



# *3D Simulation of Quantum Dot Devices*

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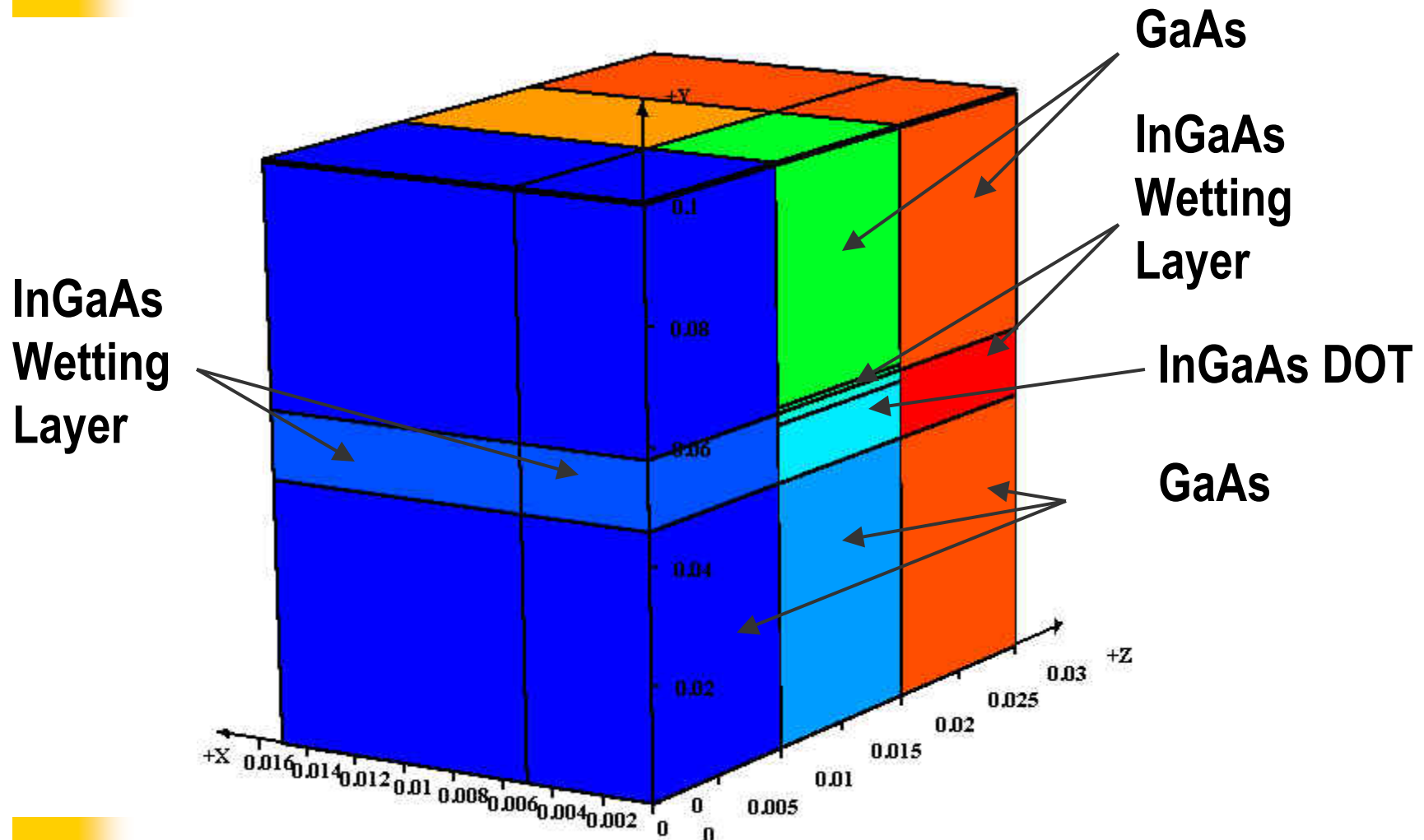
## Physical Models

- **Quantum dot structure offers delta-like density of states that facilitates population inversion → Better emitters.**
- **Better temperature stability and lower threshold are expected.**
- **Modeling is separated into two parts (1) microscopic model that solves all the quantum states in a dot; (2) macroscopic model that uses (1).**

