Microscopic Modelling of the Optical Properties of Bi Containing GaAs Based Quantum Wells

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- **OVERVIEW**
  - Outline of Theory
  - Gain/Absorption
  - Luminescence
  - Radiative and Auger losses
- **COLLABORATORS**
  - Ch. Bückers, Marburg
  - A. Thränhardt, S. Imhof, Chemnitz
  - J. Hader, J. V. Moloney et al., Tucson

Basic Assumptions

- current Bi containing GaAs based materials have a certain amount of disorder
- local Bi concentration fluctuations, clustering etc.
- dominate optical properties at low temperatures and low densities

discussion next talk: Sebastian Imhof

in this talk: room temperature, elevated densities

⇨ Bloch like behavior of the electrons

Bi incorporation via valence-band anti-crossing model

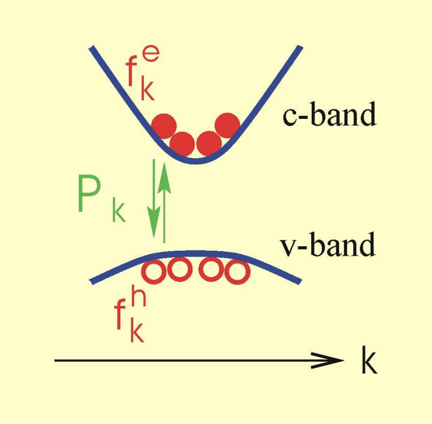
Semiconductor Optics: Semiclassical Theory

MAXWELL'S WAVE EQUATION

$$\left[\frac{\partial^2}{\partial z^2} - \frac{n^2(z)}{c^2}\frac{\partial^2}{\partial t^2}\right] E = \mu_0 \frac{\partial^2}{\partial t^2} P$$

macroscopic optical
polarization
(material response)

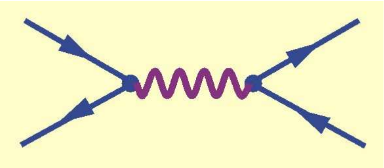
semiconductors: Bloch basis $P = \sum_k d_{cv}^* P_k + c.c.$

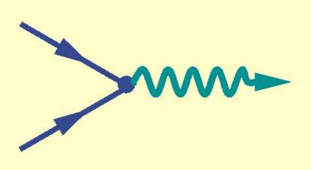


Microscopic Model

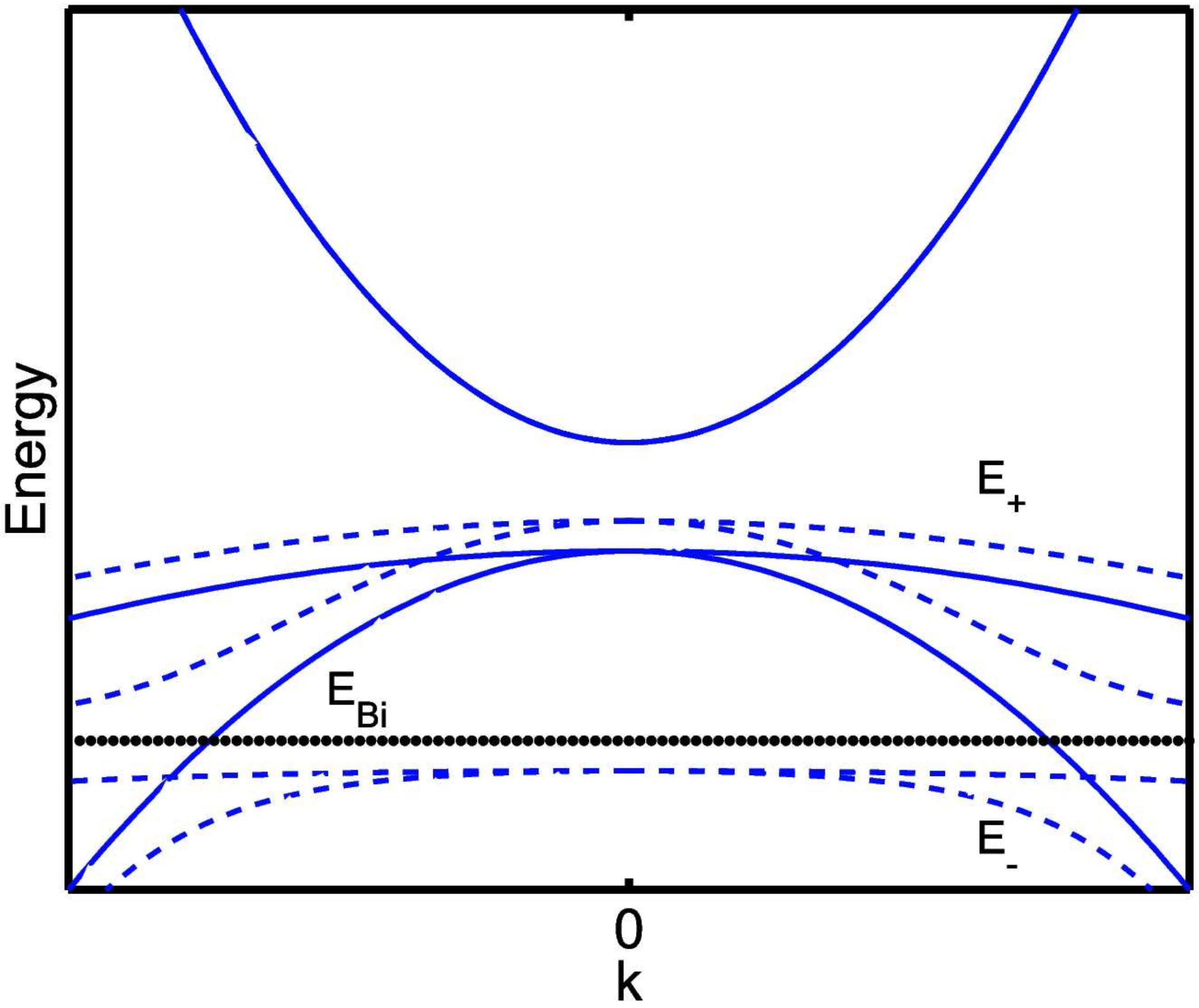
$$H = H_0 + H_{Coul} + H_{dip} + \dots$$

