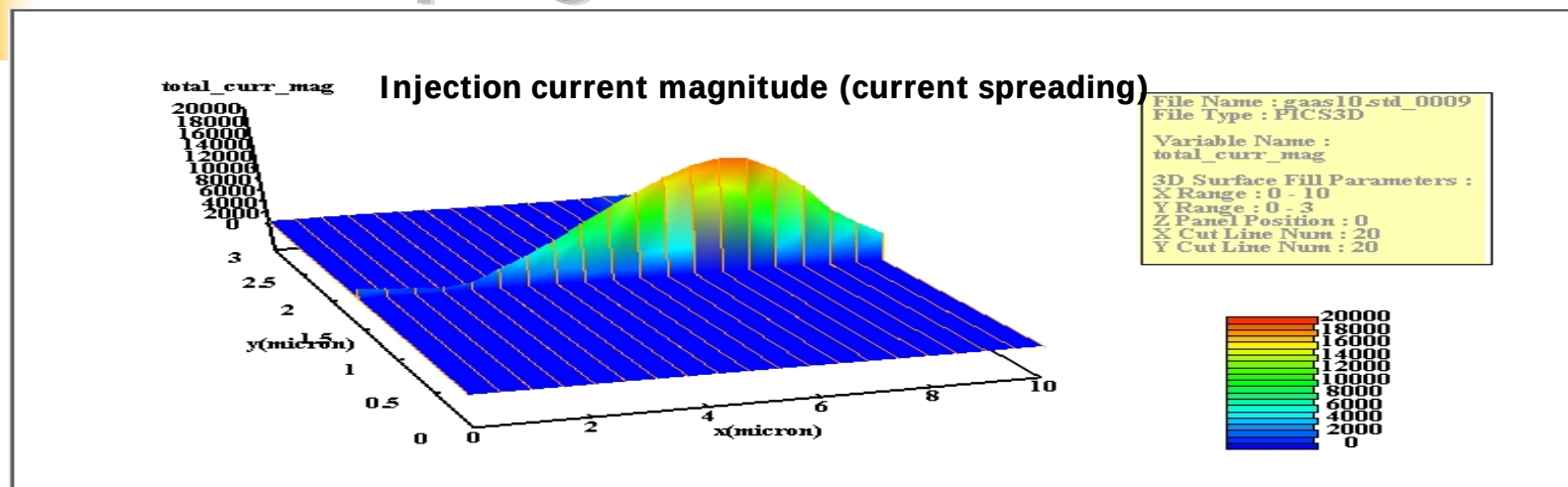


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- Multiple section tunable DFB/DBR laser.
 - **Multiple lateral/longitudinal mode simulation.**
 - Lateral mode competition in VCSEL.
 - Different k.p theories.

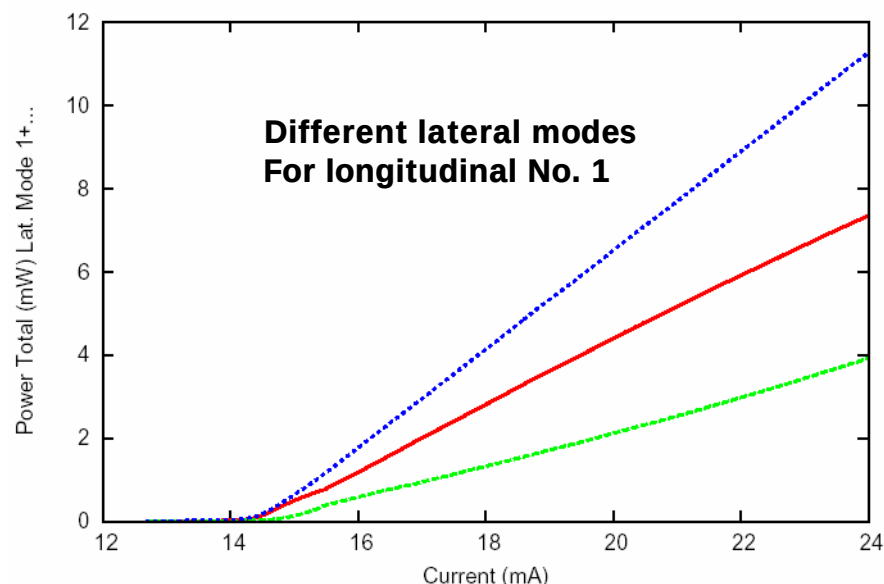
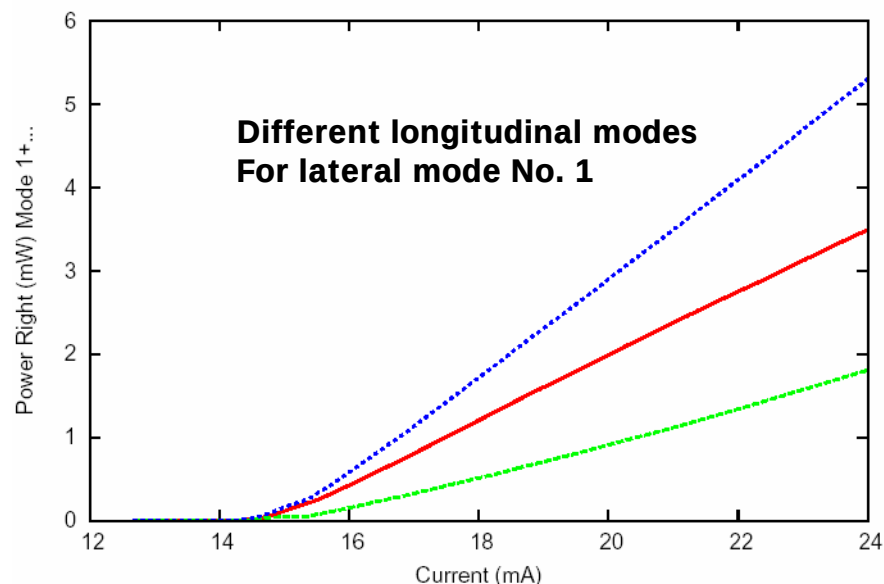
Broad-area laser with adjustable stripe



Pumping of different modes



Multi-mode considerations

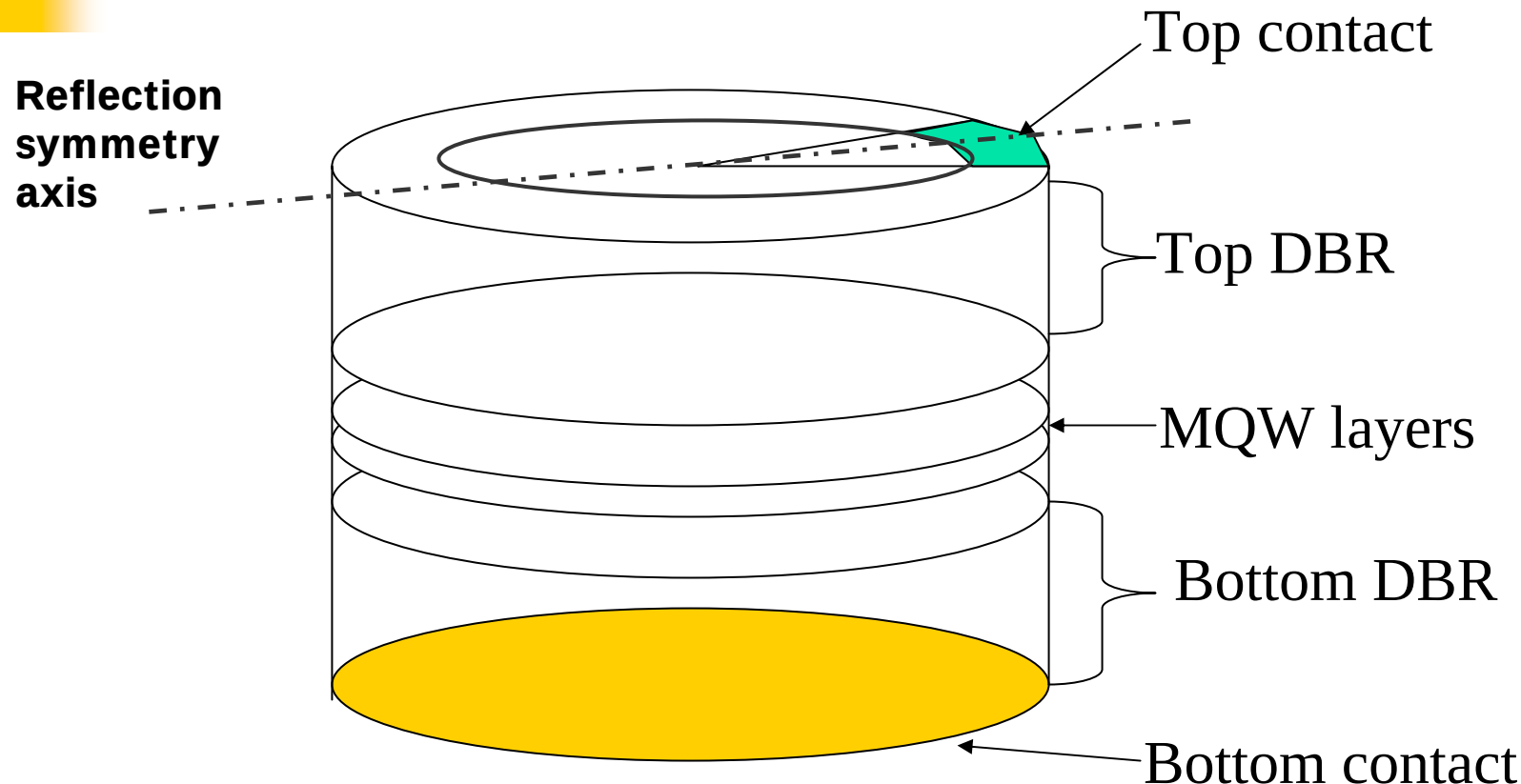


- **Must solve a whole different set of longitudinal modes using modal indices of different lateral modes.**
- **Each longitudinal mode is always associated with a particular lateral mode.**
- **Must consider longitudinal and lateral spatial hole burning effects for different lateral/longitudinal modes.**



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- Multiple section tunable DFB/DBR laser.
 - Multiple lateral/longitudinal mode simulation.
 - **Lateral mode competition in VCSEL.**
 - Different k.p theories.

Symmetric v. asymmetric VCSEL



Models required:

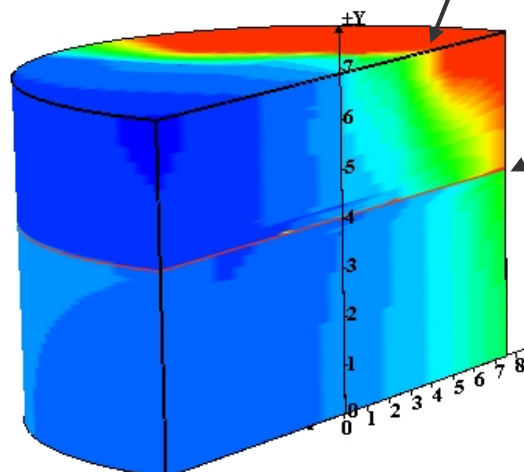
- Full 3D drift-diffusion model: cylindrical symmetry no longer available.
- Lateral mode model with both ϕ and θ dependence.
- MQW gain model as usual.
- Transfer matrix model for longitudinal modes as usual.