## Microscopic Model

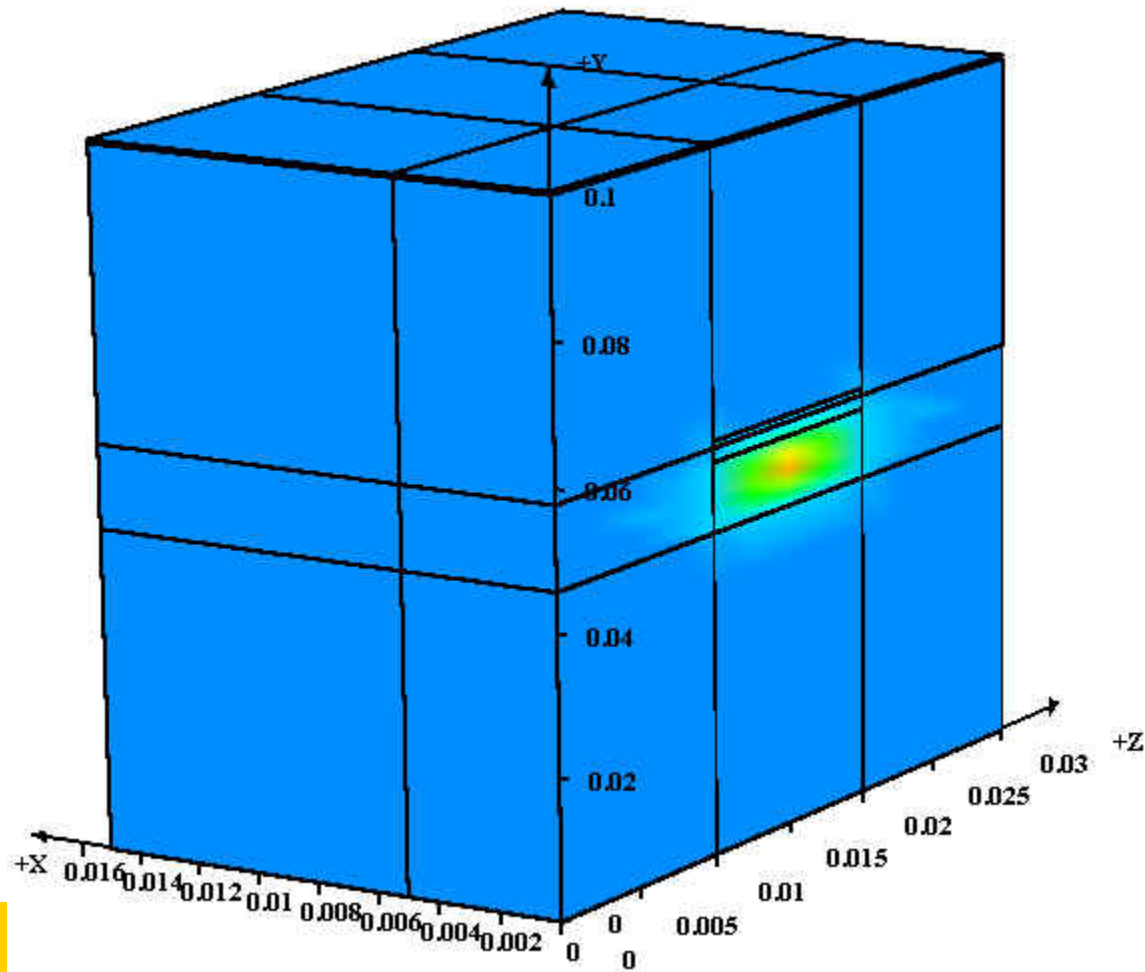
- **3D structure of QDOT as set up with Layer3D/GeoEditor3D.**
- **Use of rectangle coordinates for QDOT shapes of boxes and pyramids, etc.**
- **Use of cylindrical coordinates for QDOT of columnar or cone shapes.**
- **Schrodinger equation is discretized in 3D and solved with sparse eigen matrix techniques.**
- **Strain effects are taken into account by using strain dependent potential profiles and anisotropic effective masses for different band valleys (HH,LH,CH, etc.)**
- **Applicable for wurtzite structure (GaN-based) as well as for zincblende structure.**

# A simple QDOT of a box



Use only  $\frac{1}{2}$  of the symmetric structure

# Quantum wave function of a box



File Name : box.sid\_0001

File Type : LASTIP

Variable Name :

Wave\_Intensity 1

3D Cube Contour Parameters :