H_0	single particle (band structure)
H_{Coul}	Coulomb interaction between carriers
H_{dip}	dipole interaction with optical field
…..	phonon coupling etc.





k . p Bandstructure for Bismides

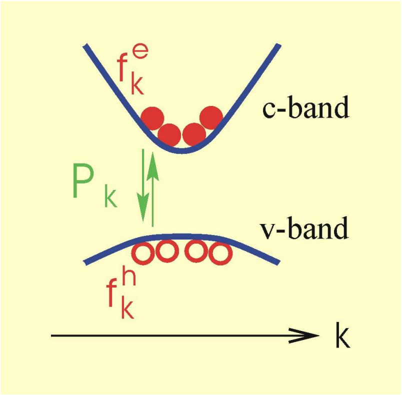


→ anticrossing of Bi-level and valence bands

Semiconductor Bloch Equations

$$\left[i\hbar\frac{\partial}{\partial t}-\epsilon^e_k-\epsilon^h_k\right]P_k=\left[1-f^e_k-f^h_k\right]\Omega_k+\frac{\partial}{\partial t}P_k|_{corr}$$

$$i\hbar\frac{\partial}{\partial t}\,f^a_k=-\Omega_k(t)P^*_k+\Omega^*_kP_k+\frac{\partial}{\partial t}f^a_k|_{corr}$$



field renormalization $\Omega_k(t)=d_{cv}\;E^{QW}(t)+\sum_{k'}\;V_{k-k'}\;P_{k'}(t)$

energy renormalization $\epsilon^a_k(t)\;=\;\varepsilon^a_k-\sum_{k'}\;V_{k-k'}\;f^a_{k'}(t)$

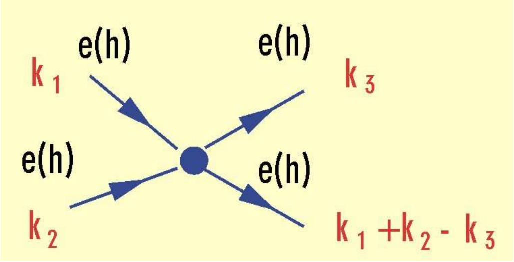
- nonlinearities: phase-space filling, gap reduction, Coulomb enhancement
- correlation contributions: scattering, dephasing, screening

Correlation Effects

Carriers: Quantum Boltzmann Equation

$$\frac{\partial}{\partial t}\, f_k^a(t)|_{corr} = \Sigma_k^{in,a}(t)[1 - f_k^a(t)] - \Sigma_k^{out,a}(t) f_k^a(t)$$

scattering rates:



$$\frac{\partial}{\partial t}\, f_k^a|_{corr} \approx \sum_{k_1 \dots k_3} |W|^2\, f_{k_1} f_{k_2}[1 - f_{k_3}][1 - f_k^a] - \dots$$

quasi-equilibrium: $$\frac{\partial}{\partial t}\, f_k^a|_{corr} = 0$$

detailed balance

Fermi-Dirac distribution: $f_k^a = F_k^a = \dfrac{1}{e^{(E_k - \mu_a)/k_B T} + 1}$

Correlation Effects

Polarization: Excitation Induced Dephasing

$$\left[i\hbar\frac{\partial}{\partial t}-\varepsilon^{e}_{\mathbf{k}}(t)-\varepsilon^{h}_{\mathbf{k}}(t)\right]P_{\mathbf{k}}(t)-\left[1-f^{e}_{\mathbf{k}}(t)-f^{h}_{\mathbf{k}}(t)\right]\Omega_{\mathbf{k}}(t)$$

$$=i\left[\Gamma_{\mathbf{k}}(t)P_{\mathbf{k}}(t)+\sum_{k'}\Gamma_{\mathbf{k},\mathbf{k}'}(t)P_{\mathbf{k}'}(t)\right]$$

Re $\Gamma_k(t)$ … diagonal dephasing
⇒ generalized T_2 time

Im $\Gamma_k(t)$ … diagonal energy shift
⇒ generalized band-gap shift

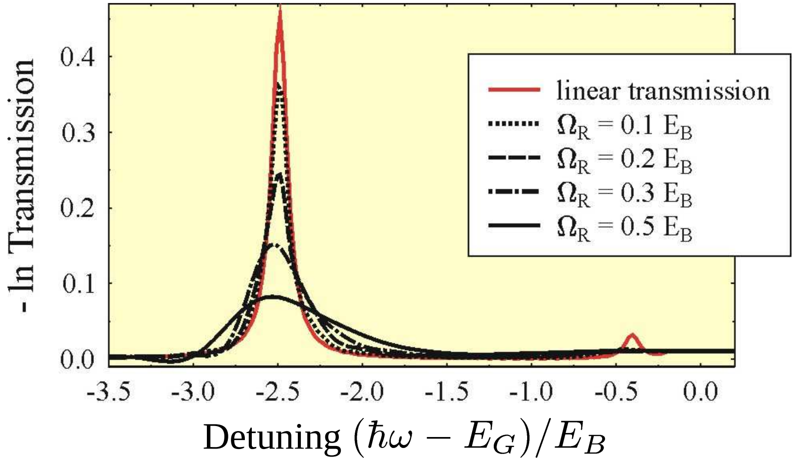
Re $\Gamma_{k,k'}(t)$ … off-diagonal dephasing