Asymmetric VCSEL injection

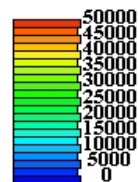
Current magnitude

Contact

QW's

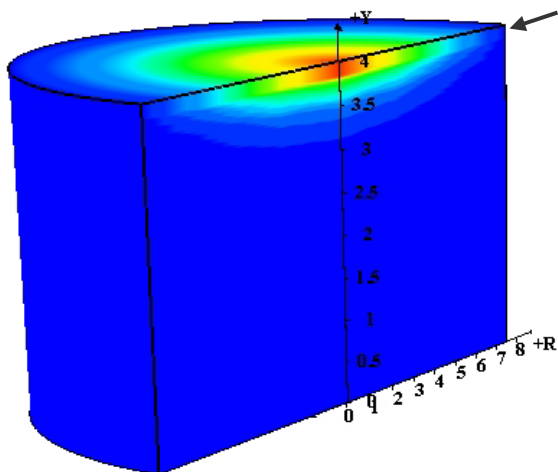


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File Type : PICS3D
Variable Name :
total_curr_mag
3D Cube Contour Parameters :
X Range : 0 - 7.5
Y Range : 0 - 6.8959
Z Range : 0 - 180
X Cut Line Num : 20
Y Cut Line Num : 20
Z Cut Line Num : 20



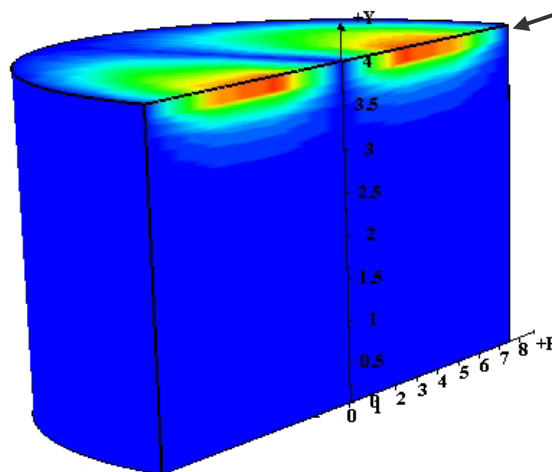
Fundamental mode

QW's

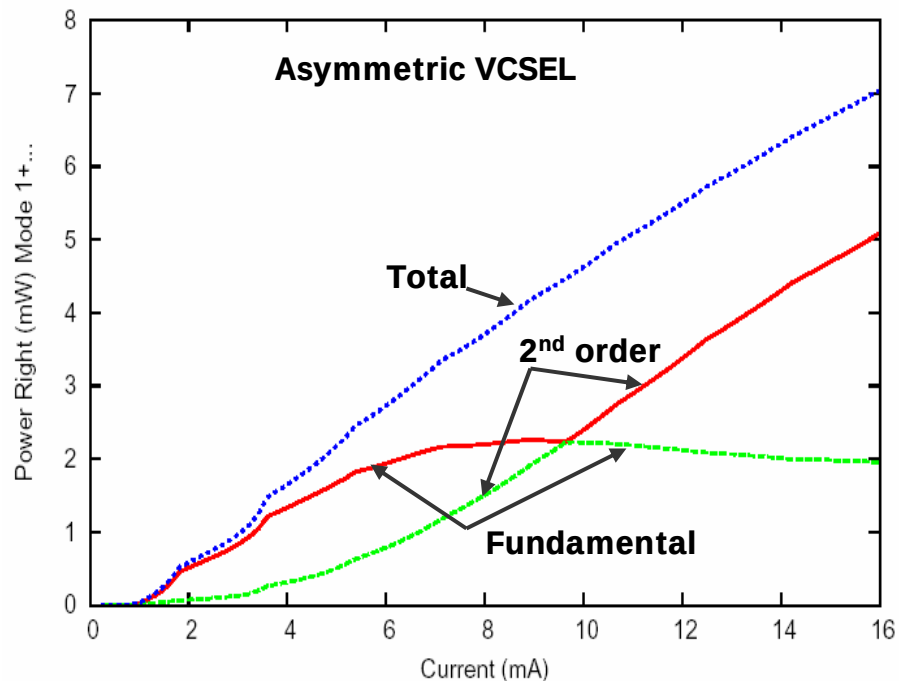


2nd order mode

QW's

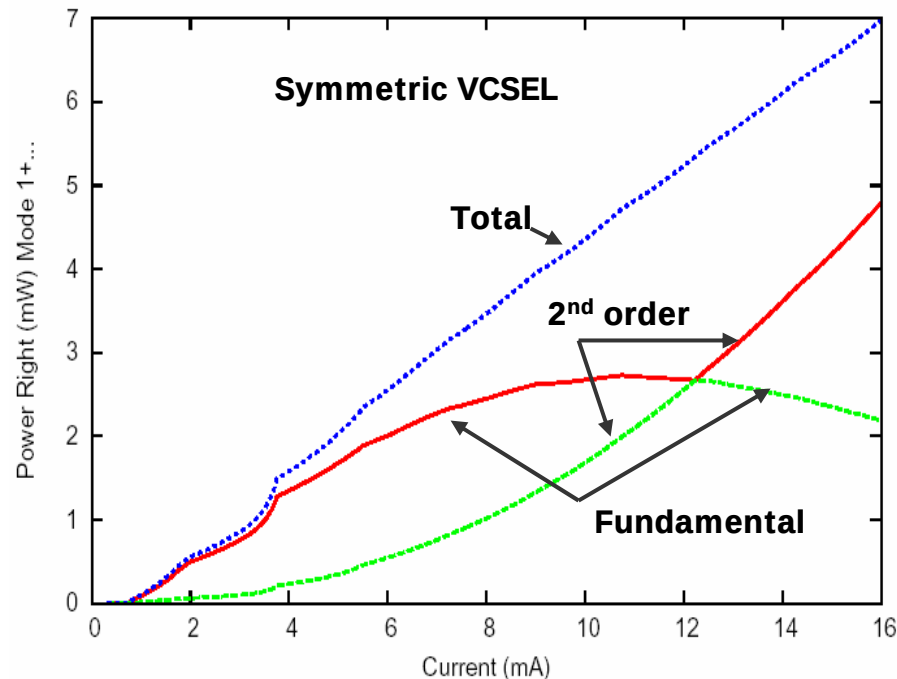


Mode competition behavior



Conclusions

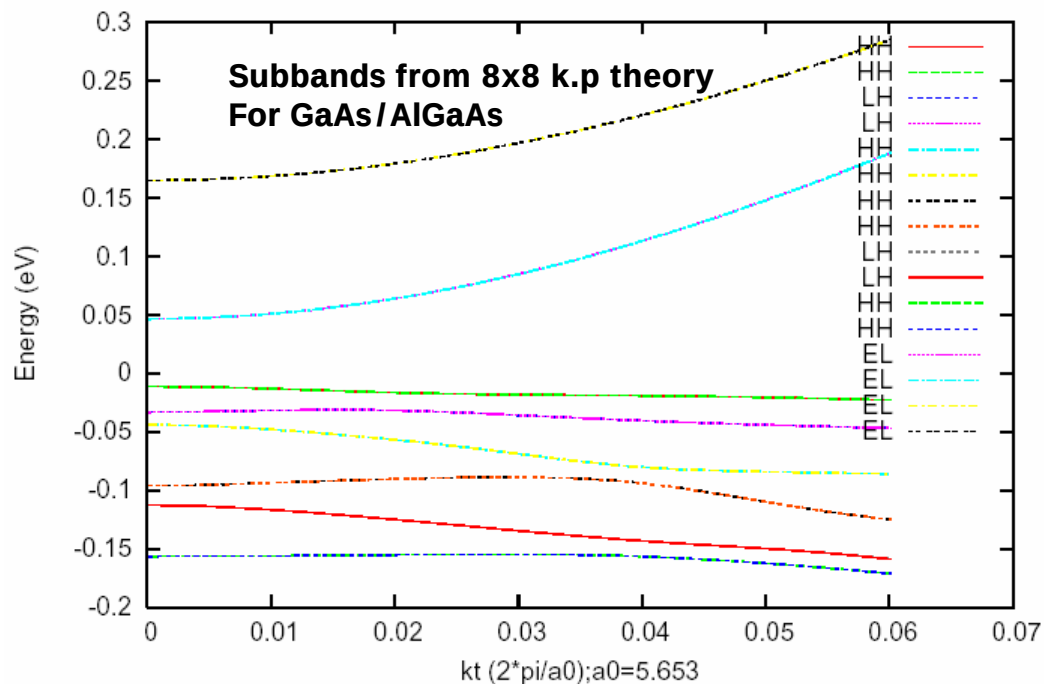
- a) VCSEL has similar lateral mode competition behavior as edge laser;
- b) Asymmetric VCSEL mode is necessary to simulate multi-lateral mode behavior.



- Multiple section tunable DFB/DBR laser.
- Multiple lateral/longitudinal mode simulation.
- Lateral mode competition in VCSEL.
- **Different k.p theories.**

k.p theories for zinc-blende

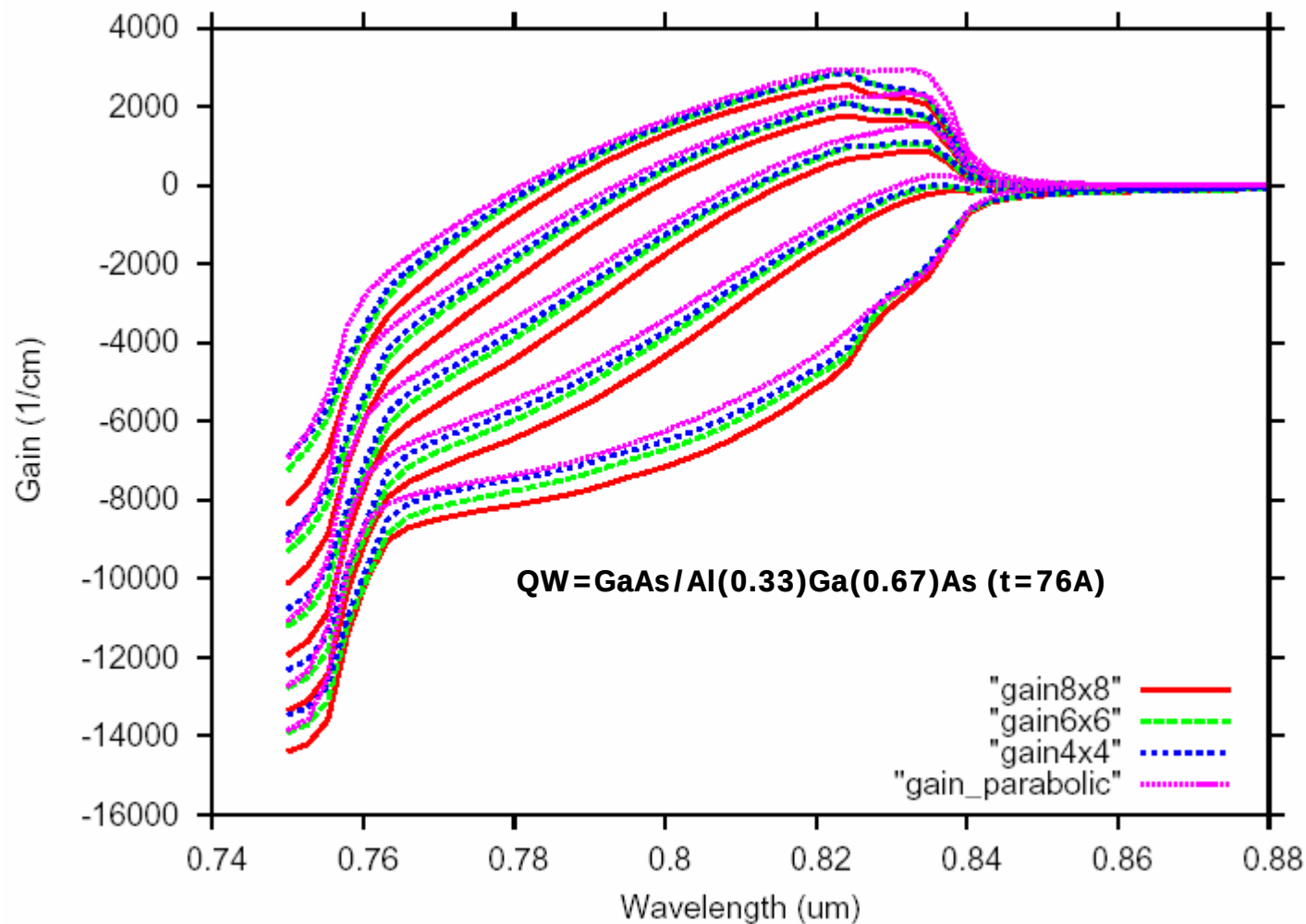
4-band k.p Model, Conduction and Valence Subbands versus kt