X Range : 0 - 0.015

Y Range : 0 - 0.1

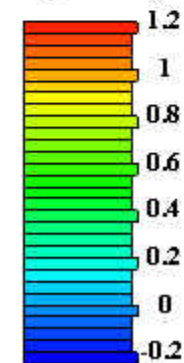
Z Range : 0 - 0.03

X Cut Line Num : 40

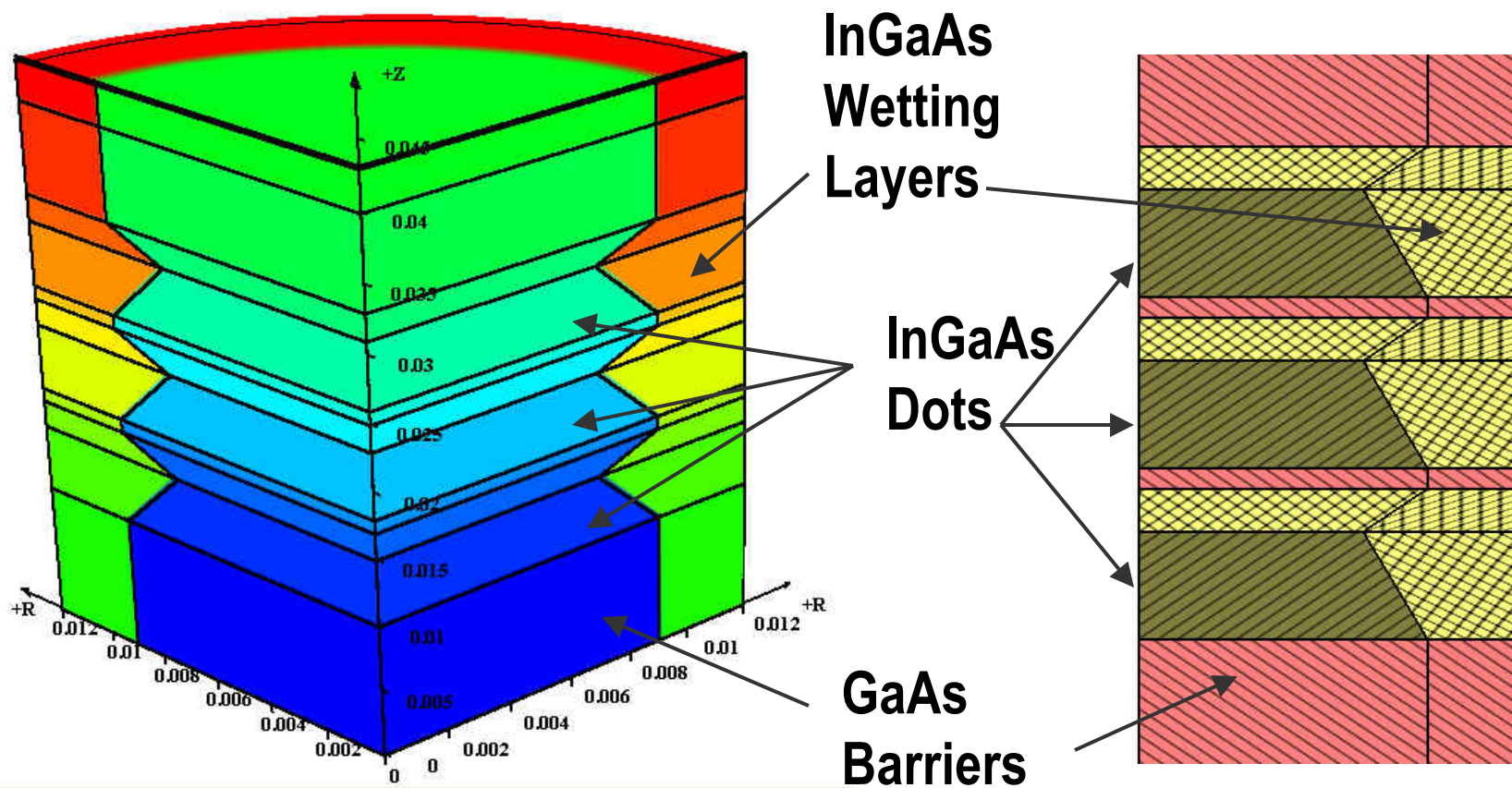
Y Cut Line Num : 40

Z Cut Line Num : 40

Wave\_Intensity 1

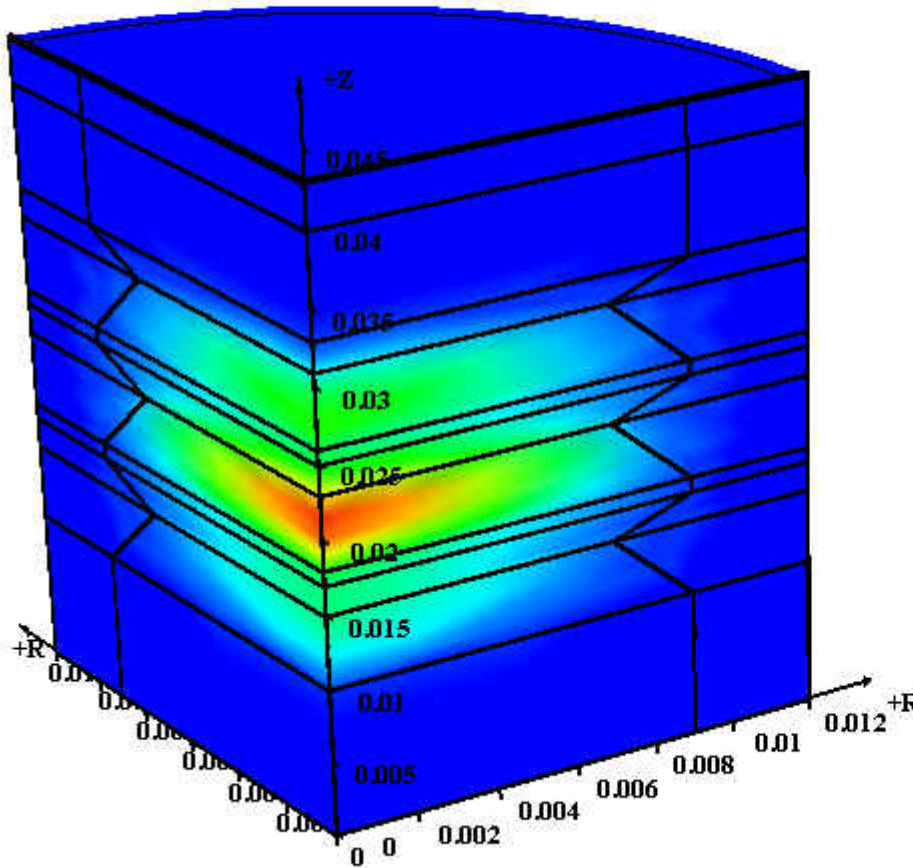


# Coupled columnar dots

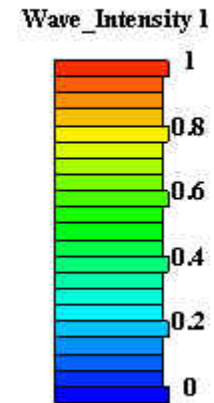


Remark: It is a simplified structure. Real structure Of QDOT may have composition grading from InGaAs To InAs at the center of the dot.

