

Many-Body, exciton and Inhomogeneous Broadening Effects In Device Simulation

CROSSLIGHT
Software Inc.

Copyright 2004-7 Crosslight Software Inc.
www.crosslight.com

Many-body effects on gain

- Coulomb attraction between e-h pair enhances radiative recombination → enhanced optical gain and spontaneous emission.
- Band-gap reduction due to Coulomb-hole self energy and screened-exchange shift.
- Coulomb enhancement is more pronounced in wide band-gap materials, CdZnSe and GaN
- It has been reported that many body effects are important in prediction of laser characteristics.

Exciton effects on absorption

- Same coulomb attraction between e-h pair more pronounced in low carrier density/absorption when carrier screening effect is less.
- Results in excitonic peaks in absorption spectra.
- Many-body/exciton model critical for device simulation when active layer carrier density is low (such as EAM).

Inhomogeneous broadening tail states

- Fluctuation in quantum well thickness and composition, defects and impurities all contribute to inhomogeneous broadening of optical spectra.
- Manifests itself in an exponential tail in band gap.
- Results in reduced effective band gap and modification in gain/spontaneous emission spectra shape (more symmetrical)

Physical Models

- Semiconductor Bloch equations with screened Hartree-Fock approximation
- First-order Pade approximation.
- Band-gap renormalization
 - Coulomb-hole self-energy $\Delta\mathcal{E}_{CH}$
 - Exchange energy $\Delta\mathcal{E}_{SX}$
- Optical gain enhancement

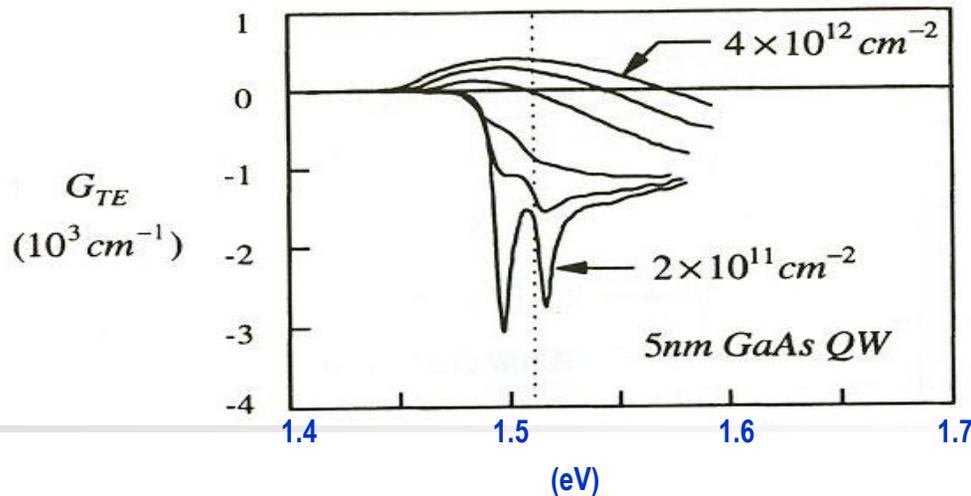
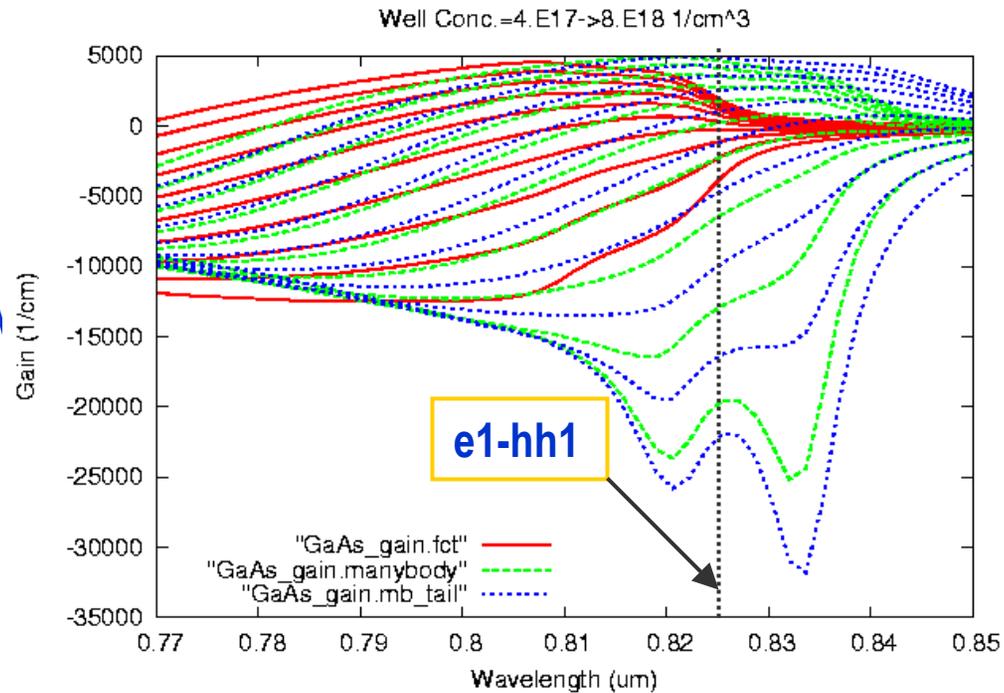
$$g(E) \propto \int g_0(E) \times CE_factor(E) dE$$

Reference:

'Semiconductor Laser Fundamentals', by W.W. Chow and S.W. Koch

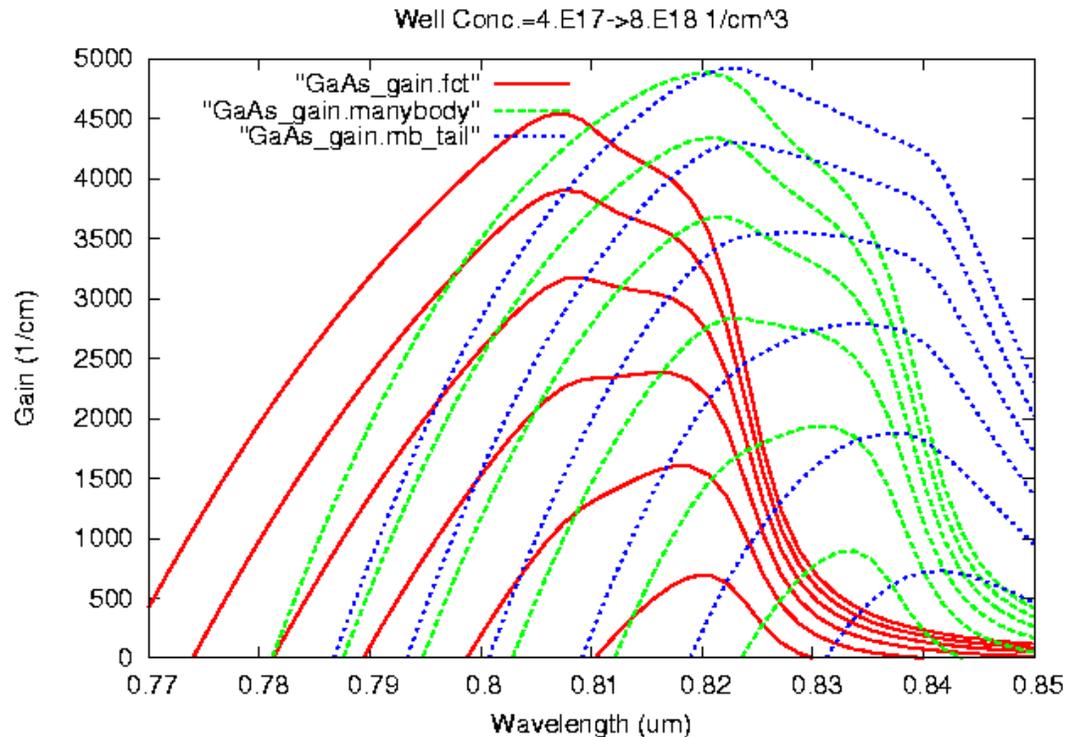
GaAs/AlGaAs, Gain spectrum

5nm GaAs/Al_{0.2}Ga_{0.8}A
 Fct: free carrier theory
 Manybody: Coulomb
 mb_tail: Coulomb+tail
 states