Im $\Gamma_{k,k'}(t)$ … off-diagonal energy shift

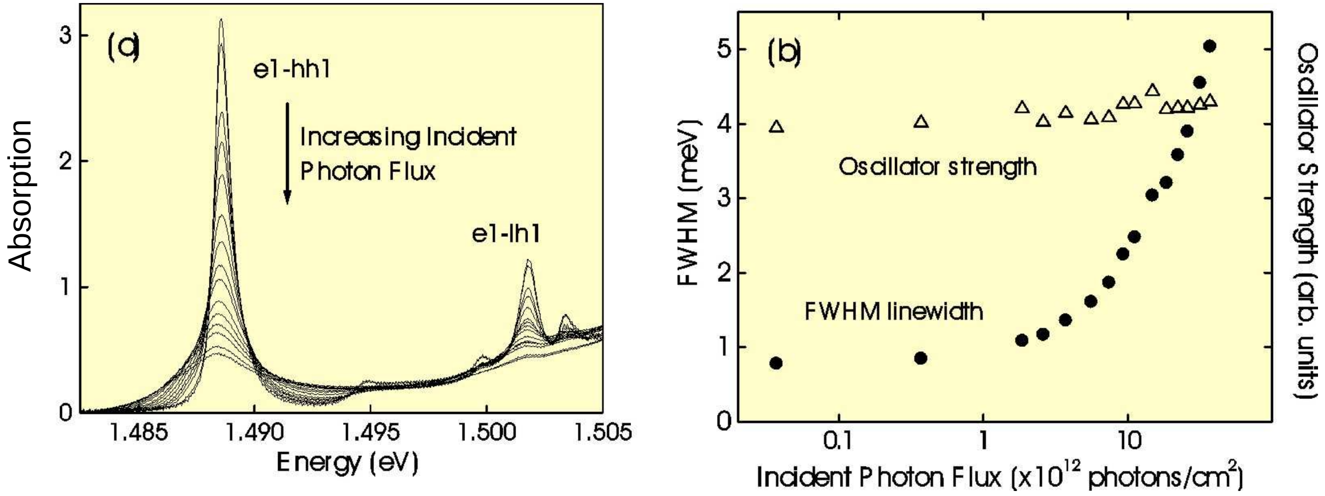
- $\Gamma_k(t)$ and $\Gamma_{k,k'}(t)$ are calculated from all terms quadratic in the screened Coulomb interaction
- strong compensation between diagonal and off-diagonal terms

⇒ important for excitation saturation: Jahnke *et al*., PRL 77, 5257 (1996).
and gain calculations: Haug/Koch Quantum Theory of … (World Scientific, 5th ed., 2009).

Exciton Saturation

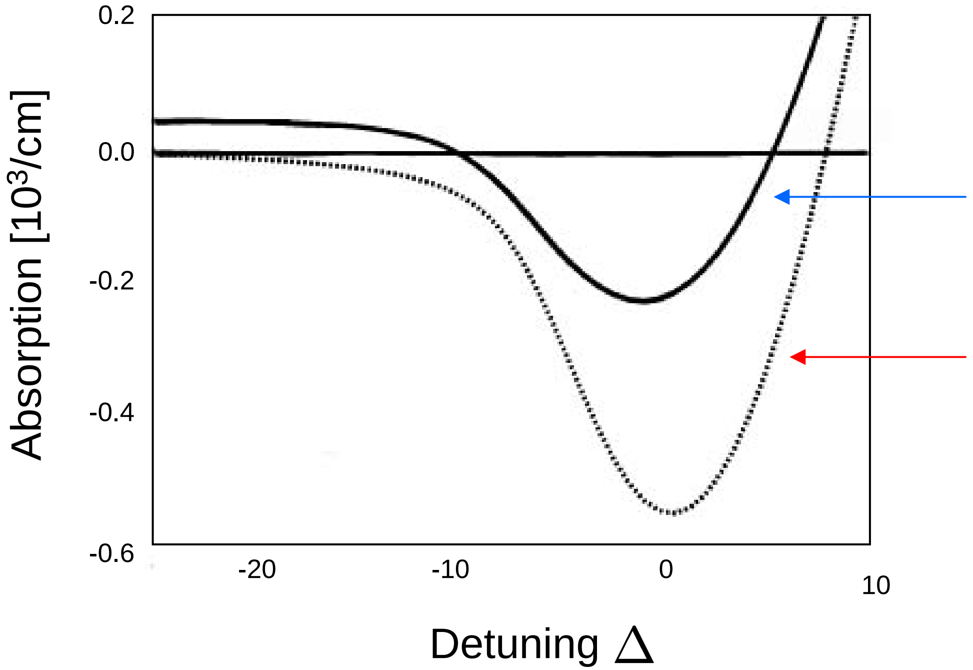


F. Jahnke, M. Kira, and S.W. Koch,
Z. Physik B 104, 559 (1997)



- experiment: InGaAs/GaAs QW
- Khitrova, Gibbs, Jahnke, Kira, Koch, Rev. Mod. Phys. 71, 1591 (1999)
- EID first observed in 4-wave mixing, Wang *et al.* PRL 71, 1261 (1993)

Lineshape Problem

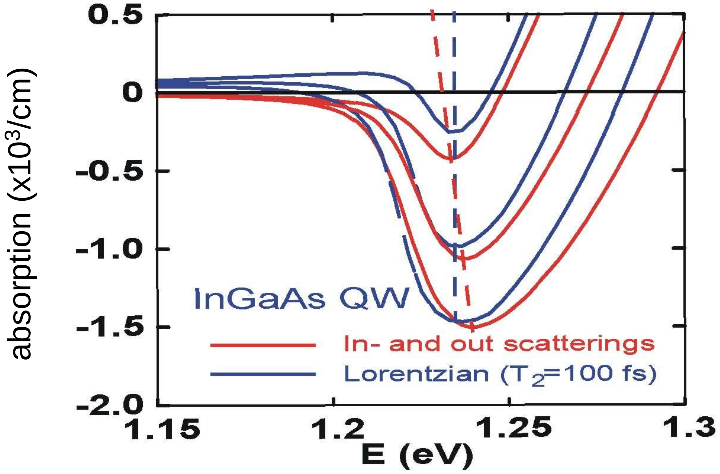


dephasing rate approx.