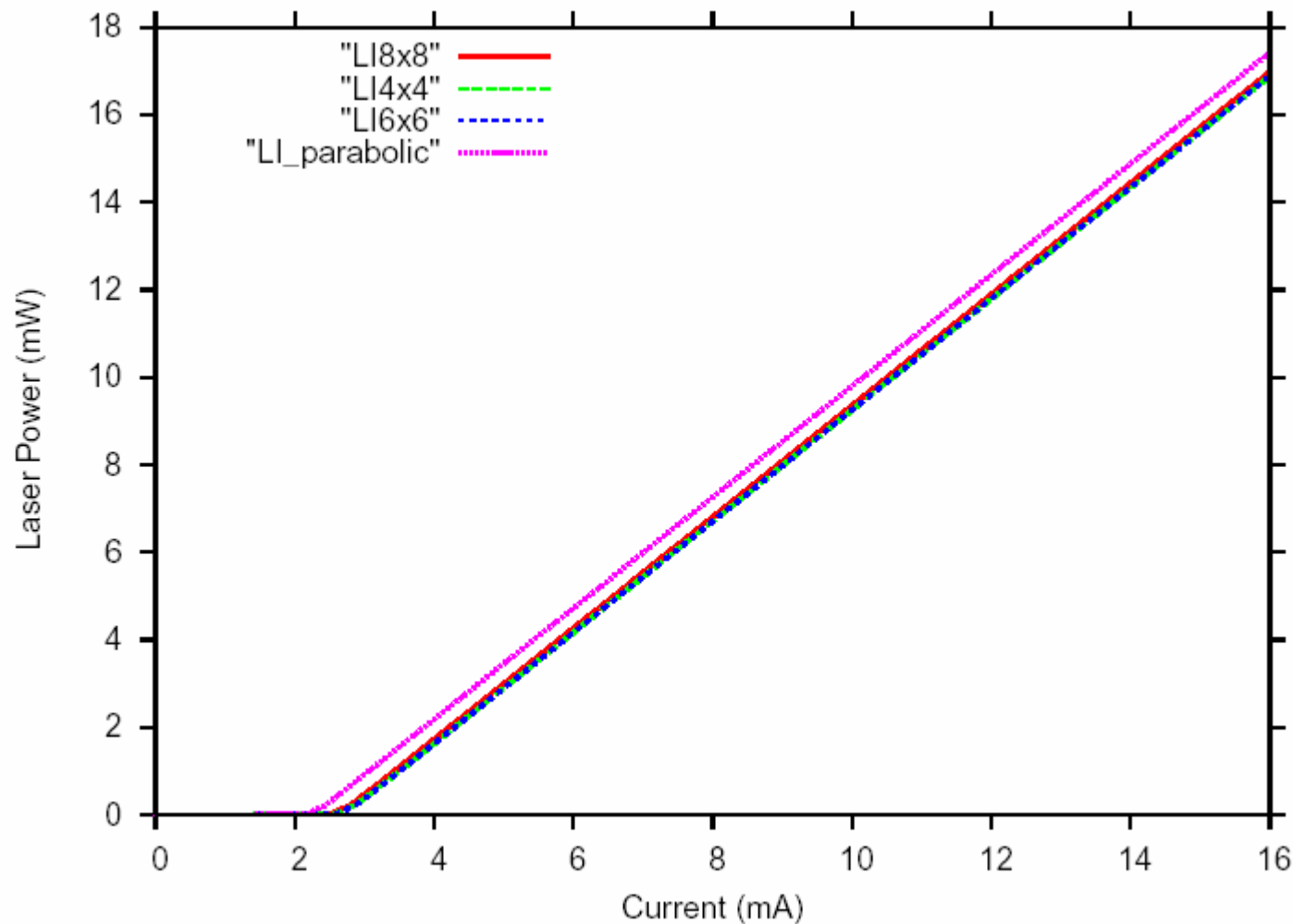
Motivations:

- When conventional parabolic gain model does not fit experiment, we need to try something else.
- Need to determine whether it is worth the trouble to go to higher order k.p theories.

Comparison for GaAs / AlGaAs QW

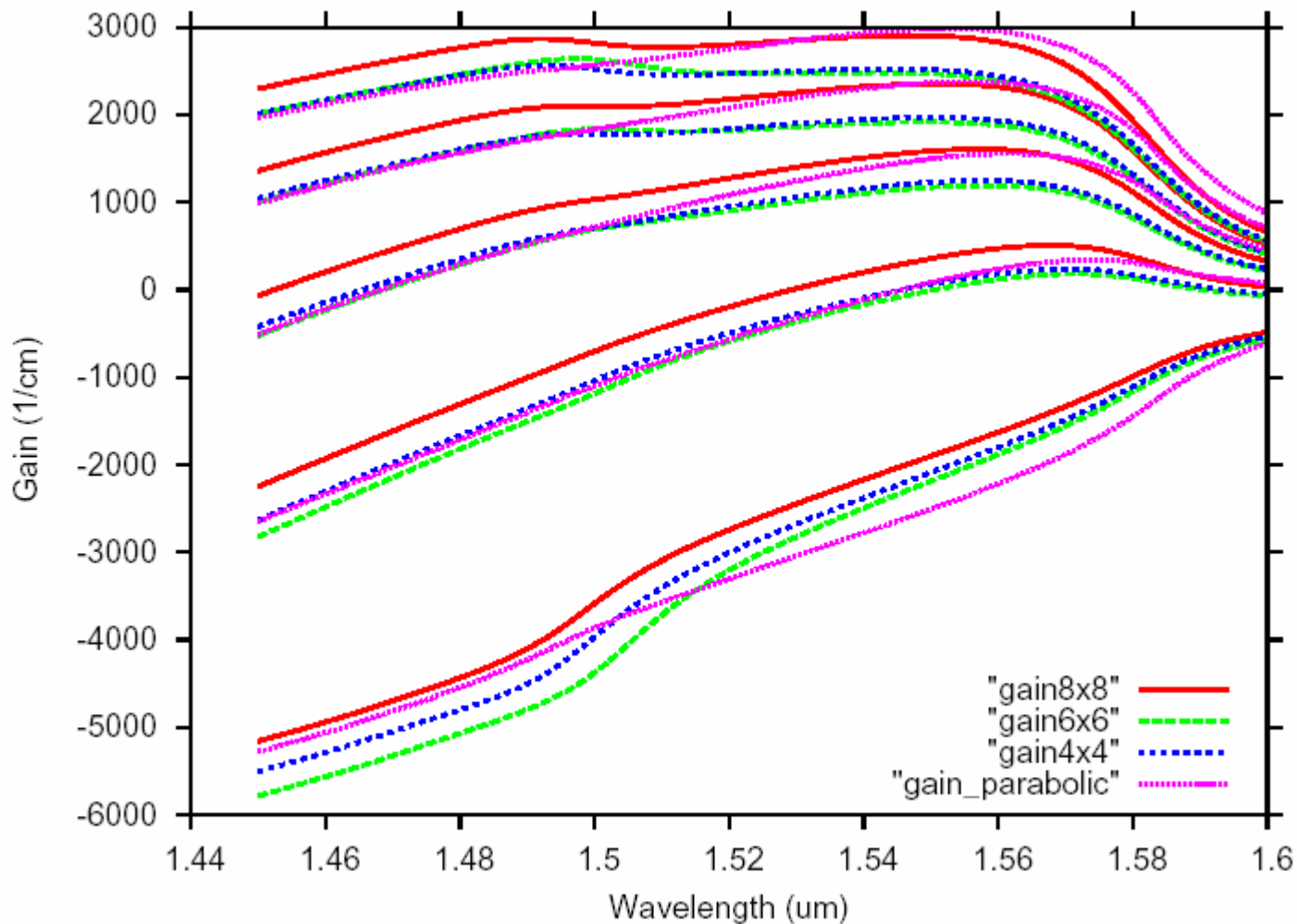


Light v. current



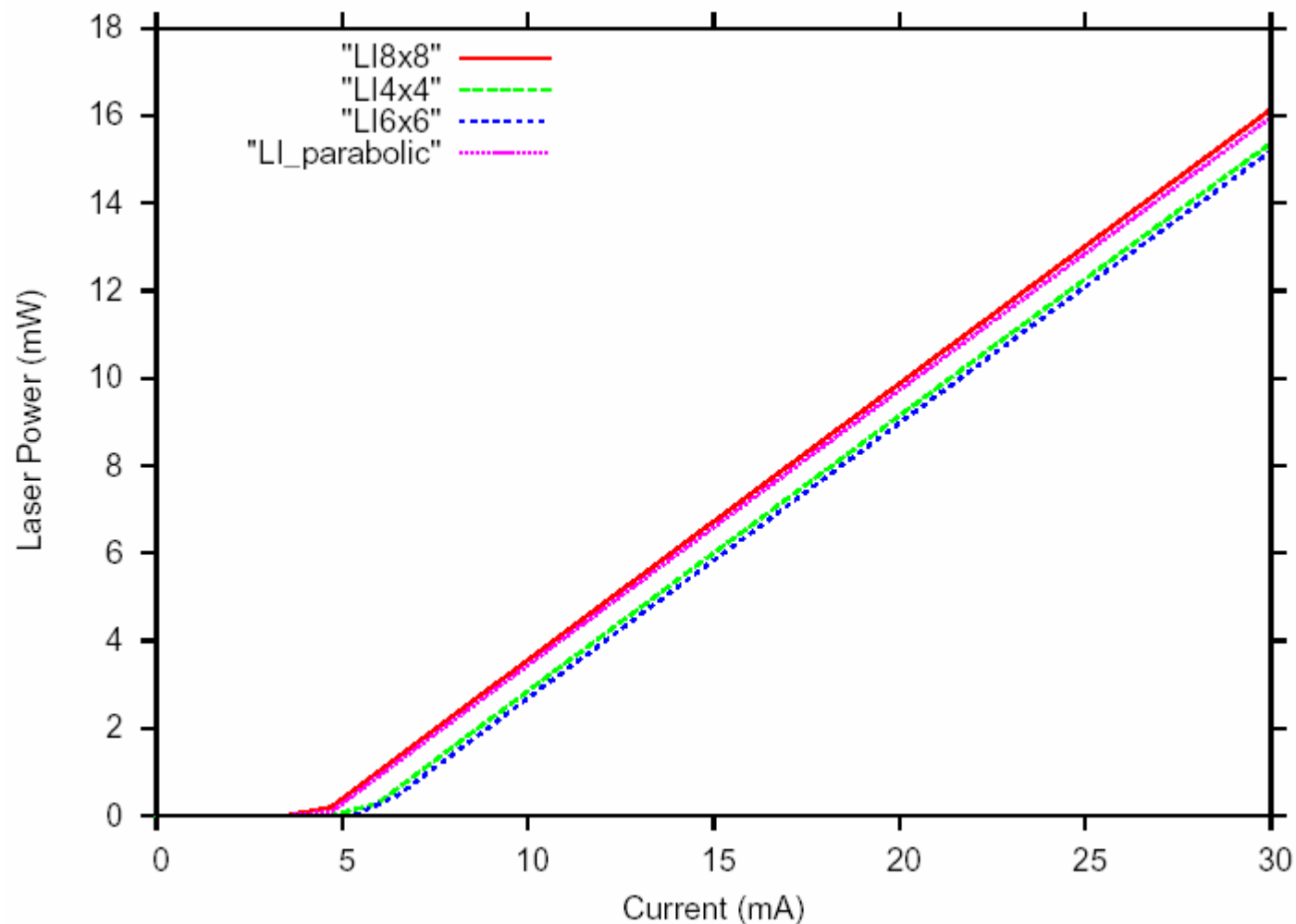
QW=GaAs/Al(0.33)Ga(0.67)As (t=76Å)