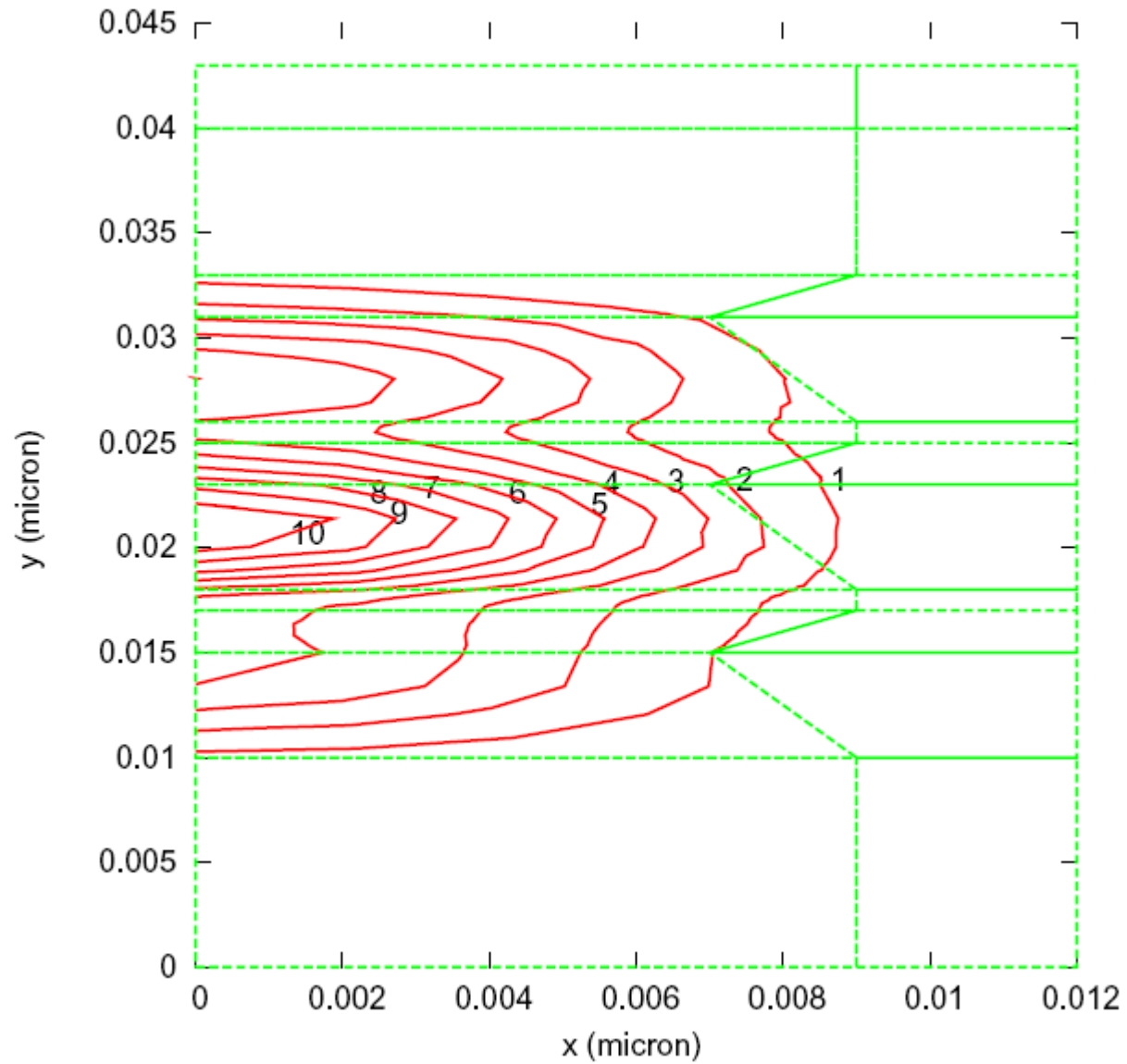
# Results for columnar dots



File Name : cone.std\_0001  
File Type : LASTIP  
  
Variable Name :  
Wave\_Intensity 1  
  
3D Cube Contour Parameters :  
X Range : 0 - 0.012  
Y Range : 0 - 0.043  
Z Range : 0 - 0  
  