'Semiconductor Laser
 Fundamentals', by W.W.
 Chow and S.W. Koch

Zoom in Positive Gain

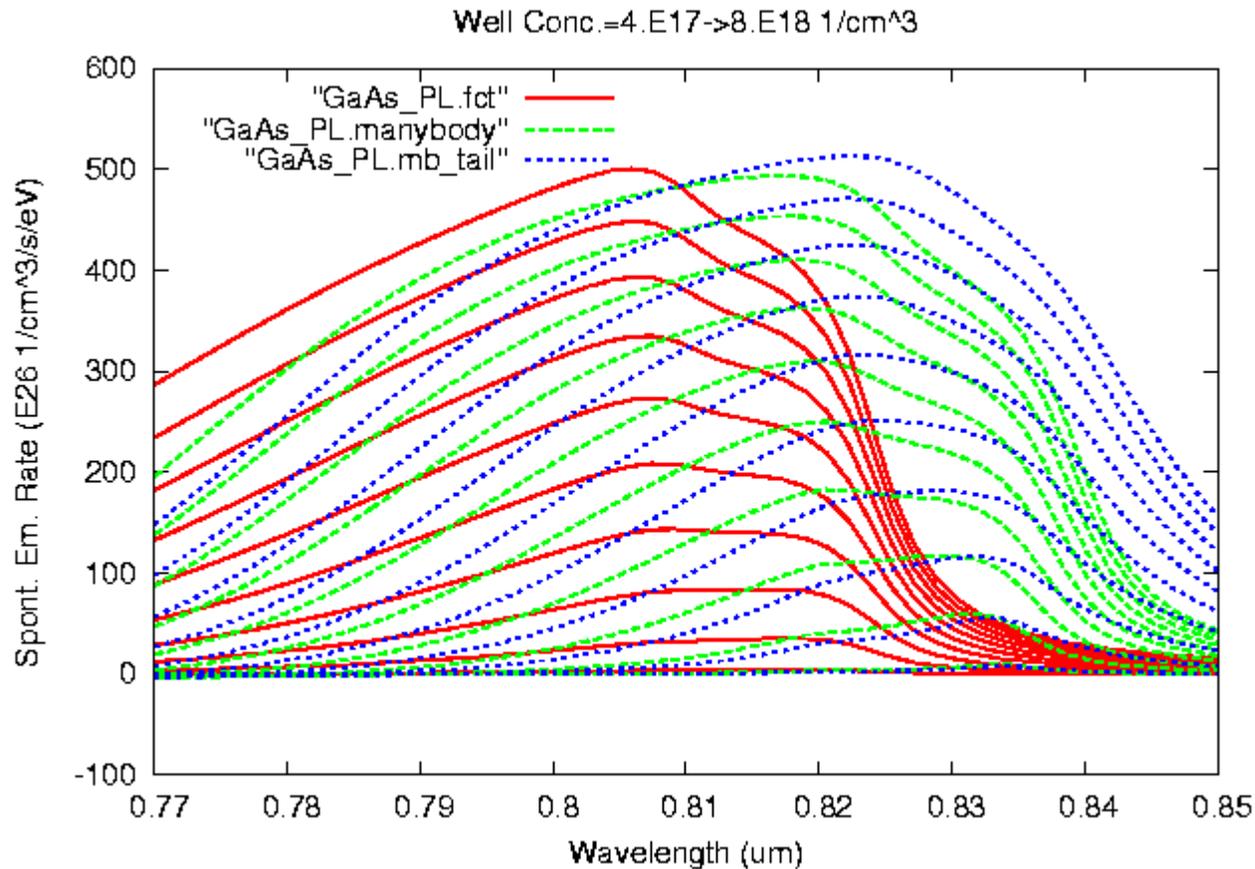


Coulomb enhancement (about 10%-20%) is not so strong for GaAs at high carrier density, but band-gap renormalization reduces the band-gap.

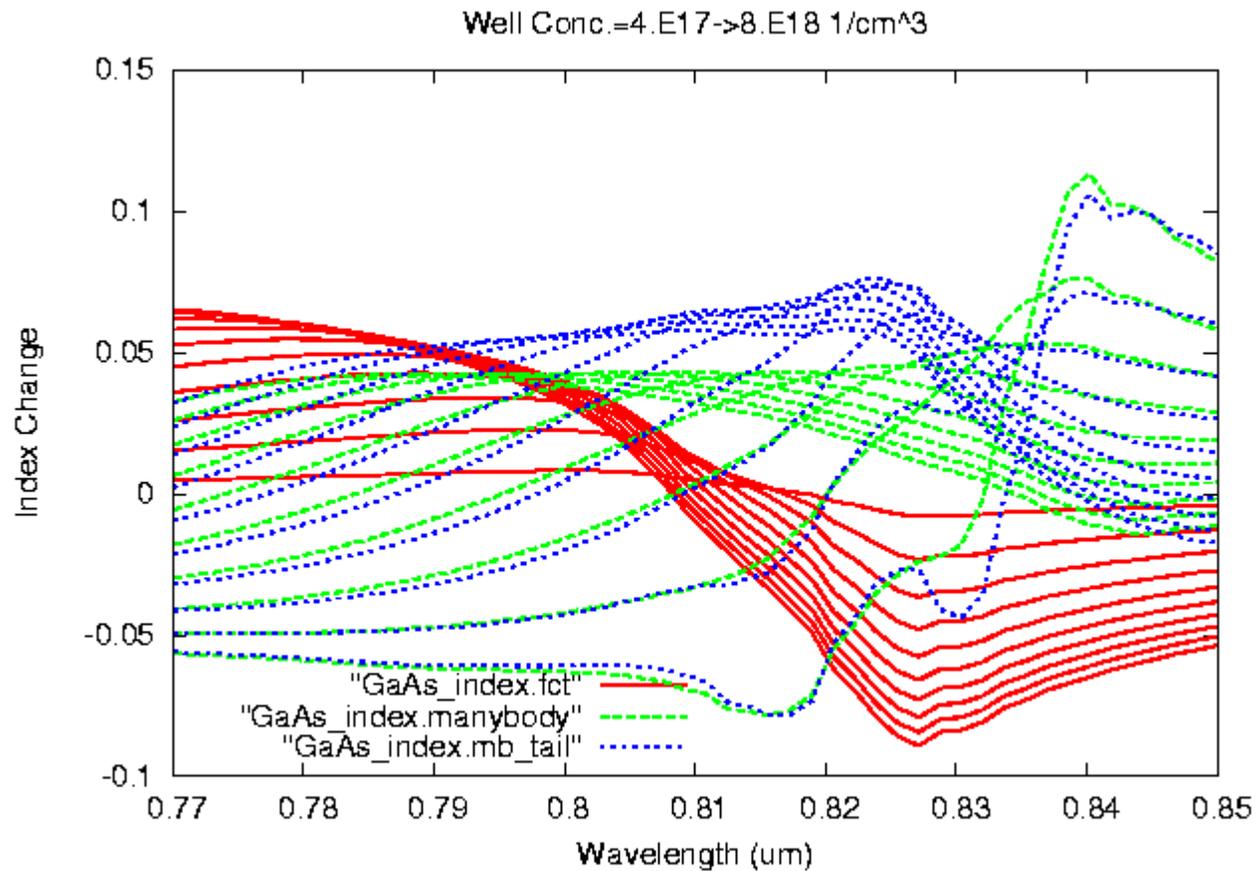
Many-body effects make big difference at low density gain spectra. The appearance of sharp exciton resonance is correctly predicted. 1s exciton binding energy is 18meV.

At high density inhomogeneous broadening shifts the gain peak to longer wavelength.