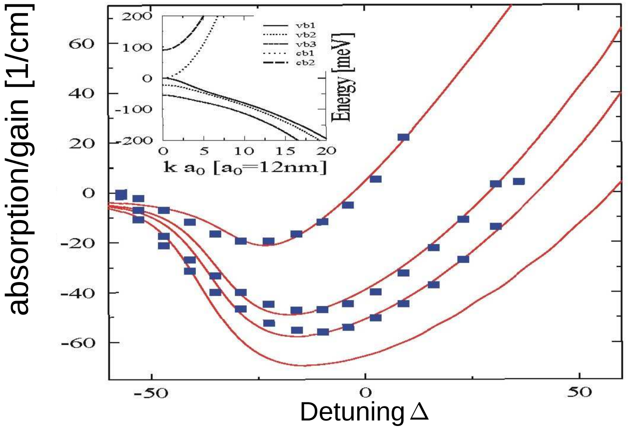
full calculation

- $\Delta = (\hbar\omega - E_G)/E_B$
- gain of two-band bulk material
- nondiagonal scattering contributions $\rightarrow$ lineshape modification, no absorption below the gap

Optical Gain in Semiconductors: Theory and Experiment



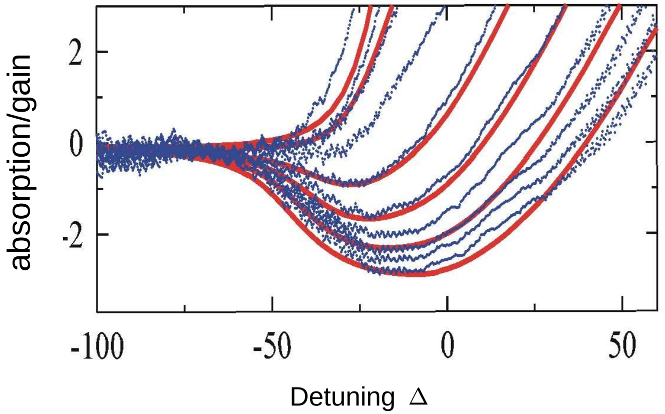
10nm (9.2nm) InGaAs/AlGaAs



N=1.6, 2.2, 2.5, 3.0*10^{12}/cm^2

exp: D. Bossert et al., theory: A. Girndt et al., Marburg

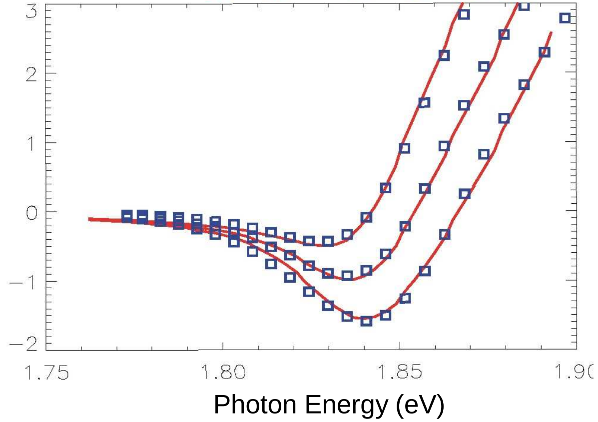
8nm InGaAs/AlGaAs



Current 0-20mA… Density 0.6-3.0x10^{12}cm^{-2}

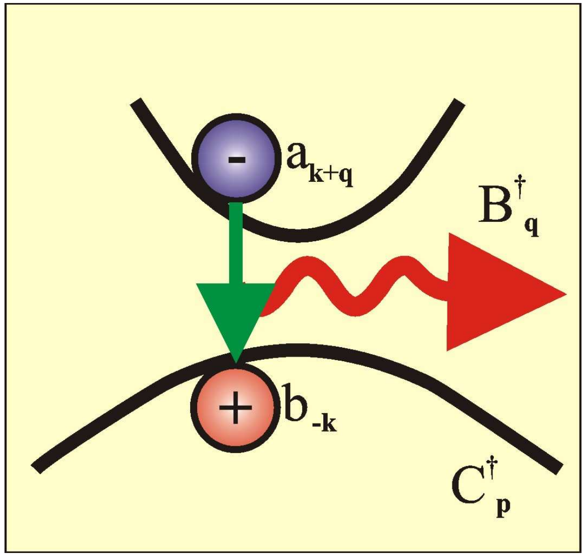
exp: C. Ellmers et al., theory: A. Girndt et al. Marburg

6.8 nm $In_{0.4}Ga_{0.5}P/(Al_{0.5}Ga_{0.5})In_{0.51}P_{0.49}$



Courtesy of W.W. Chow, P.M. Smowton, P. Blood, A. Grindt, F. Jahnke, and S.W. Koch

Luminescence: Quantized Light-Matter Interaction



$$H^{qm}_{cf} = \sum A(k,q) a_{k+q_{||}} b_{-k} B^\dagger_q + \mathrm{h.c.}$$

$A(k,q)$ proportional to dipole matrix element and mode strength in quantum wells