X Cut Line Num : 40  
Y Cut Line Num : 40  
Z Cut Line Num : 40



# Columnar dots (contours)



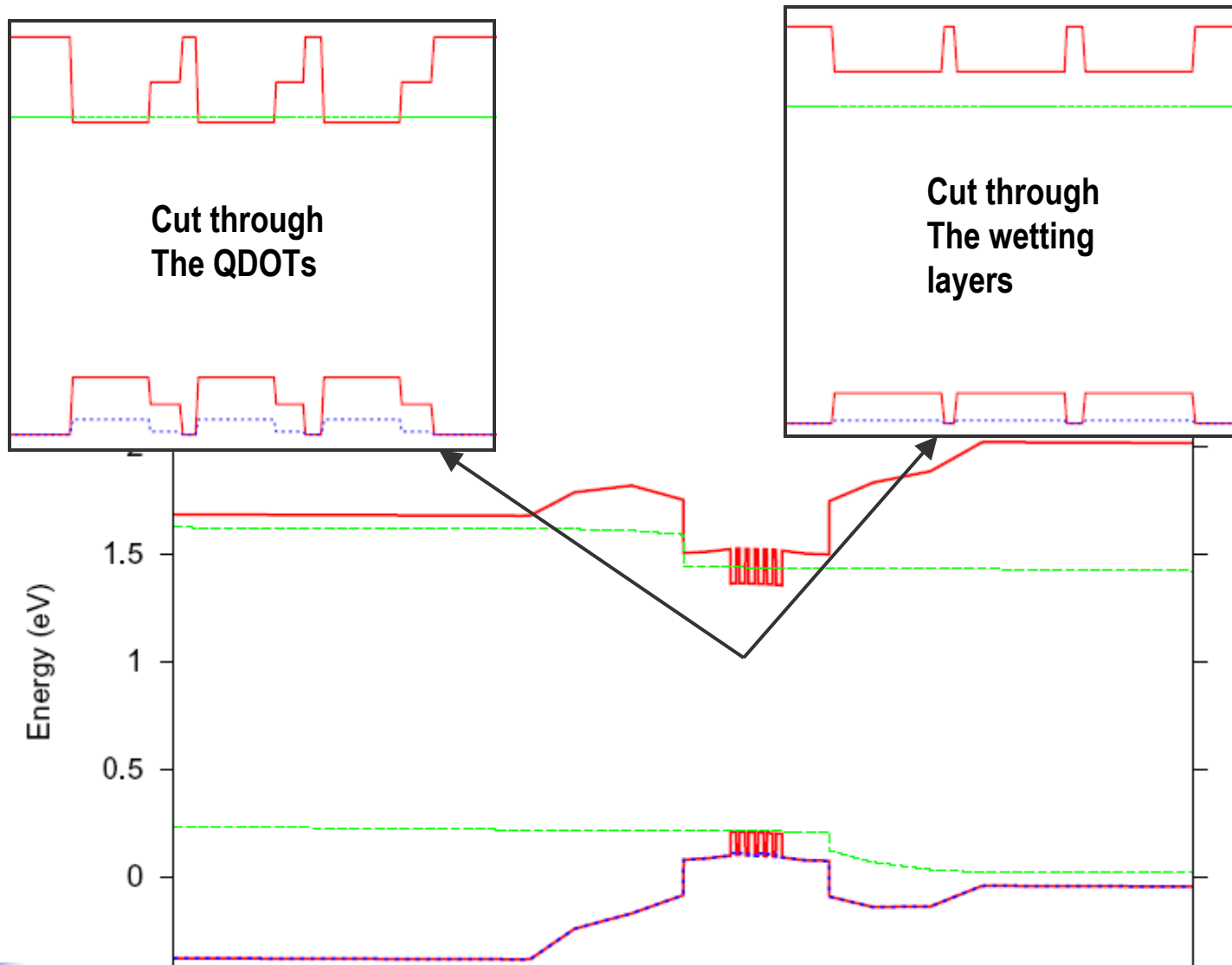


## **Macroscopic Model**

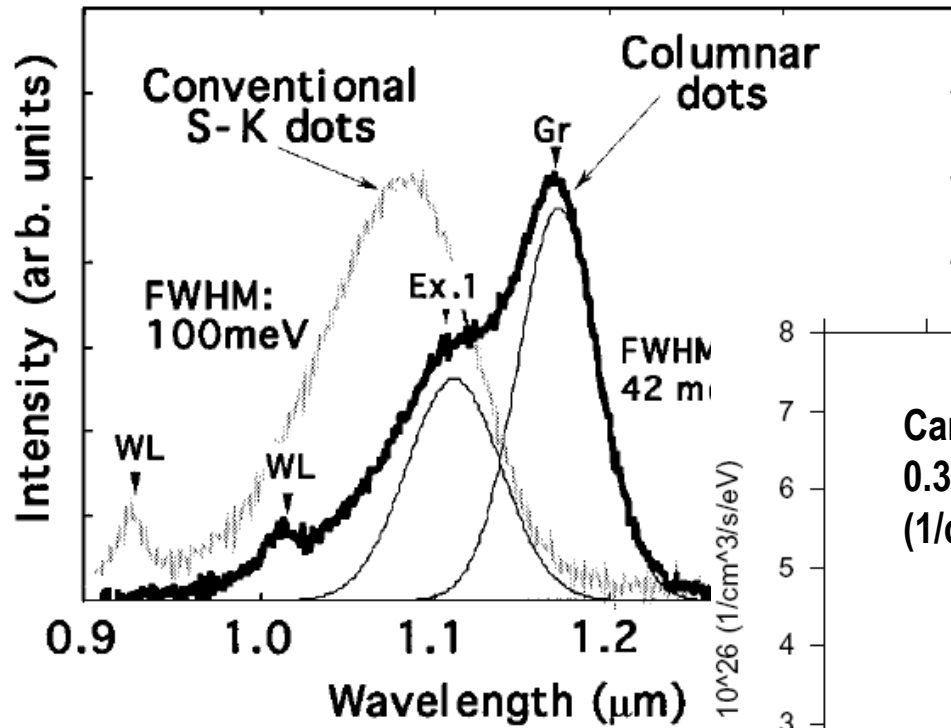
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- **Set up 2D/3D larger laser diode/LED/PD structure as usual.**
- **Import quantum levels and optical transition overlaps from microscopic solutions. If necessary, correct potential profile at the dot model.**
- **Use of delta-like density of states for optical gain, spontaneous emission and carrier concentration calculation.**
- **Use wetting layer as a reference to compute optical confinement and carrier sheet concentration for the dots.**