Spontaneous emission



Index change



InGaN/InGaN Quantum Well

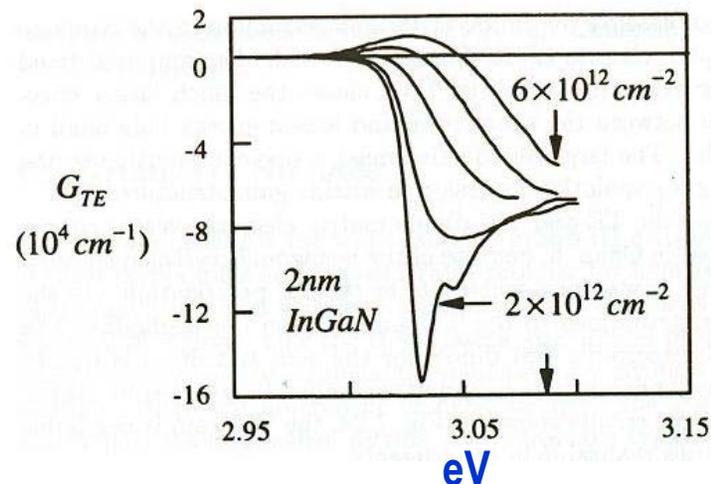
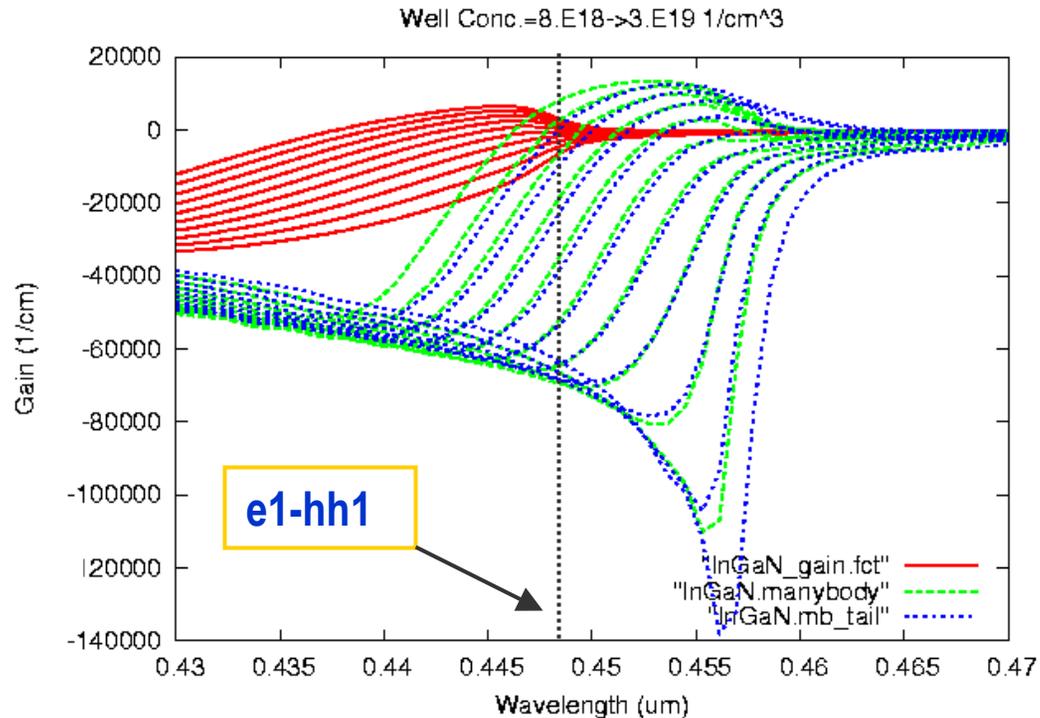
2nm In_{0.2}Ga_{0.8}N/GaN