Comparison for InGaAsP QW



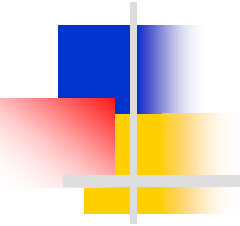
QW = InGa(.47)As / In(.74)Ga(.26)As(.57)P(.43) t = 60Å

InGaAsP QW L-I curve

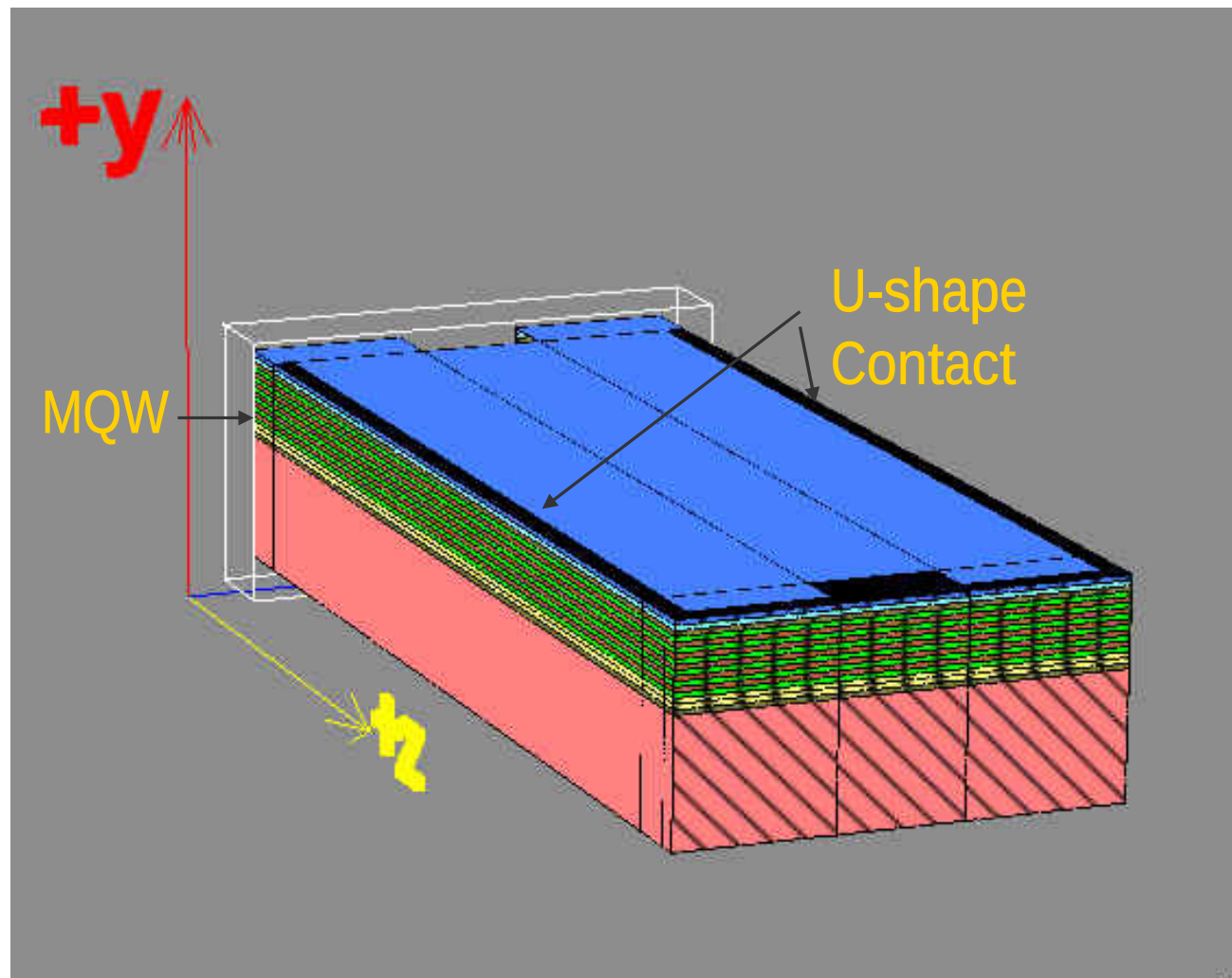


QW = InGa(.47)As / In(.74)Ga(.26)As(.57)P(.43) t = 60Å

Simulation of InGaN/GaN MQW LED with U-shape Contact



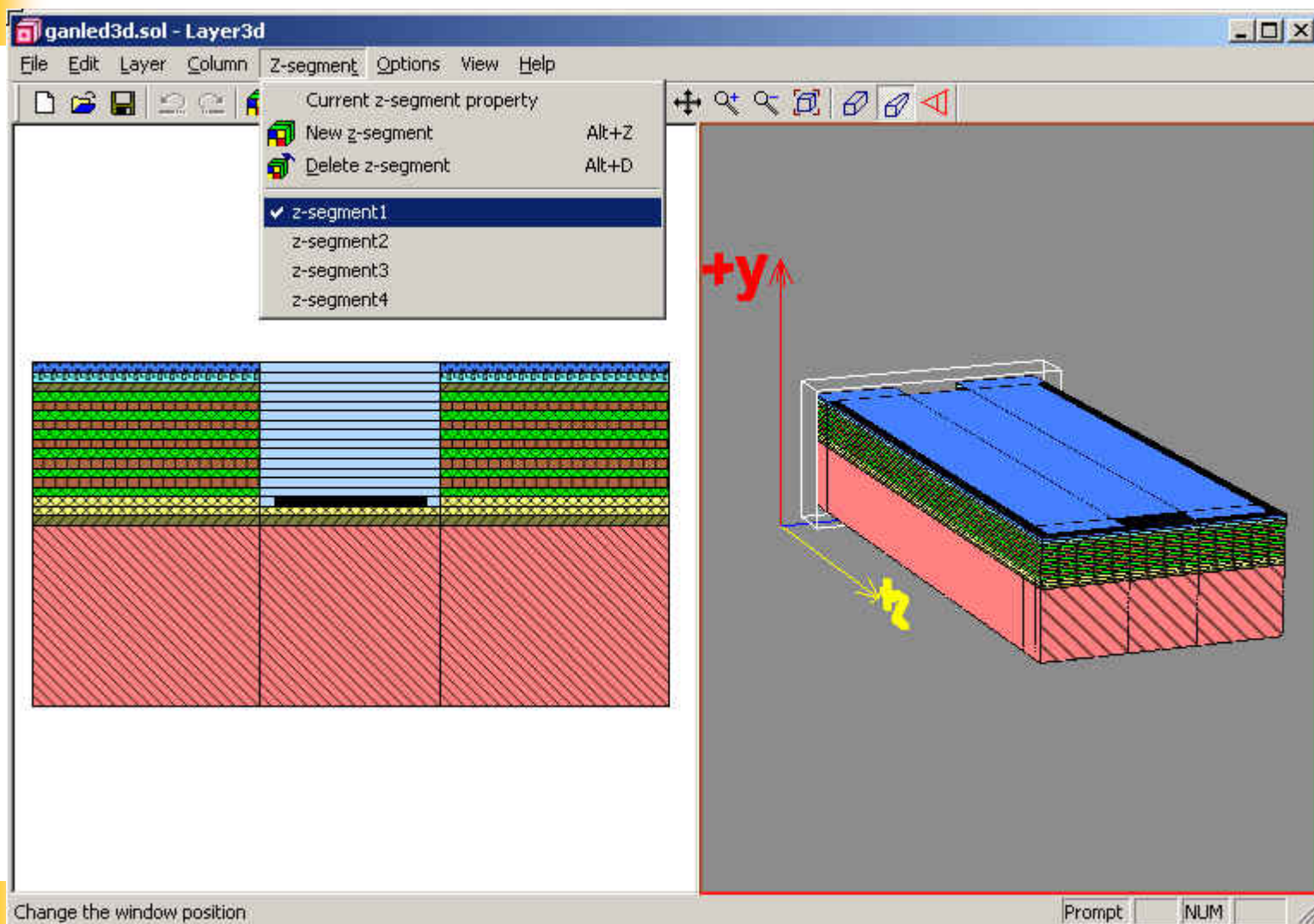
Structure



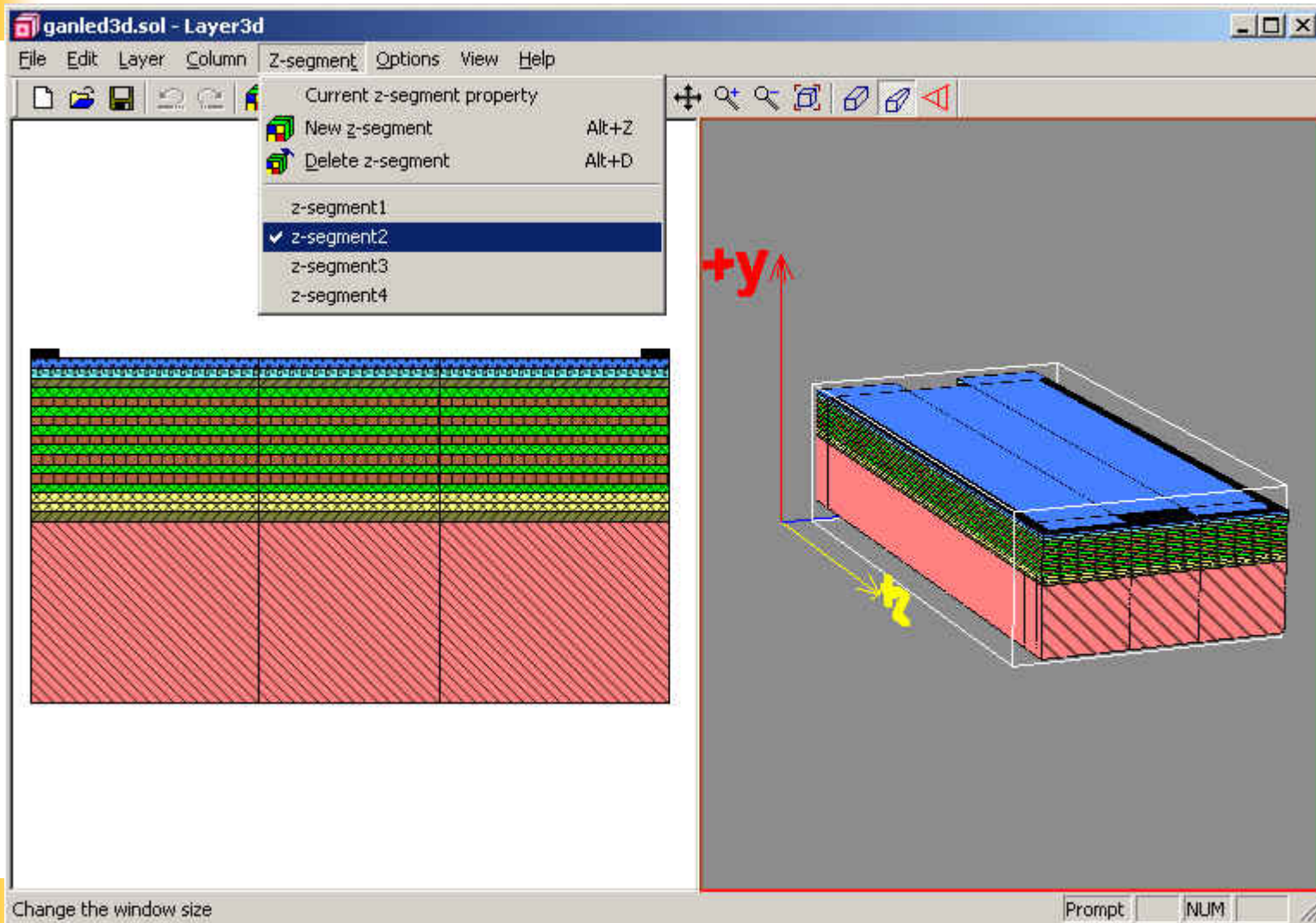
Physical Models

- Quantum drift-diffusion model for current flow/spreading (included).
- MQW quantum well gain/spontaneous emission model with effective mass approximation (included).
- 3D ray-tracing model (included).
- K.p model for MQW (optional).
- Self-heating model (optional).
- Polarization surface charge/self-consistent model (optional).