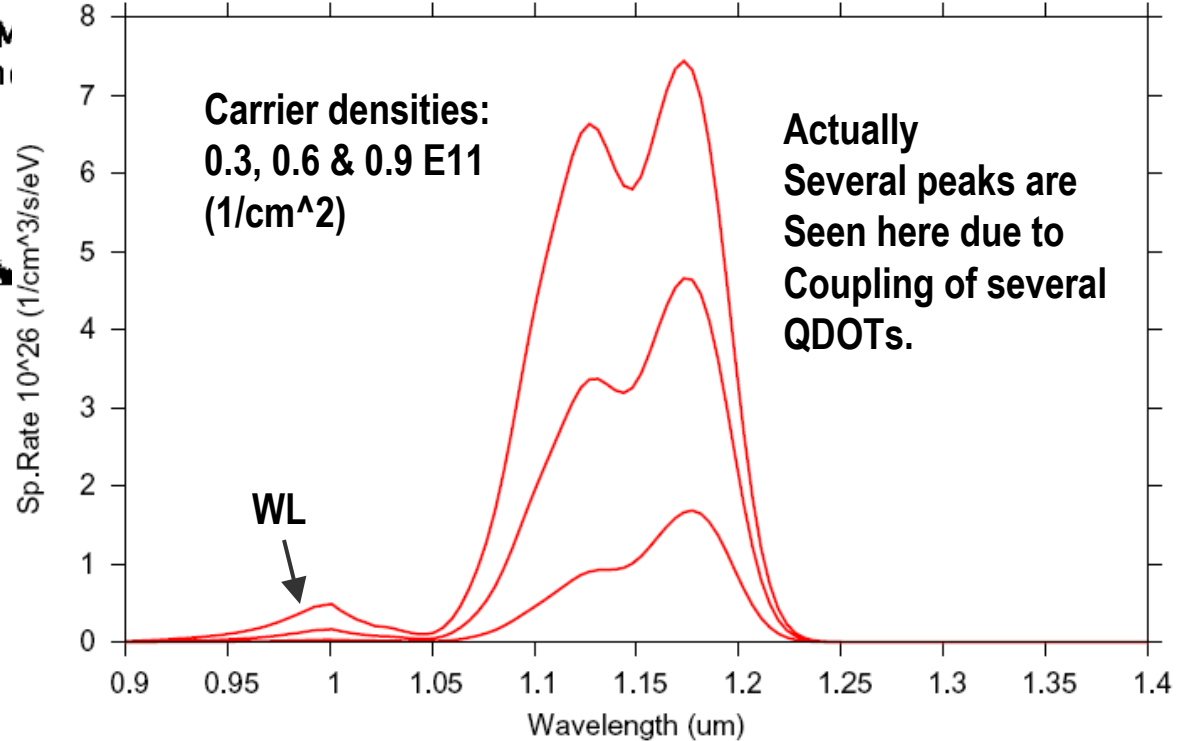
# Band diagrams



# Comparing PL with experiment

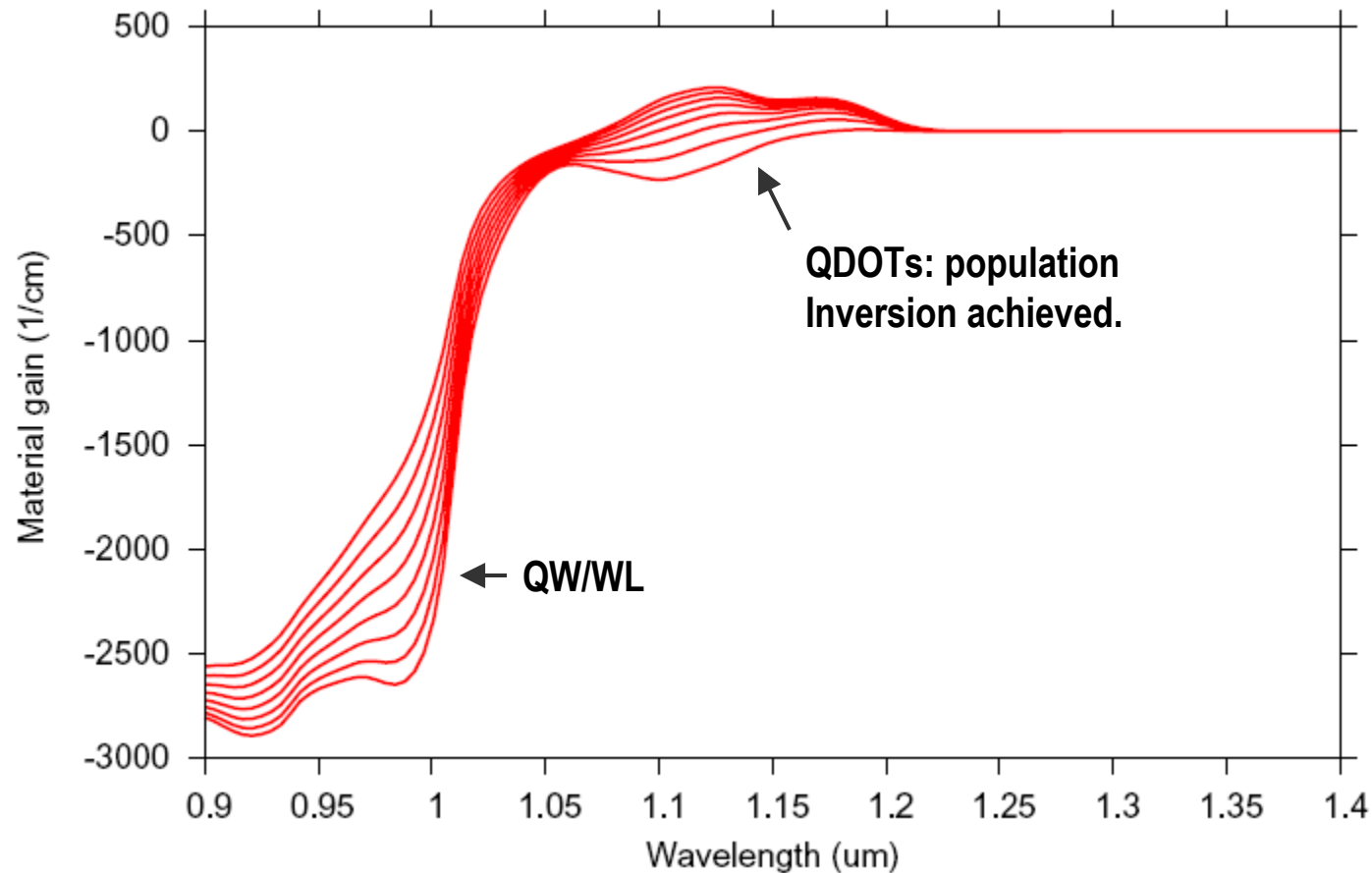


M. Sugawara, et. al.,  
IEEE J. Select. Topics in  
Quant. Electron. vol. 6,p462  
2000.



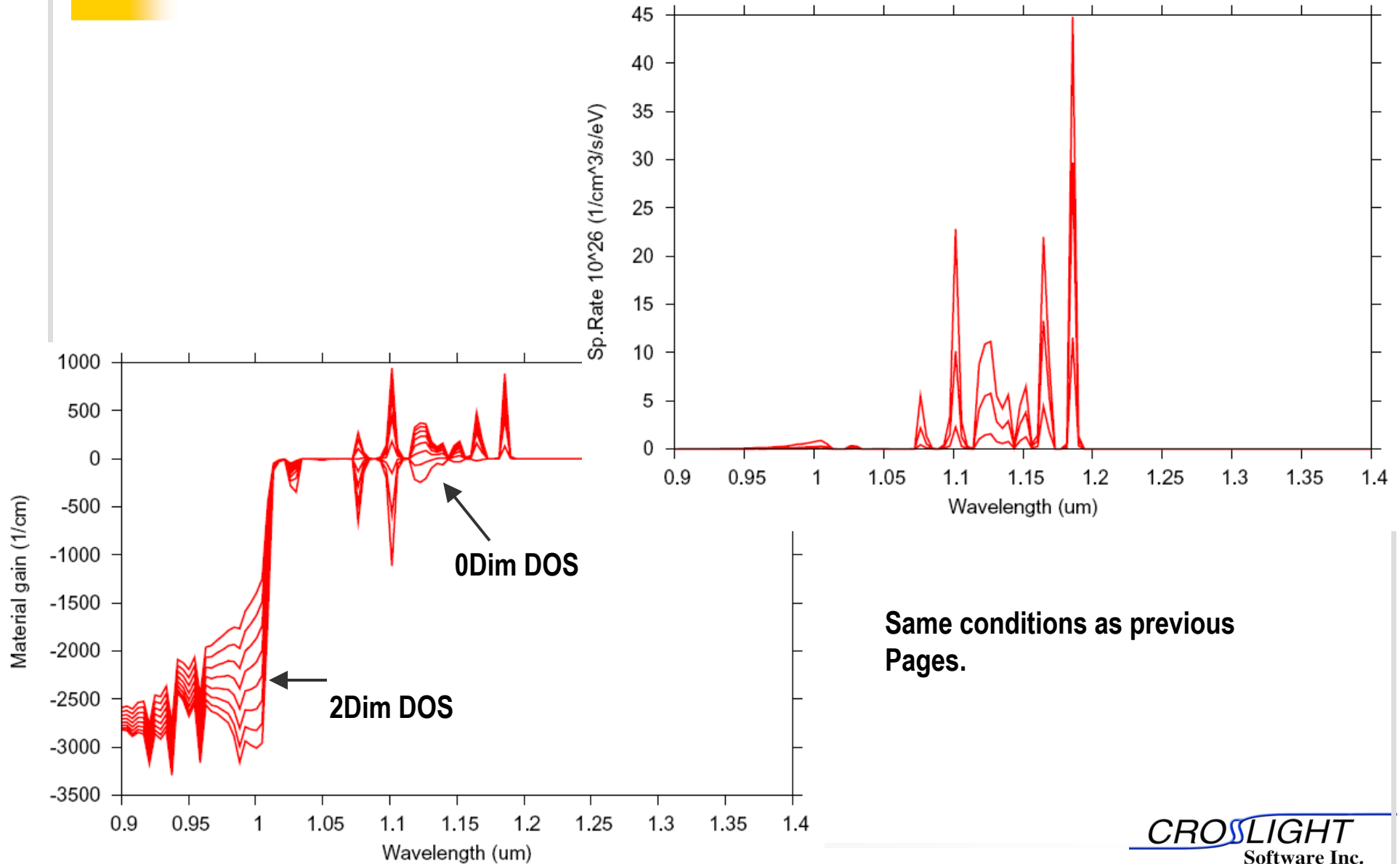
Both QW and QDOT models are needed here.