Fct: free carrier theory

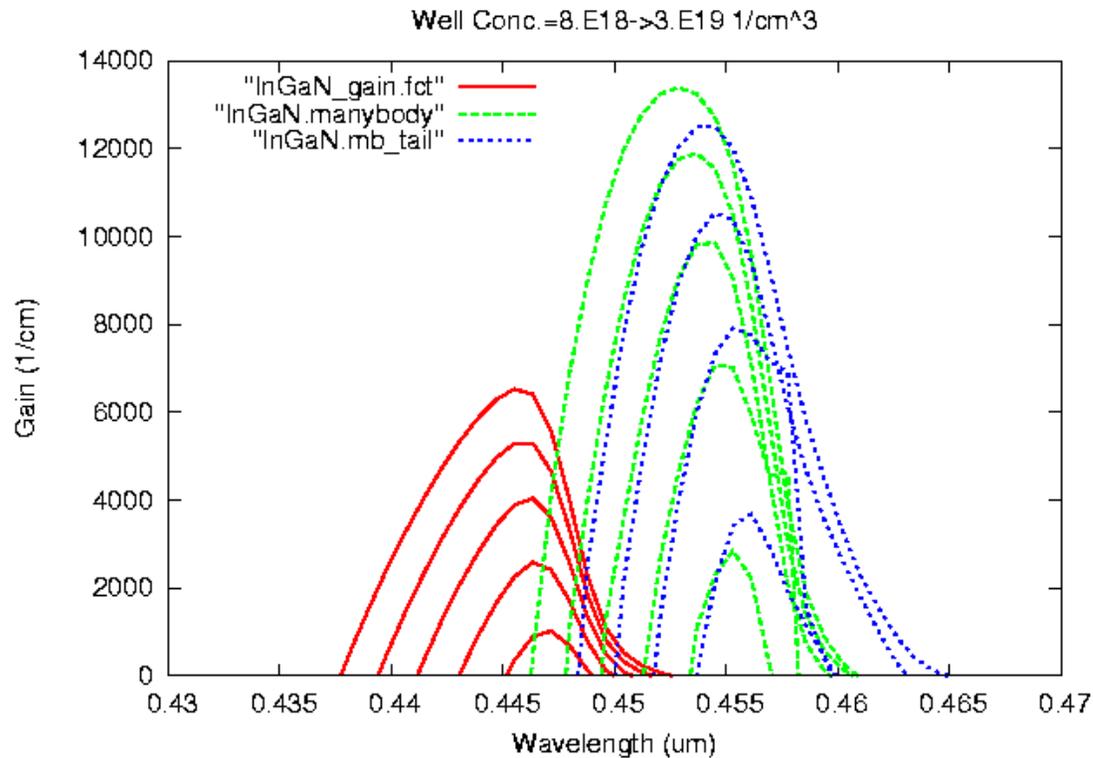
Manybody: Coulomb

mb_tail: Coulomb+tail
states

'Semiconductor Laser
Fundamentals', by W.W.
Chow and S.W. Koch

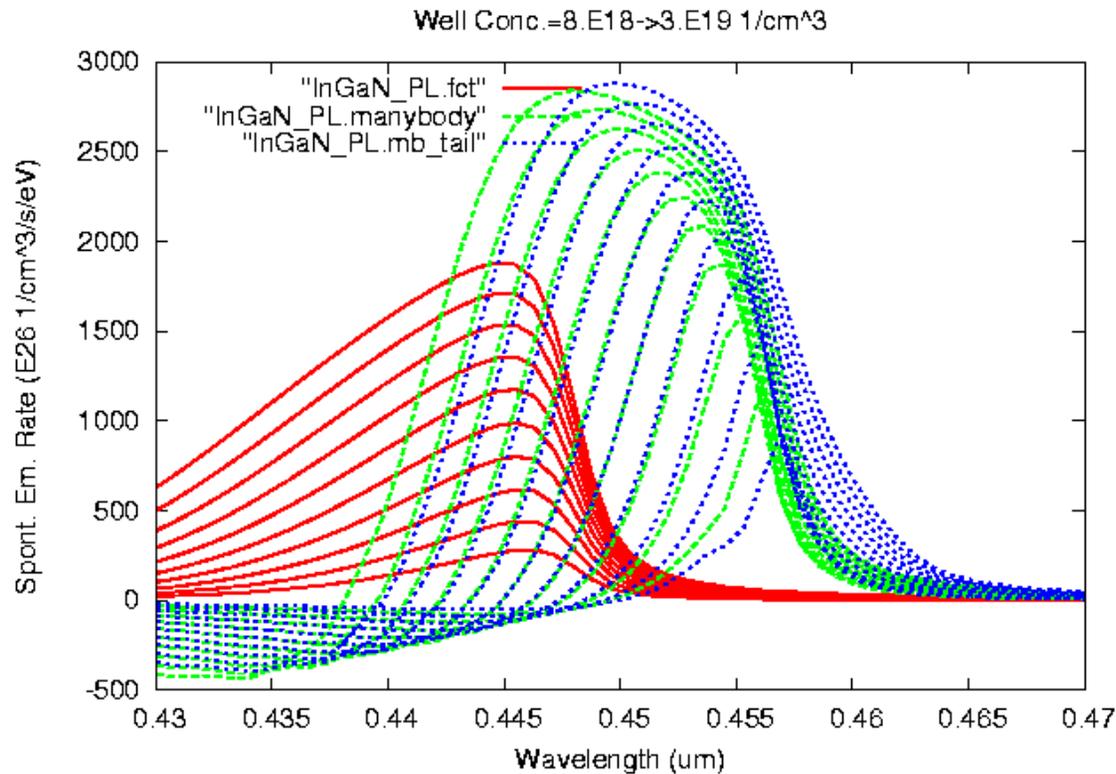


Zoom in positive gain



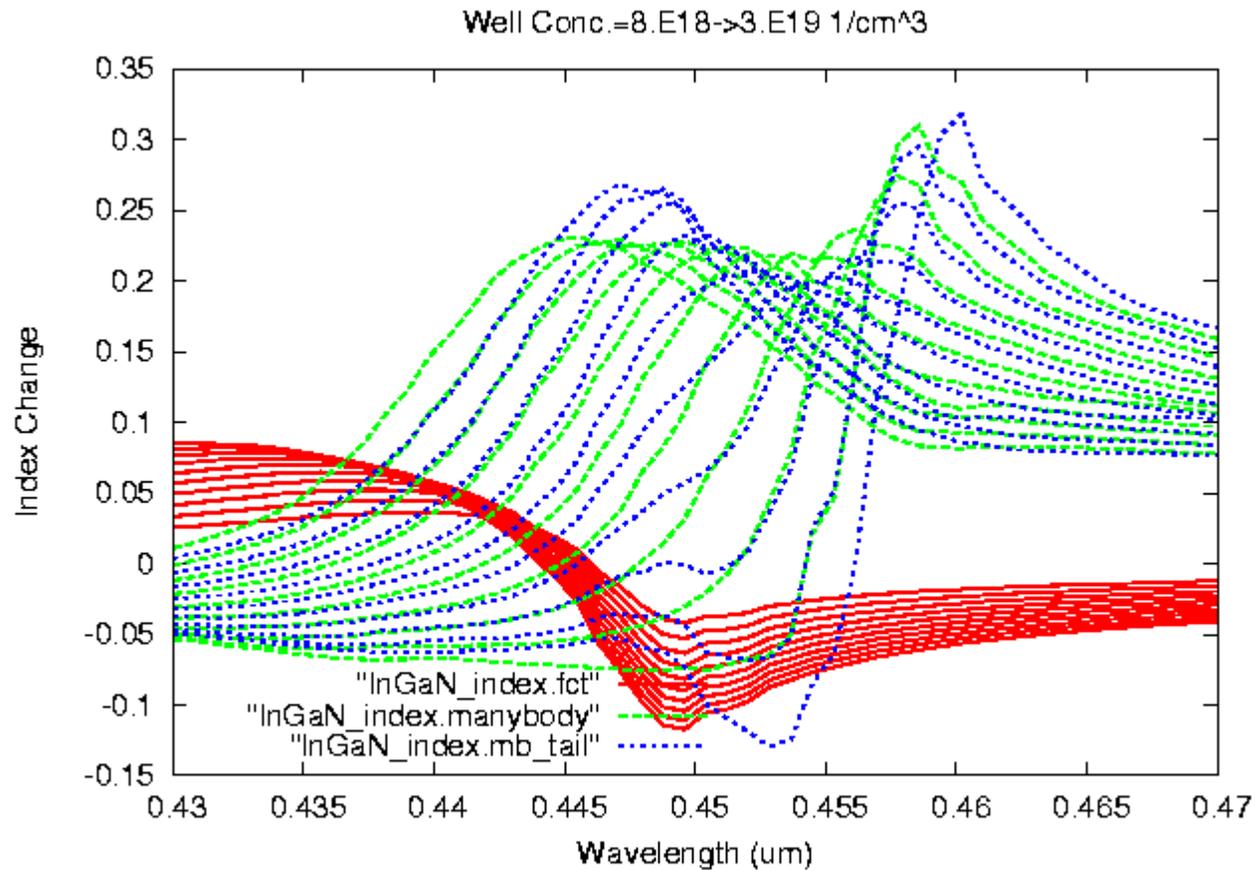
InGaN results show strong Coulomb enhancement (by a factor of 2) in the spectra and band-gap reduction. 1s exciton binding energy is about 46meV in good agreement with Chow's calculation.