Semiconductor Luminescence Equations

$$i\hbar\frac{\partial}{\partial t}\Delta\left\langle B_q^\dagger B_{q'}\right\rangle = \hbar\left(\omega_{q'}-\omega_q\right)\Delta\left\langle B_q^\dagger B_{q'}\right\rangle + \sum_k \left(F_q \Pi_{k,q}^* - \text{c.c.}\right)$$

photon assisted interband polarization $\Pi_{k,q} = \Delta\left\langle B_q^\dagger b_{-k} a_{k+q_{||}}\right\rangle$

$$\left(i\hbar\frac{\partial}{\partial t} - \tilde{E}_{k,q_\parallel} + \hbar\omega_q\right)\Pi_{k,q} = \left(1 - f^e_{k+q_\parallel} - f^h_k\right)\sum_{k'} V_{k-k'}\Pi_{k',q}$$

$$+ \left.\frac{\partial \Pi_{k,q}}{\partial t}\right|_{col} + \Omega^{coh}_{k,q} + \Omega^{stim}_{k,q} + F_q S_{k,q}$$

incoherent source $S = \left\langle a^\dagger b^\dagger a b\right\rangle = f^e f^h + \Delta\left\langle a^\dagger b^\dagger a b\right\rangle$

coherent source $\Omega^{coh} \propto P, E$

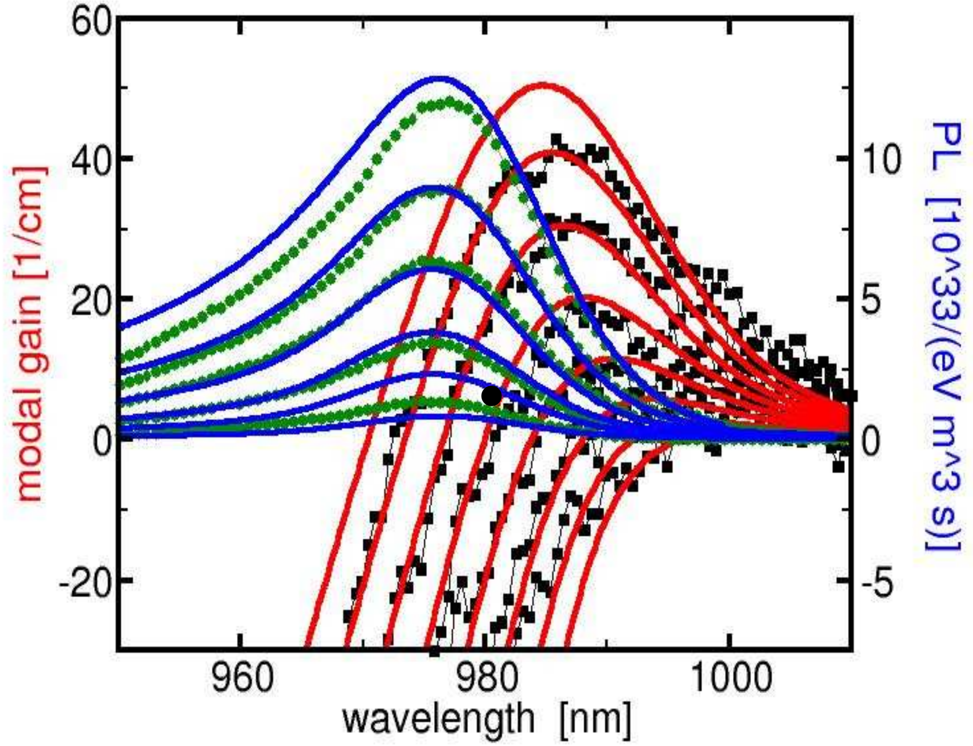
feedback (cavity) Ω^{stim}

excitonic signatures $\left(1 - f^e - f^h\right)\sum V\Pi$

Review: Kira & Koch, Prog. Quantum Electron. (2007)

Gain/Absorption and Luminescence

5nm $Ga_{0.8}In_{0.2}As/GaAs$ pin-MQW



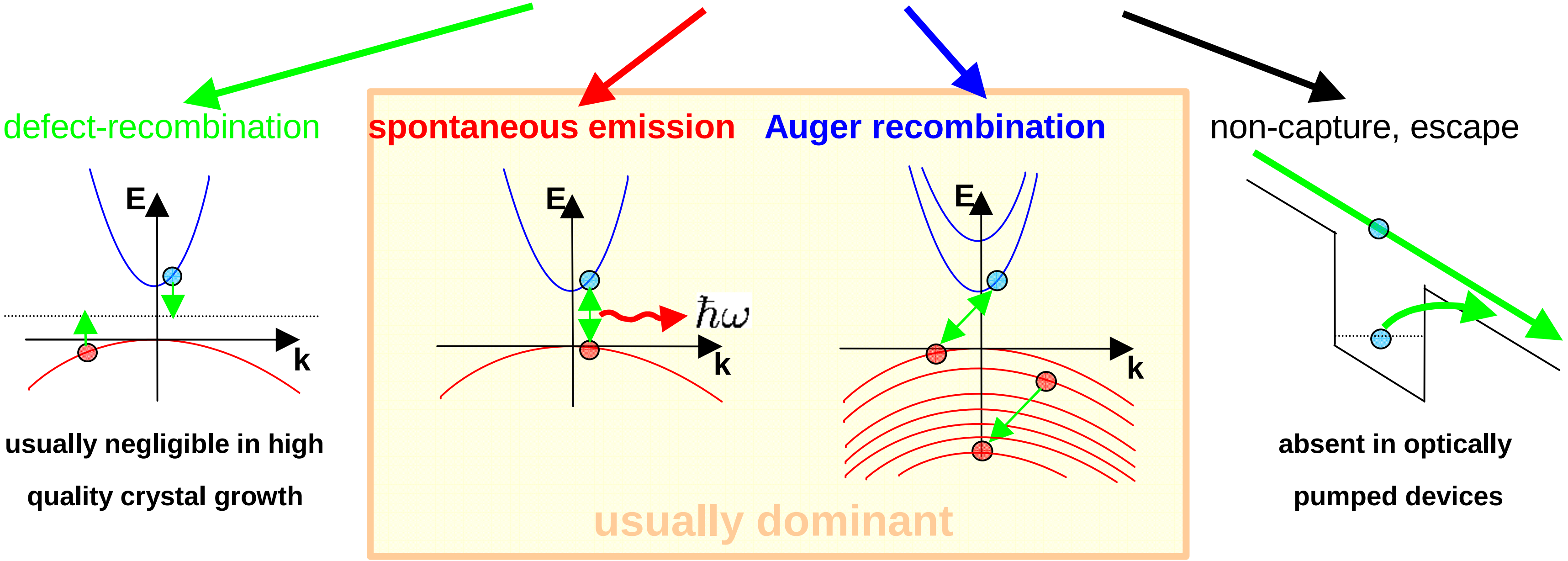
quantitative many-body theory:

detailed prediction of experiments
laser and LED etc. design

Losses in Semiconductor Lasers

classical parametrization of loss current J_{loss}:

$$J_{loss} = \mathbf{AN} + \mathbf{BN^2} + \mathbf{CN^3} + J_{rest}$$



defect-recombination

spontaneous emission

Auger recombination

non-capture, escape

usually negligible in high quality crystal growth

usually dominant

absent in optically pumped devices

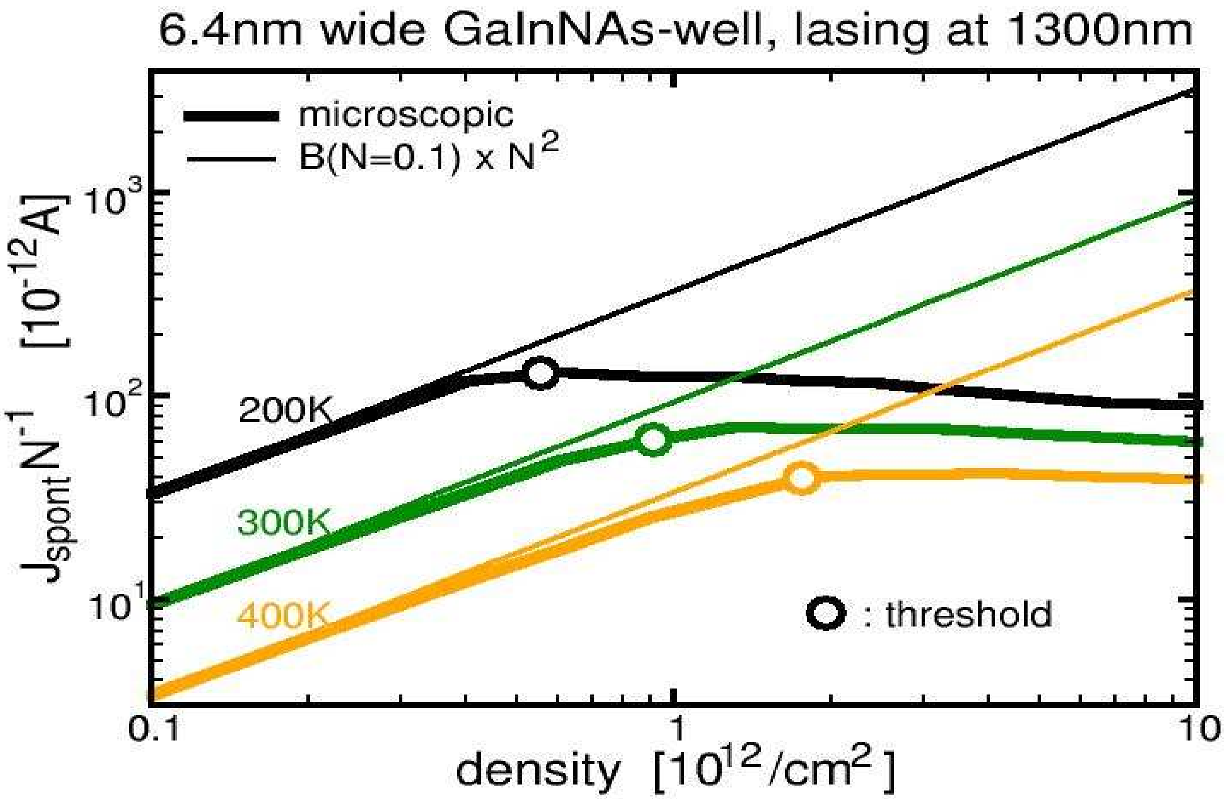
problems with A, B, C - parametrization:

- **parameters only very roughly known and only for special cases;**
  depend on well- and barrier-materials, layer widths, temperatures, densities...

- **simple density dependence far from reality**

Spontaneous Recombination Current

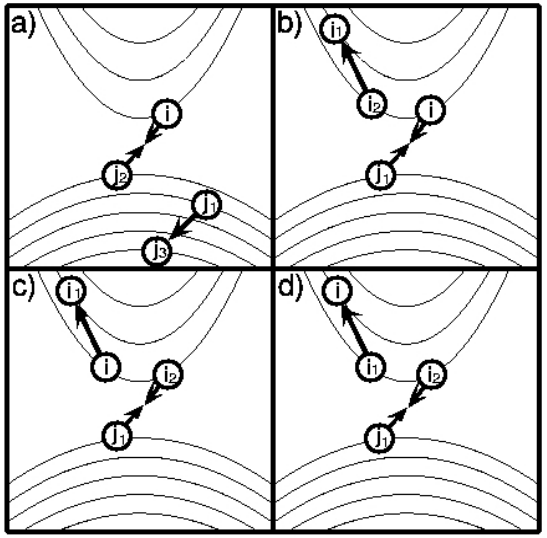
$$J_{spont} = eR_{spont} = e \int d\omega \; I_{PL}(\omega)$$



➡ J_{spont} linear N dependence at high densities

Auger Recombination

Quantum-Boltzmann scattering
in 2. Born-Markov approximation:



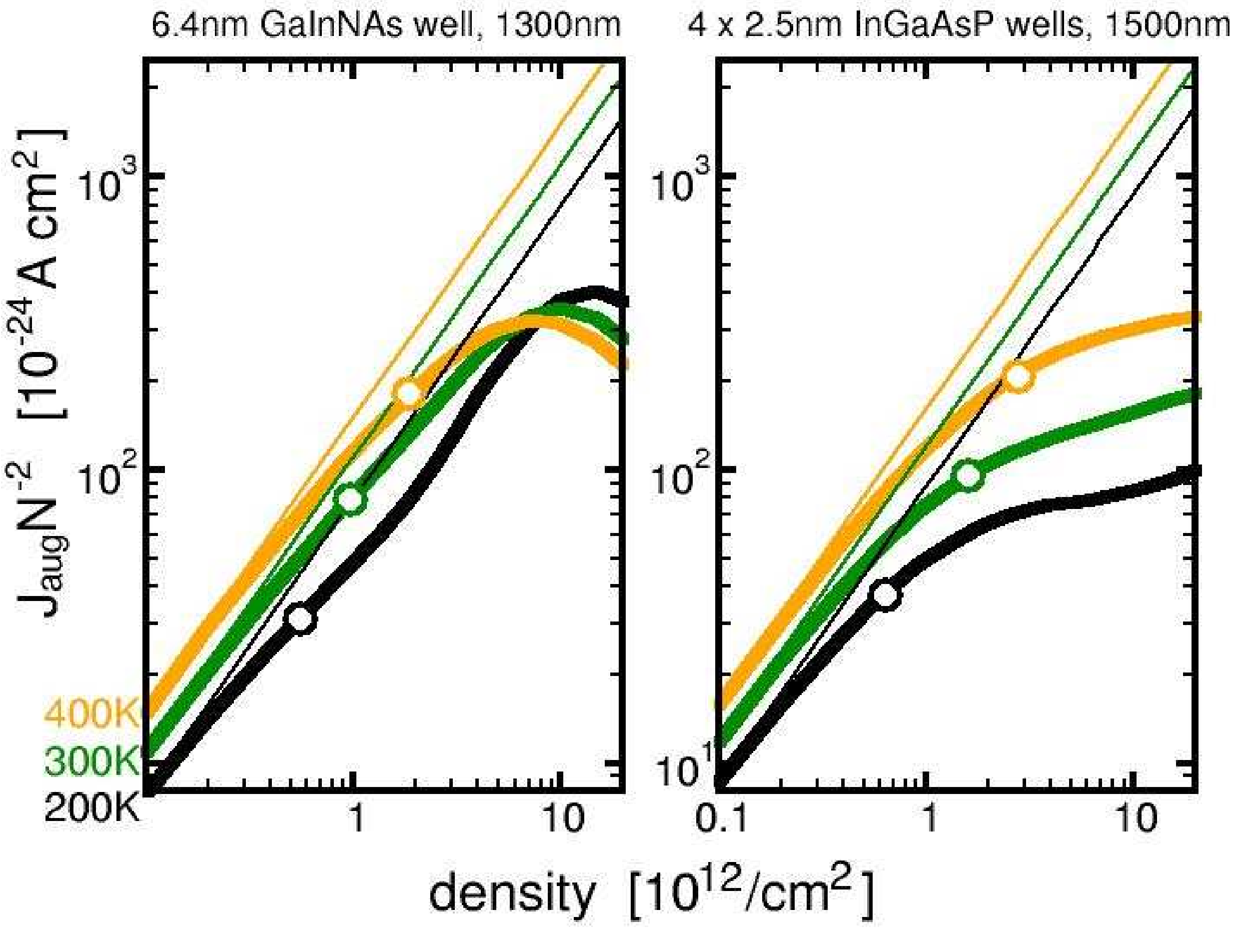
Impact Ionization

$$\frac{\partial}{\partial t} f_k^a|_{aug} = \frac{2\pi}{\hbar} \sum_{k_1,k_2,k_3,b=e,h} |W|^2 \Big[f_{k_1}^b [1 - f_{k_2}^c][1 - f_{k_3}^d][1 - f_k^a]$$