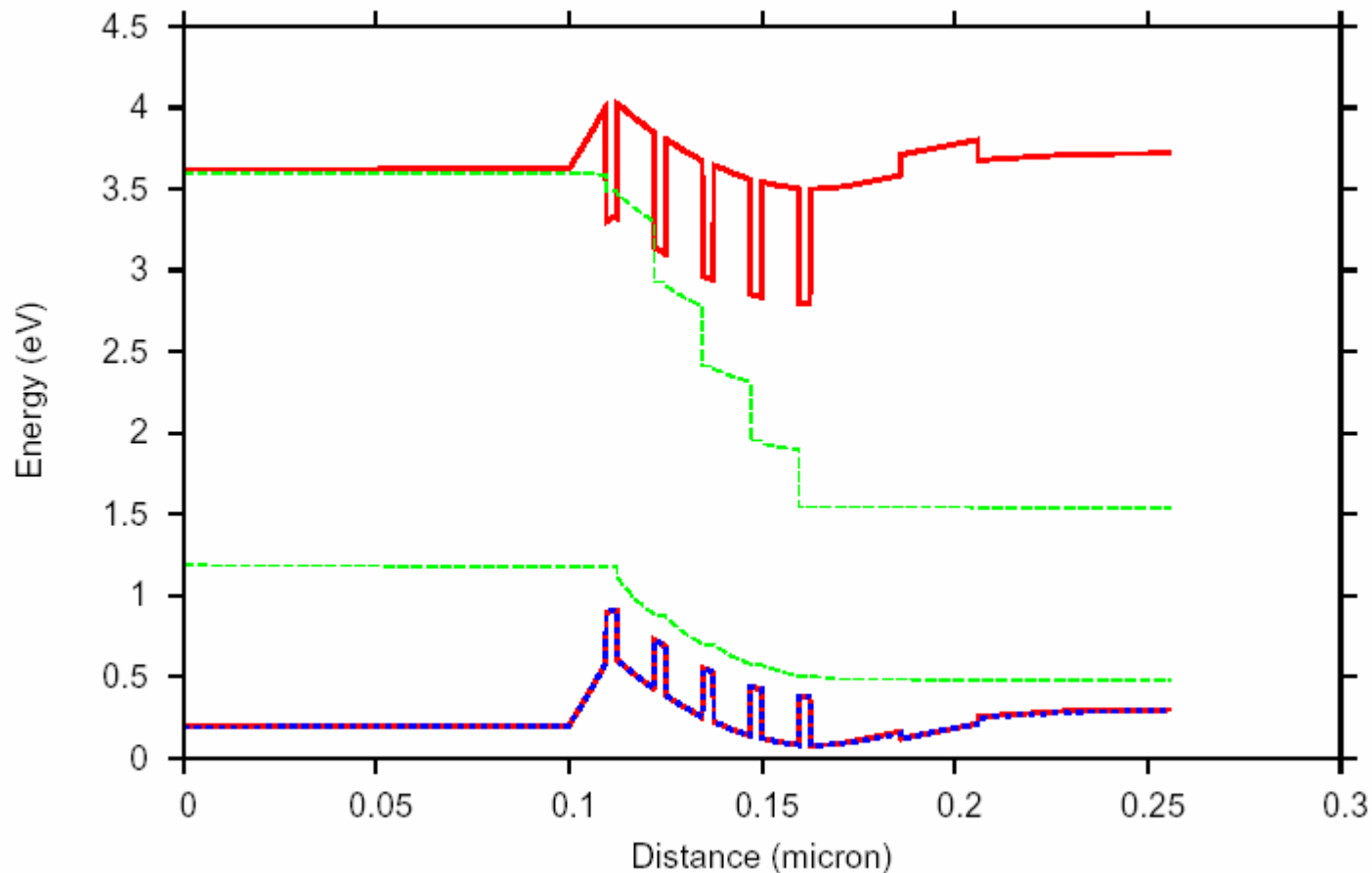
Z-segment1



Z-segment2

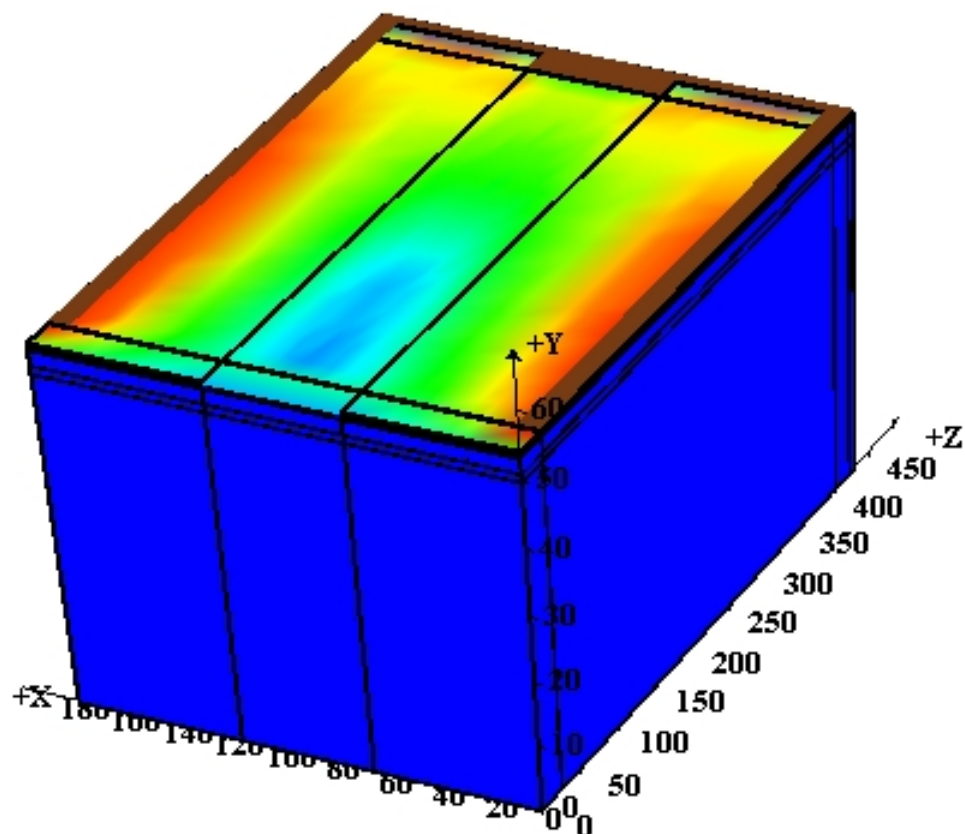


Band Diagram



May be viewed at any positions

3D View: Current at QW

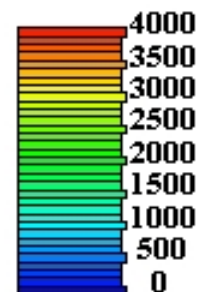


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File Type : APSYS

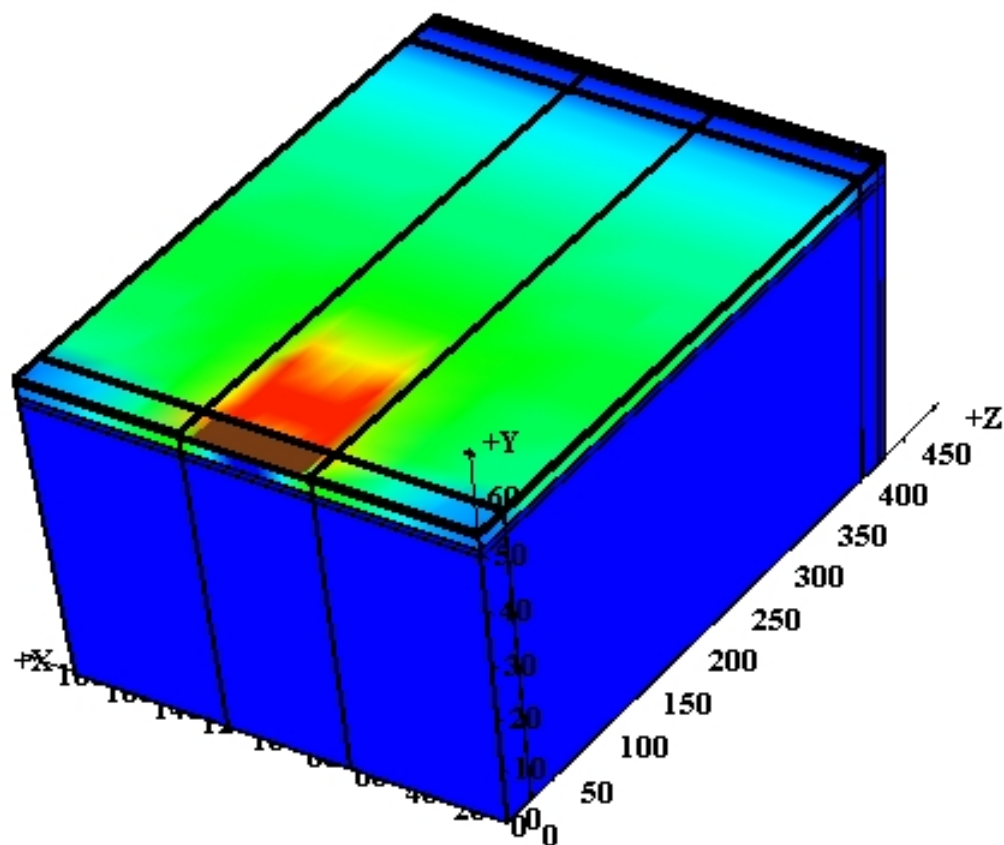
Variable Name :
total_curr_mag

3D Cube Contour Parameters :
X Range : 0 - 176
Y Range : 0 - 53.81
Z Range : 0 - 428