# Optical gain spectrum



Carrier conc. in wetting layers ranges from  $0.6E11 \rightarrow 6E11$  ( $1/cm^2$ ). For QDOT LED, this will be useful for photon-recycling model.

# Spectrum without broadening

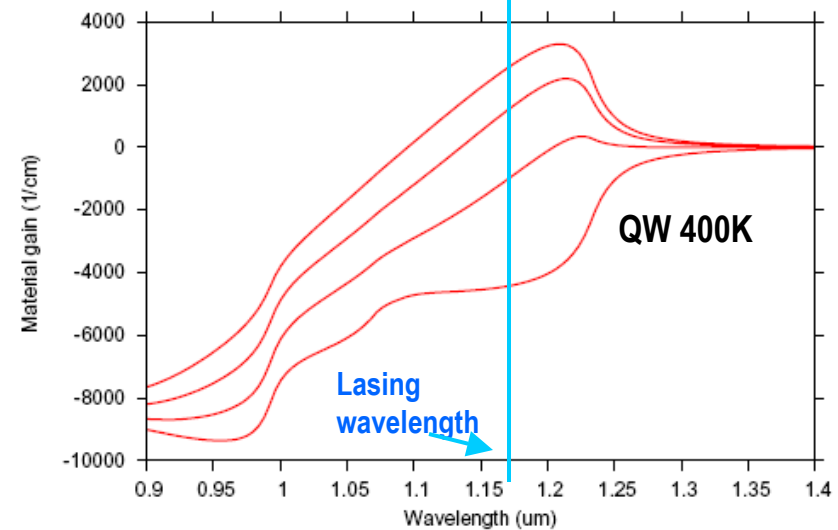
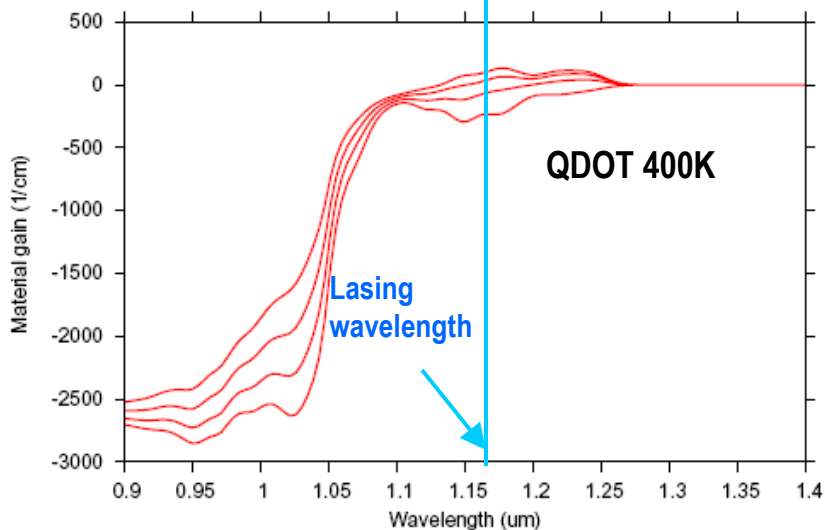
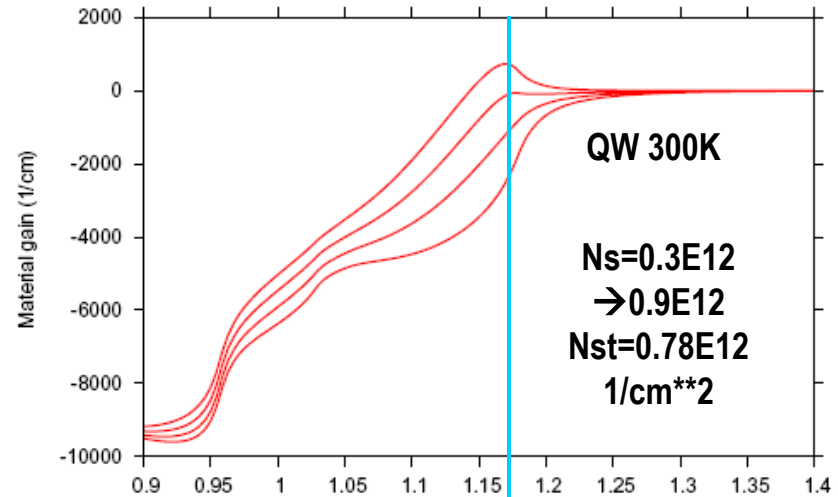
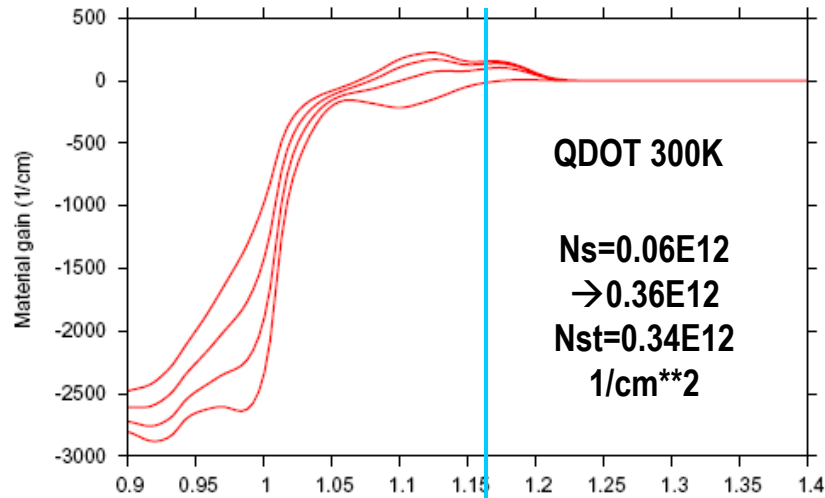