Spontaneous emission

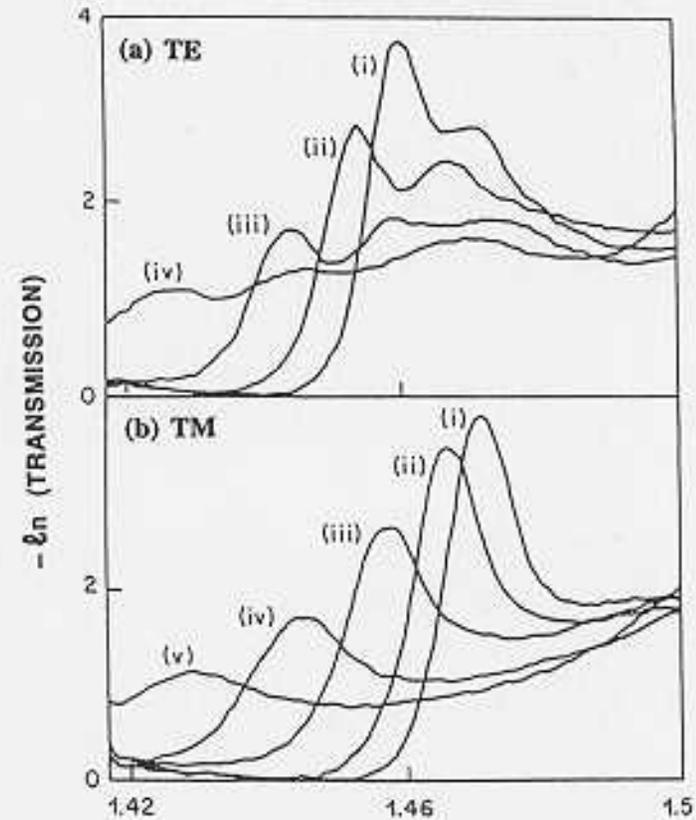
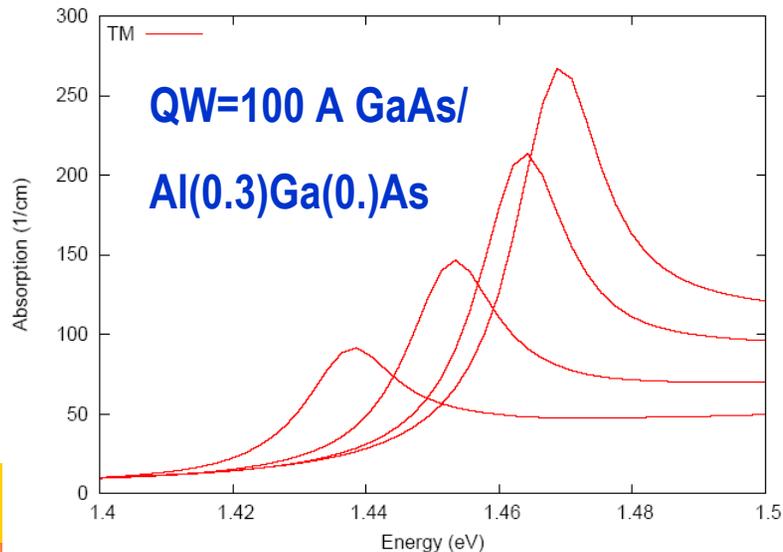
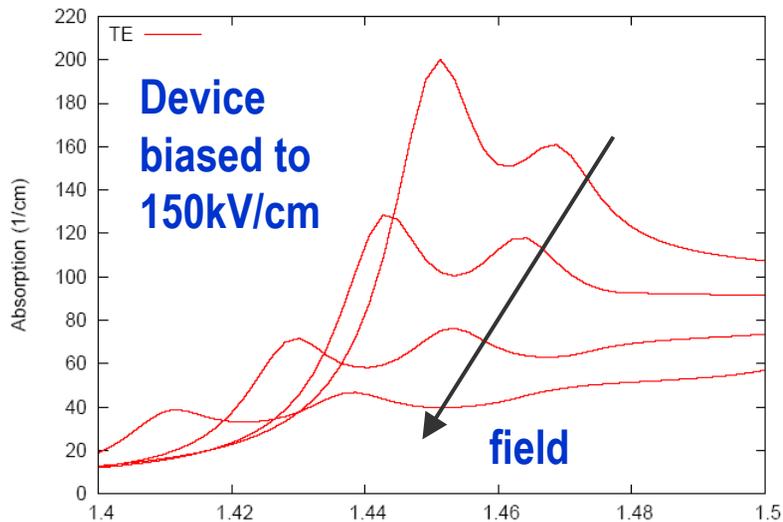