X Cut Line Num : 20
Y Cut Line Num : 20
Z Cut Line Num : 20



3D View: Current below QW

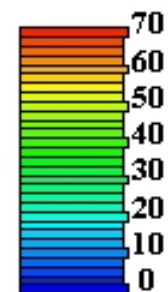


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File Type : APSSYS

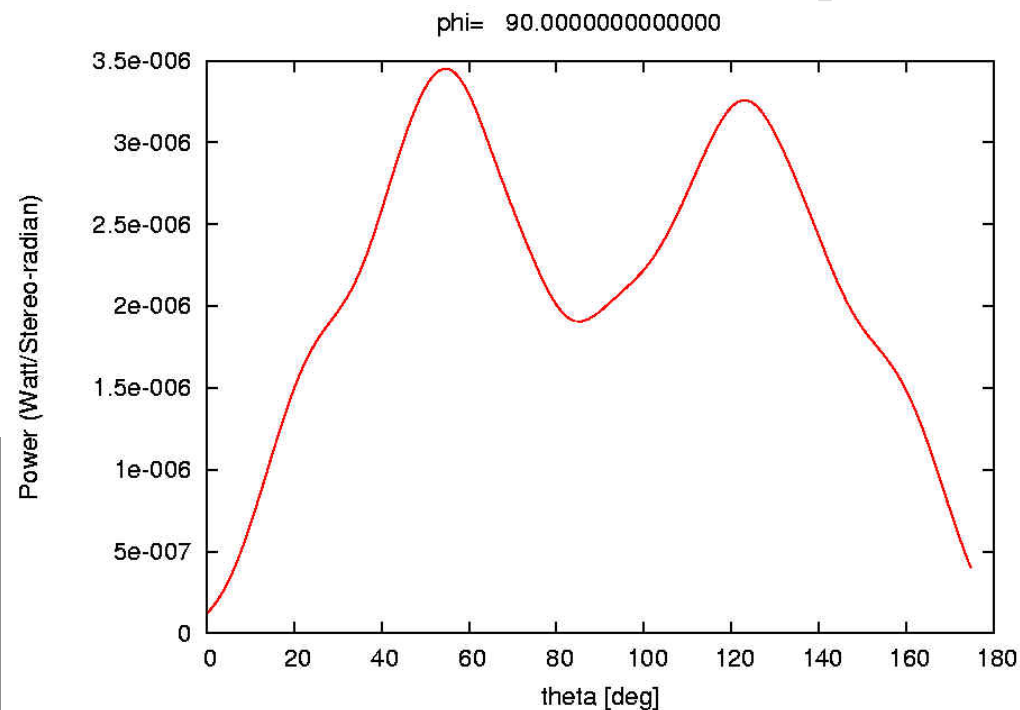
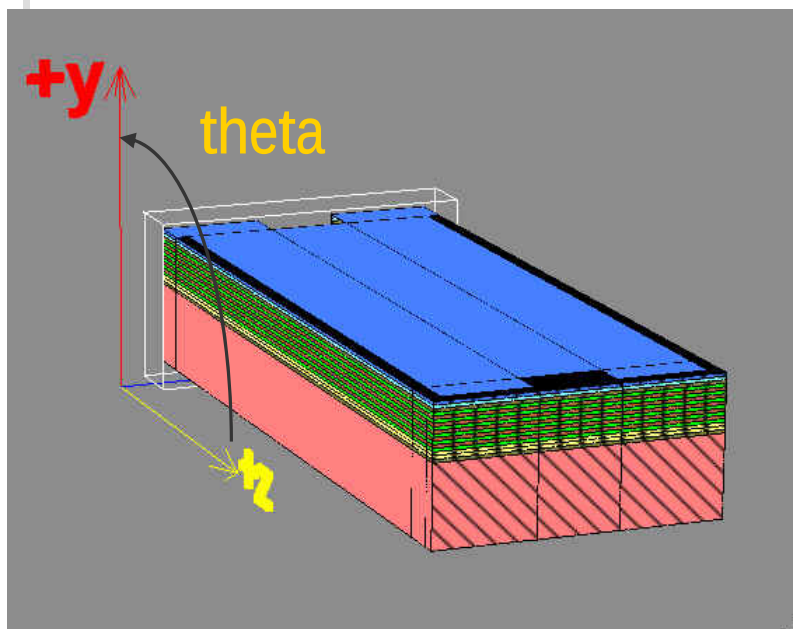
Variable Name :
total_curr_mag

3D Cube Contour Parameters :
X Range : 0 - 176
Y Range : 0 - 53.3
Z Range : 0 - 428

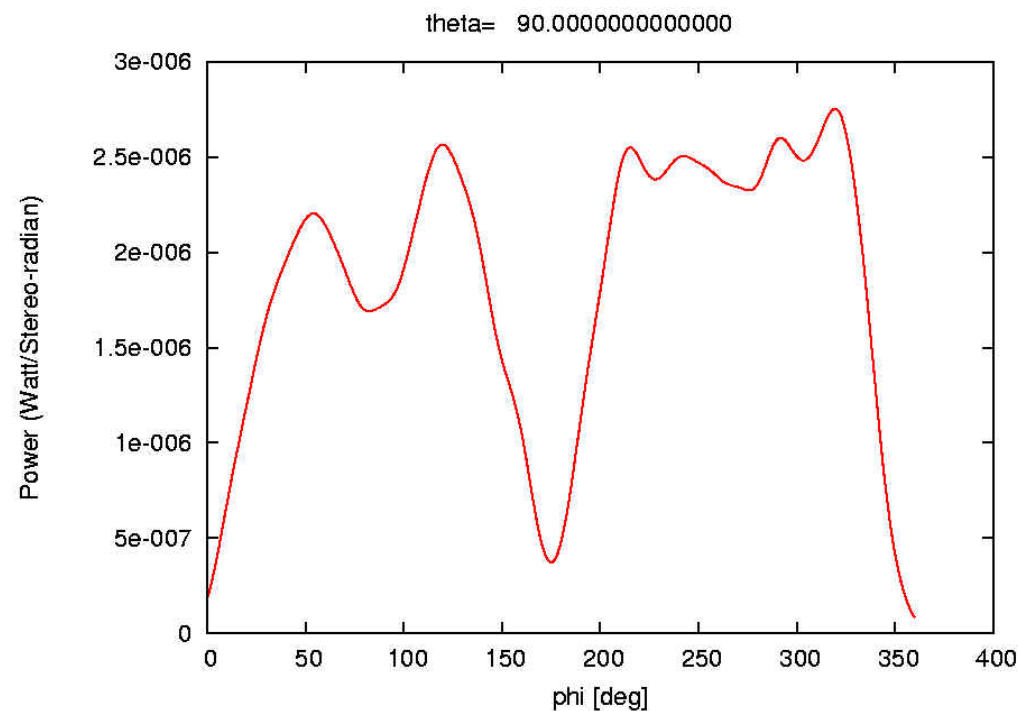
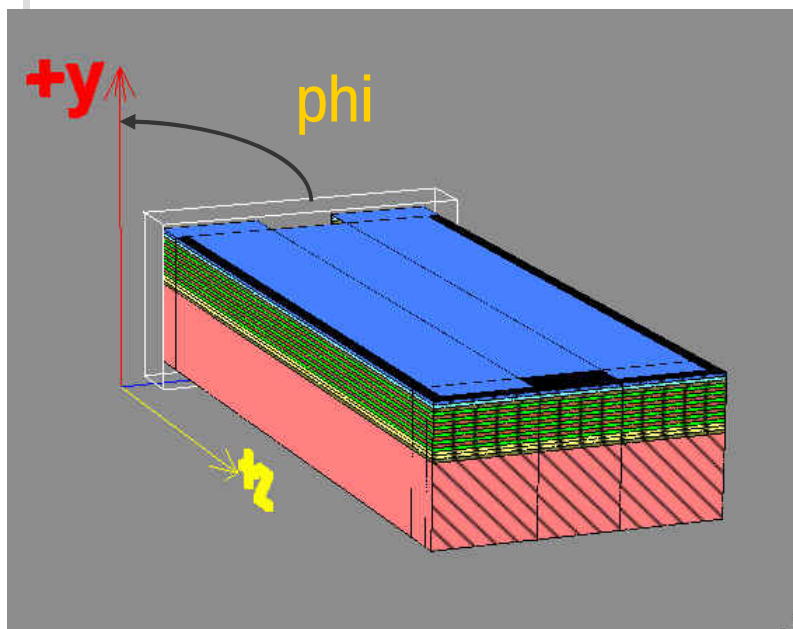
X Cut Line Num : 20
Y Cut Line Num : 20
Z Cut Line Num : 20