## Temperature dependence study

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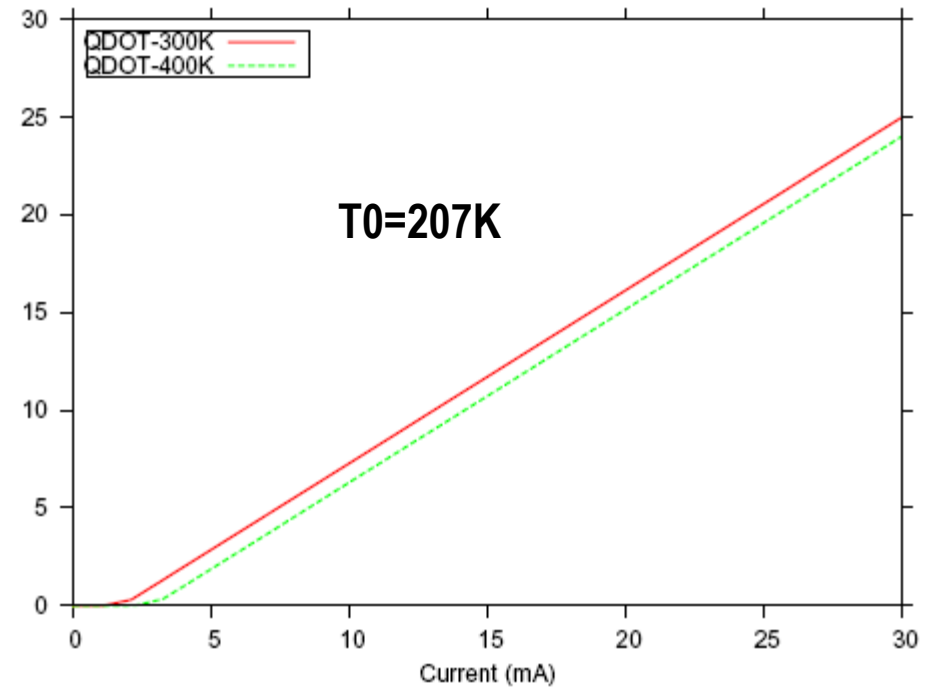
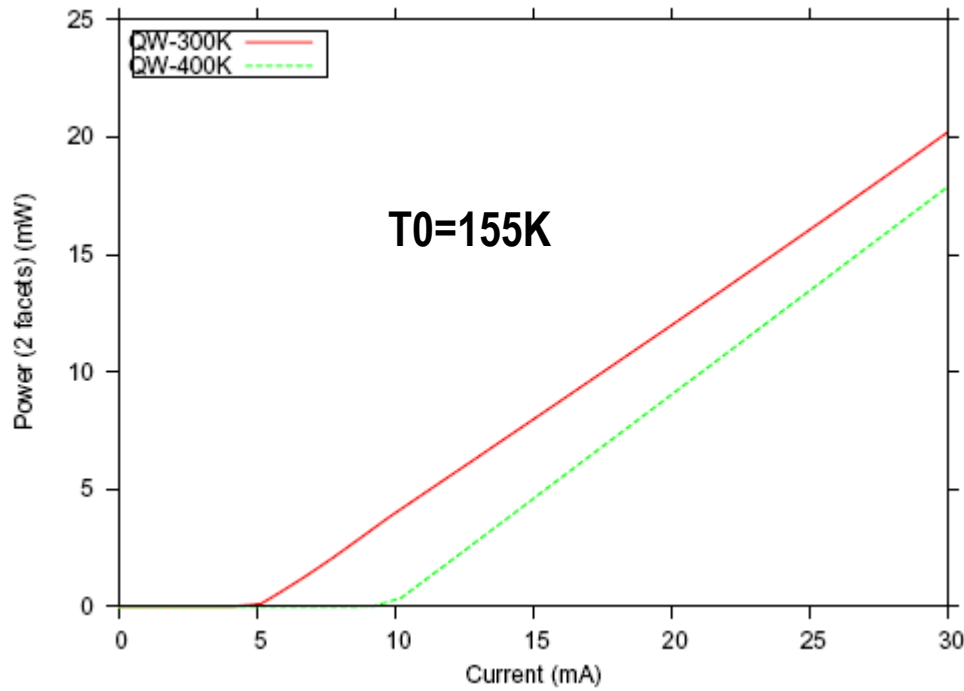
- **Objective: to compare performance of MQW and QDOT lasers at the same wavelength (1.17 microns) using the same material system (InGaAs/AlGaAs).**
- **Both QDOT and QW indium compositions are tuned to have gain peak at 1.17 microns at T=300K.**
- **Assumption of no current spreading (1D) simulation, no temperature dependence in non-radiative carrier lifetime and Auger recombination.**

# Gain Spectra



All four simulations are forced to lase at the same wavelength.  
 $N_s$  is the carrier surface density and  $N_{st}$  is threshold surface density.  
 Remark: QDOT spectra less sensitive to temperature change.

# Lasing behaviour



**Comparison of lasing behavior at 300 and 400 K. All structures are forced to lase at 1.17 microns and temperature dependences in bandgap, optical gain, carrier concentration, and radiative recombination have been taken into account. All other quantities are assumed to be temperature independent for simplicity**



## Summary

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- **An efficient QDOT model has been established for PICS3D/LASTIP/APSYS.**
- **QDOT model may be used for photo-detectors as well as for laser diodes/LED since gain/absorption model is implemented in the same way as QW model.**
- **Combination of microscopic and macroscopic modeling of QDOT offers both efficiency and accuracy.**
- **Simulated lasing behaviors for LD indicate substantial benefits for lasing threshold and temperature insensitivity.**