Many-body simulation shows that spontaneous emission peak blue shifts with carrier density, not seen in free-carrier theory

Index change

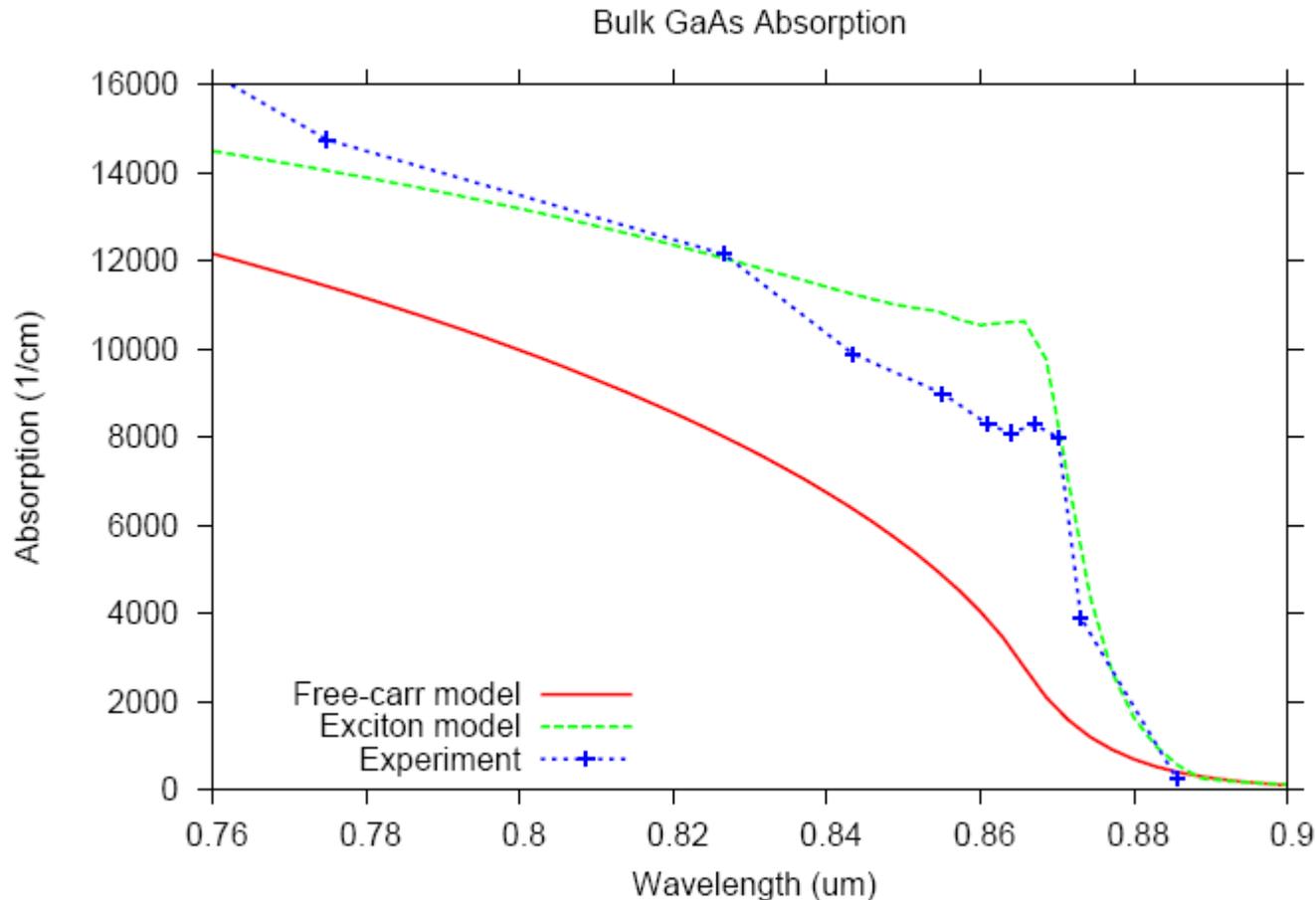


Experimental verification (I)



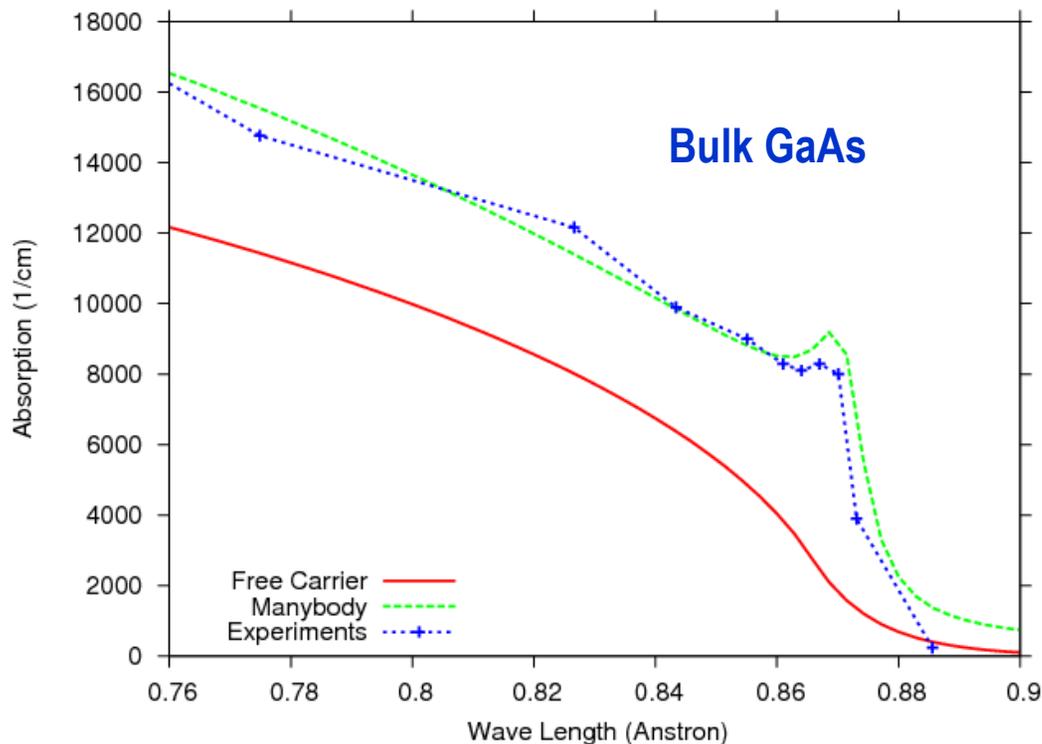
Experimental data from book of S.L. Chuang, "Physics of optoelectronic devices," Wiley & Sons, 1995.