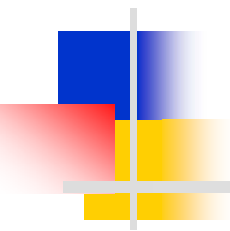
Raytracing: emission to the top



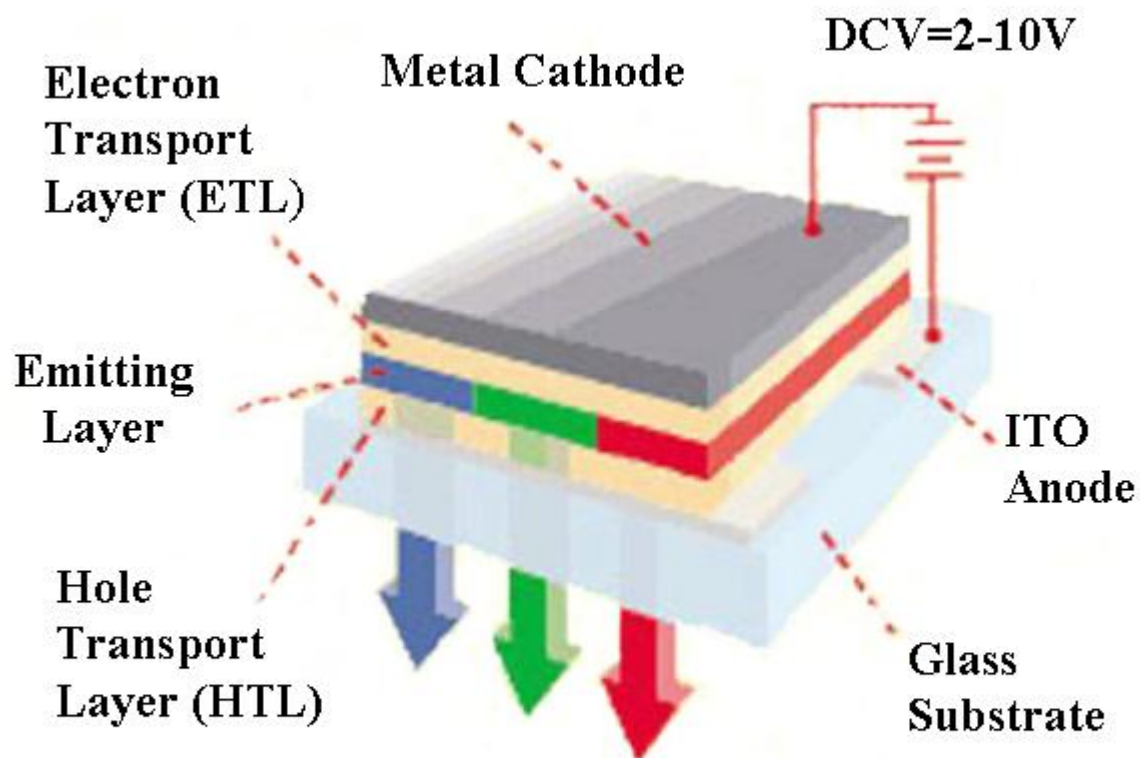
Raytracing: emission around



Simulation of an Alq3/TPD OLED

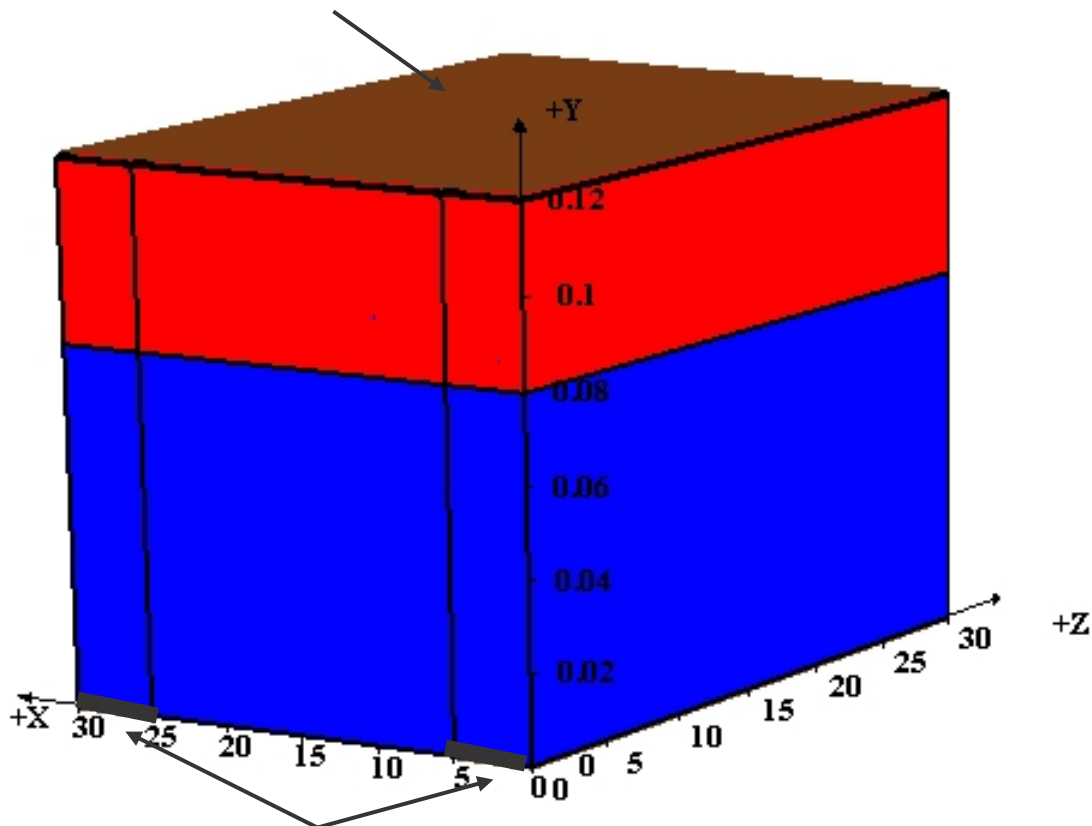


Structure



Coordinates

Metal Cathode



File Name : ol2.std_0003
File Type : APTSYS

Variable Name :
material_num

3D Cube Contour Parameters :

X Range : 0 - 30

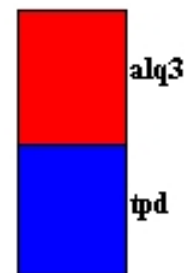
Y Range : 0 - 0.12

Z Range : 0 - 30

X Cut Line Num : 20

Y Cut Line Num : 20

Z Cut Line Num : 20

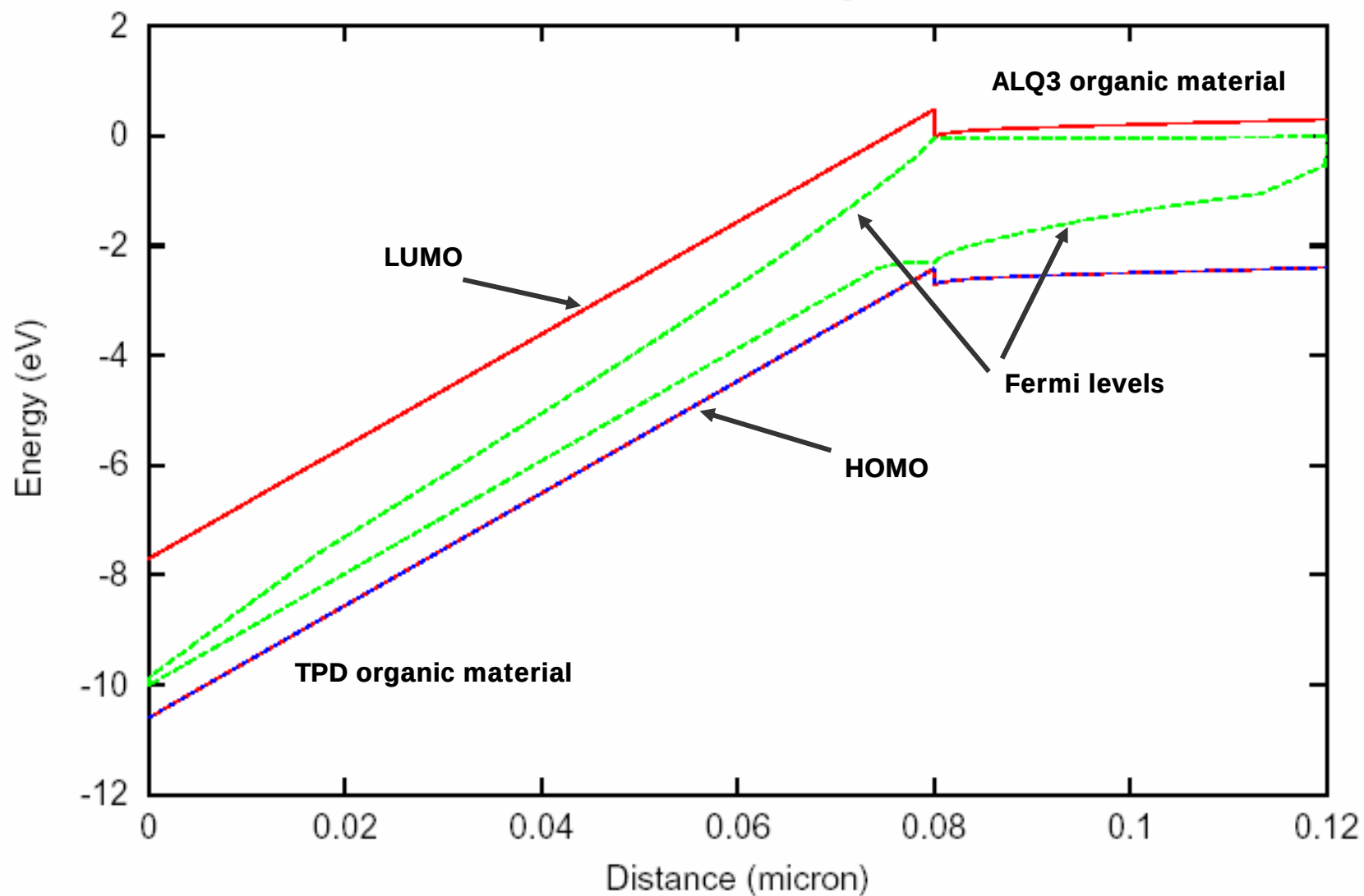


ITO Anode

Physical Models

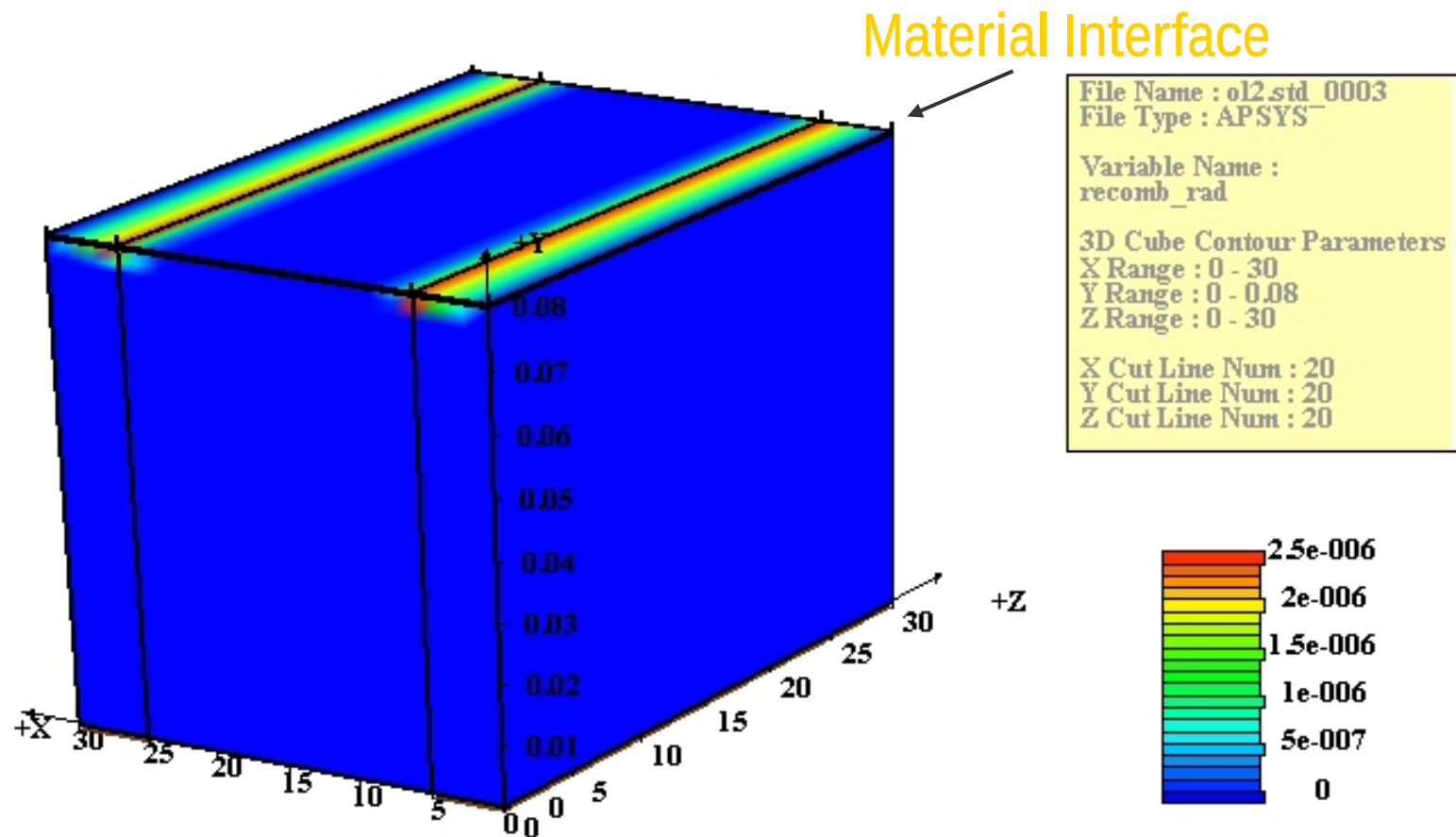
- Quantum drift-diffusion model for current flow/spreading (included).
- Poole-Frenkel field dependent mobility model (included).
- Mobility-dependent bi-molecular radiative recombination model (included).
- 3D ray-tracing model (included).
- Deep level trap model (included).
- Quantum tunneling model for Schottky barriers and heterojunctions (optional).
- Self-heating model (optional).

Band Diagram

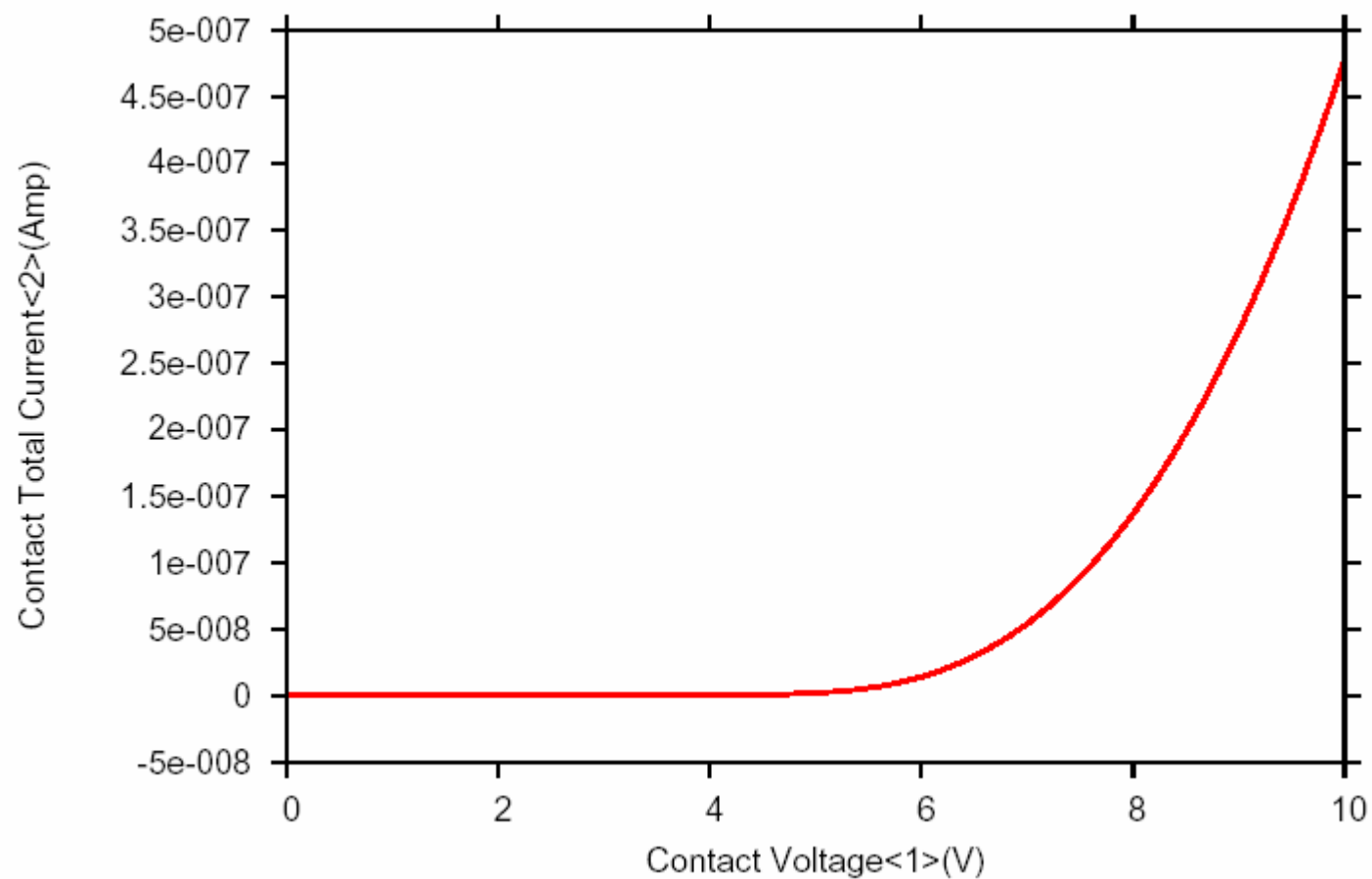


Energy band diagram of a OLED of TPD/ALQ3

3D Radiative Light Source



I-V Curve

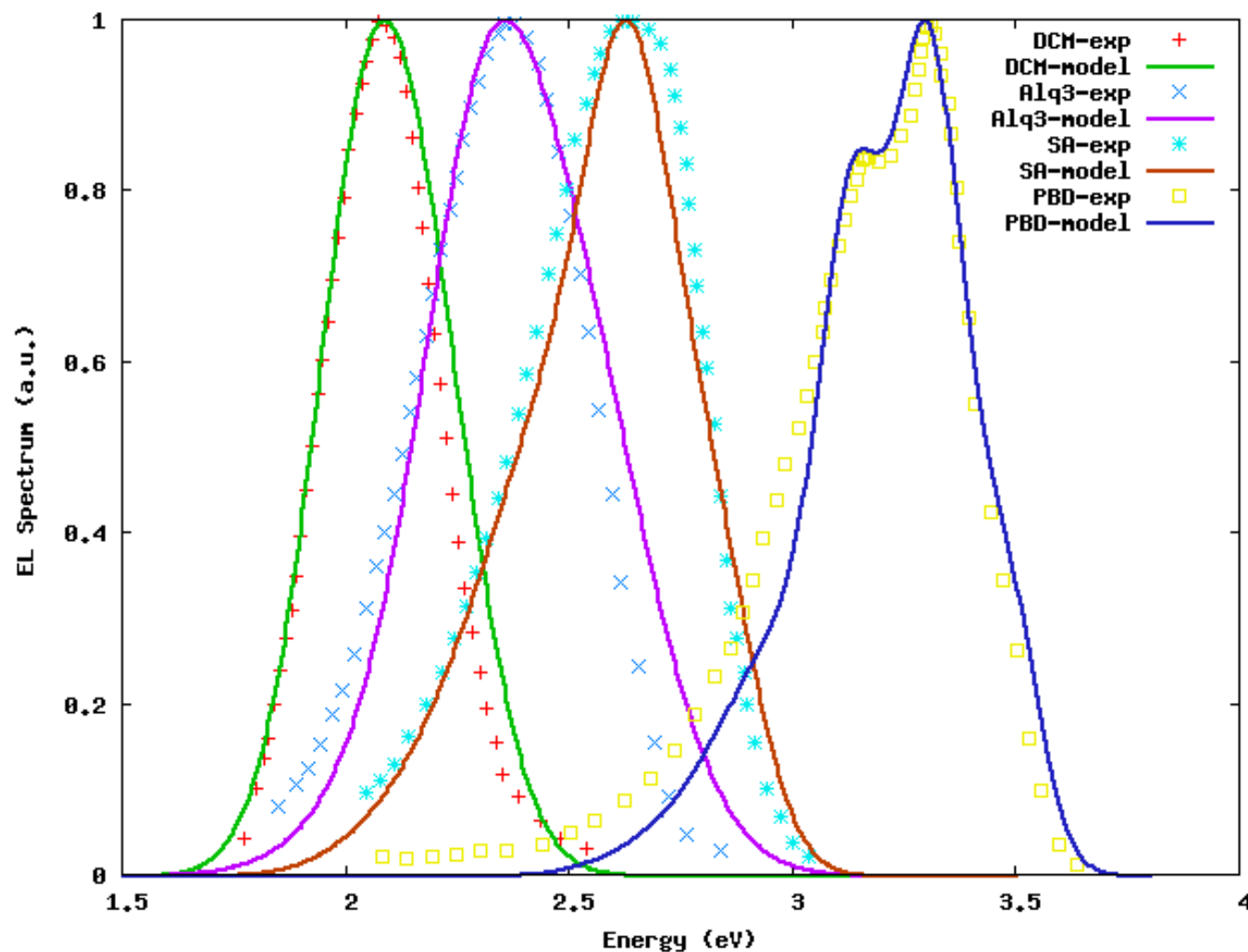




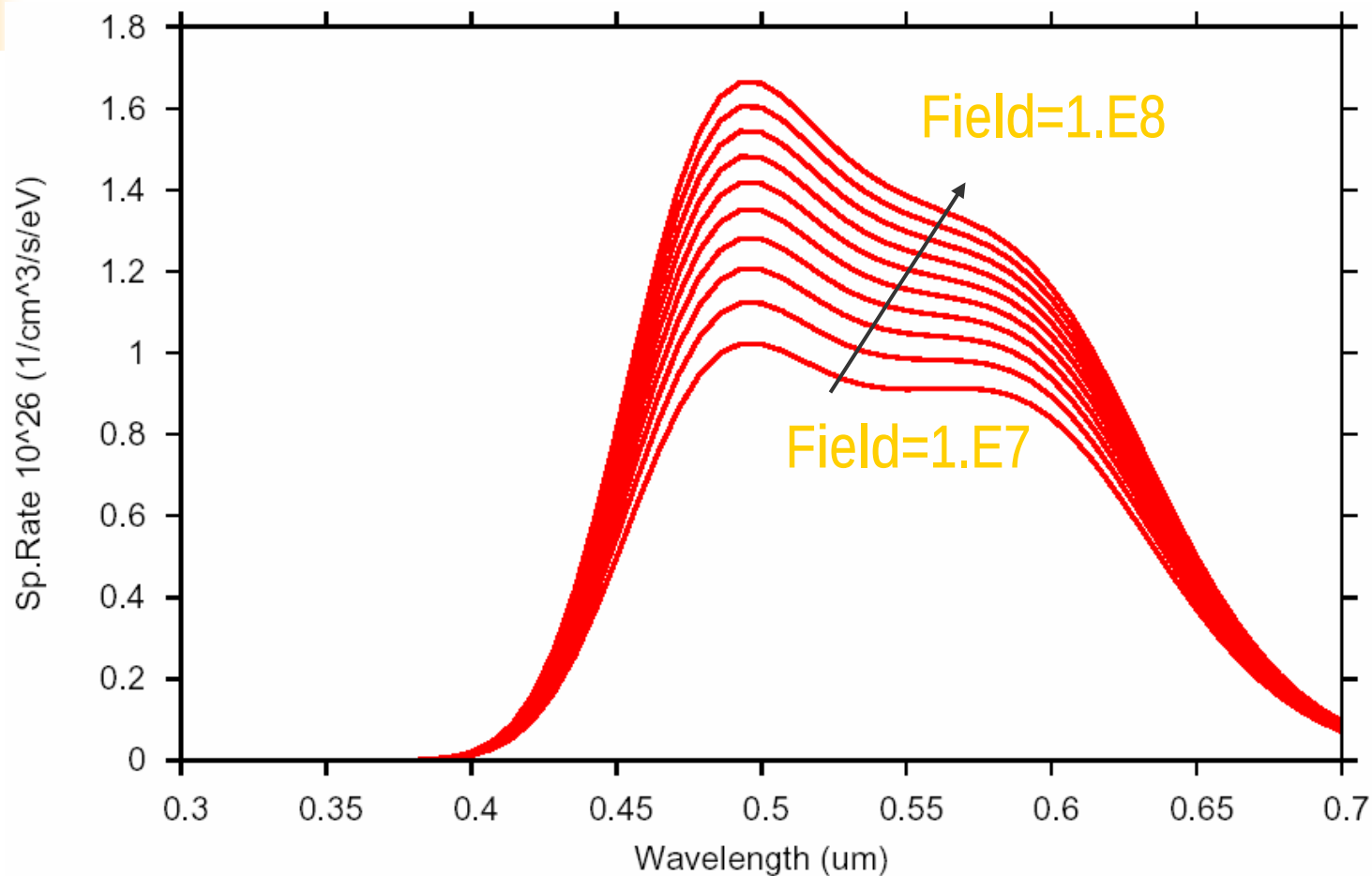
Modeling of Organic Semiconductor Electroluminescent (EL) and Absorption Spectra

- **Organic semiconductor emits light via Frenkel exciton recombination.**
- **Conventional semiconductor theories based on free-carrier / many-body interband transition are no longer valid.**
- **We have established optical spectrum model based on exciton-phonon interaction within an organic crystal.**

Some Fitted EL Spectra



EL Spectrum Model of Alq3:DCM



Applied electric field ranges from
1.E7 to 1.E8 V/m

Conclusions

- **Crosslight Software develops indebt 2/3D advance features of Laser, LED Modeling, PIC, along with other Quantum Transport modeling, specifically Quantum MOS for UHLSI CMOS technology. It can be interfaced with CSUPREM, for example with Monte-Carlo implantation modeling**
- **New non-semiconductor device modeling was successfully applied to the polymer materials, and OLED devices.**
- **New tools for modeling of MOCVD and semiconductor device fabrications will allow for more complementary TCAD design and Interfacing with Device Modeling Software.**