Experimental verification (II)



Experimental data from book of S.L Chuang, "Physics of optoelectronic devices," Wiley & Sons, 1995.

Experimental verification (III)



Free-carrier theory underestimates absorption, especially near the band edge. Manybody Coulomb enhancement based on the pade approximation gives accurate results compared with experiments.

Experimental (IV)

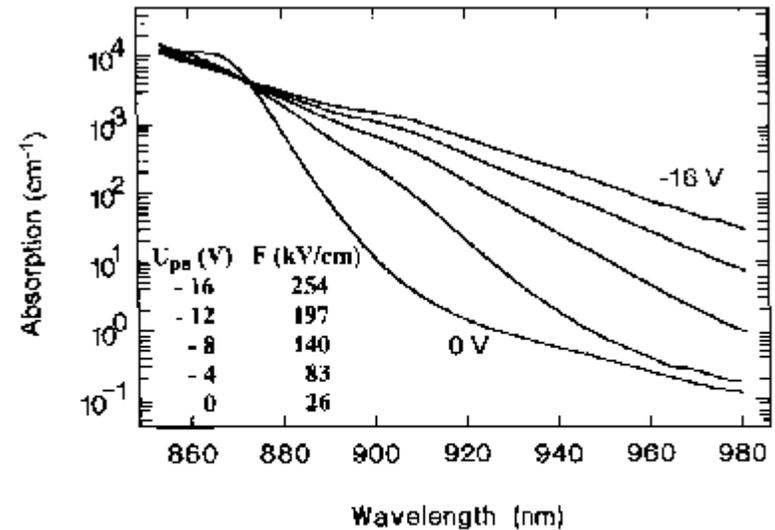
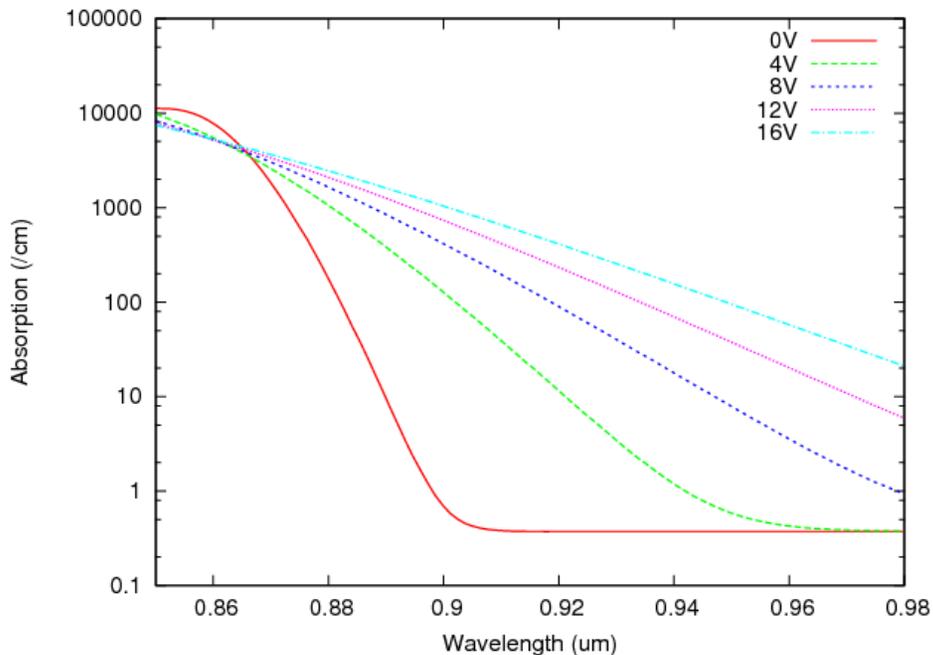


Fig. 1. Spectral dependence of the absorption coefficient $\alpha(\lambda)$ of the p-i-n DHS for a set of various voltages U_{pn} which are shown together with the corresponding electric fields in the intrinsic region.

Bulk GaAs/AlGaAs absorption $\alpha(V)$ is weighted by optical wave intensity. A dipole matrix enhancement factor from manybody calculations was used.

Recommendation/guidelines

- **Scaling/damping parameters implemented so that MB effects can be freely suppressed to reduce to conventional free-carrier gain.**
- **Easy to recalibrate existing models by adjusting scaling/damping parameters.**
- **Slight increase in computational time may be tackled using precalculated gain tables from k.p + MB models.**

Summary

- **Manybody (MB), exciton and inhomogenous broadening effects have been included in device simulators.**
- **Results agree with published theories and experimental data.**
- **Crosslight recommends new gain/absorption spectrum model to all users.**