$$- [1 - f_{k_1}^b] f_{k_2}^c f_{k_3}^d f_k^a \Big] + \ldots$$

Auger Recombination

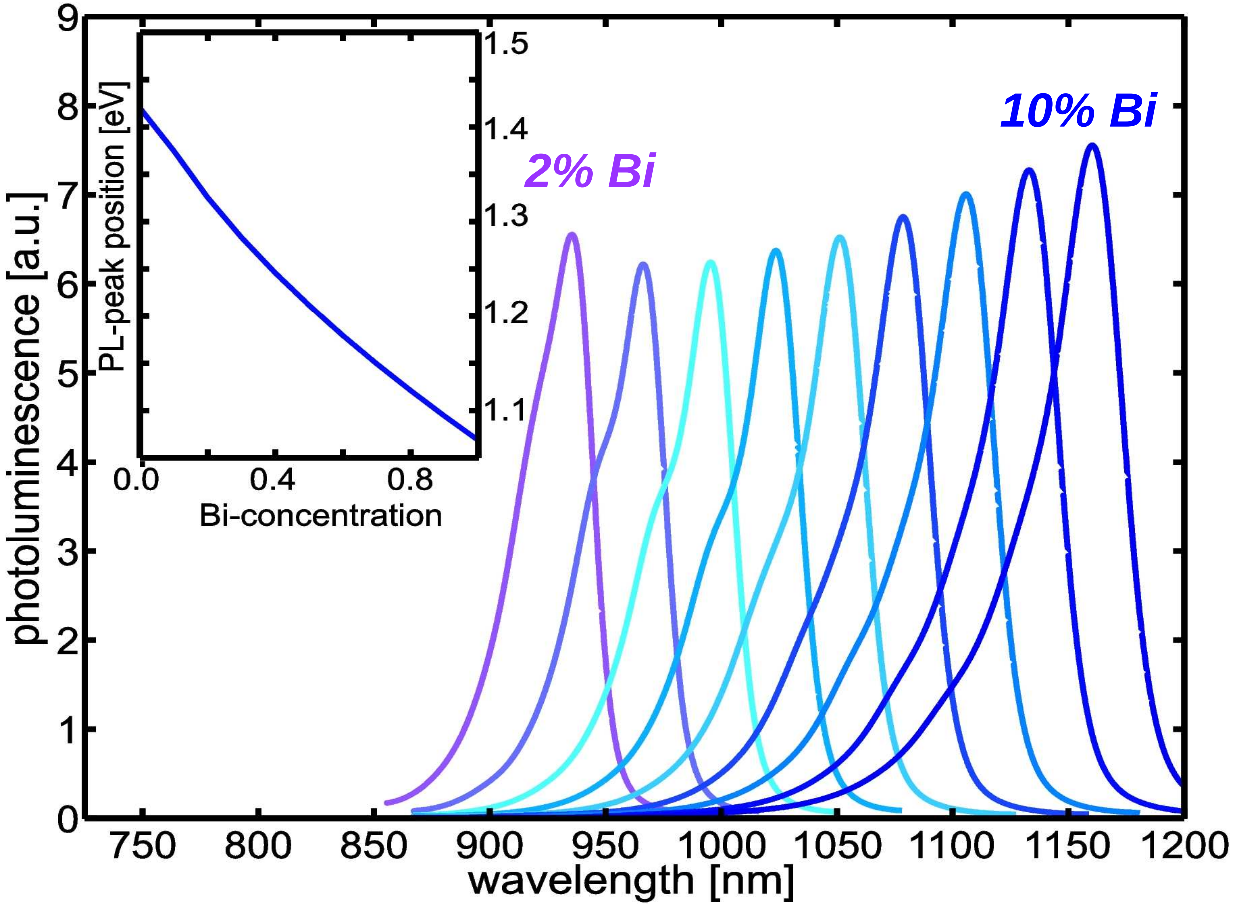
Auger Recombination: Examples



J_{aug} increase far less than cubic with N, sometimes even less than quadratic

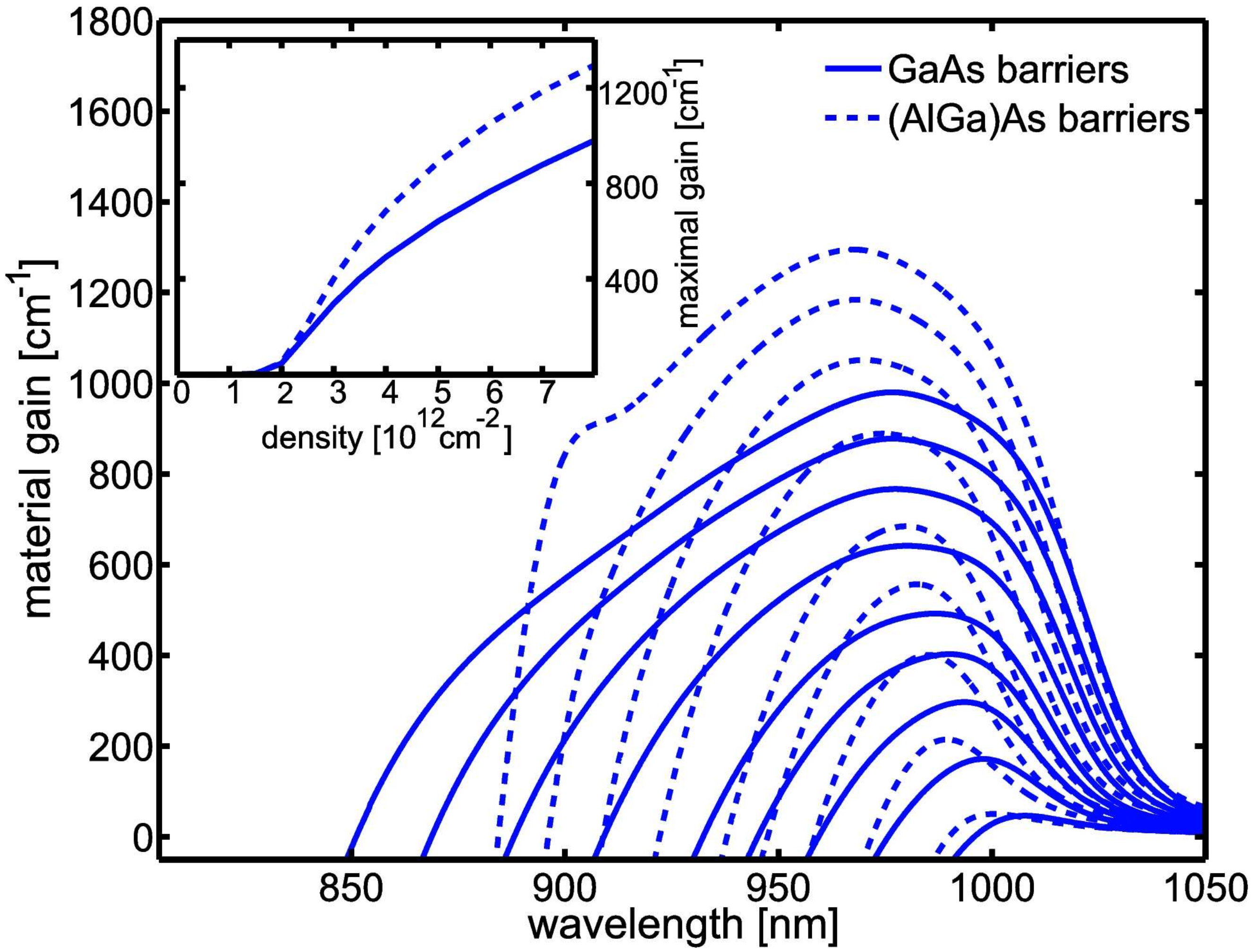
Bismides Applications

PL spectra Ga(AsBi)/GaAs quantum wells



strong red shift of PL peak with increasing Bi concentration

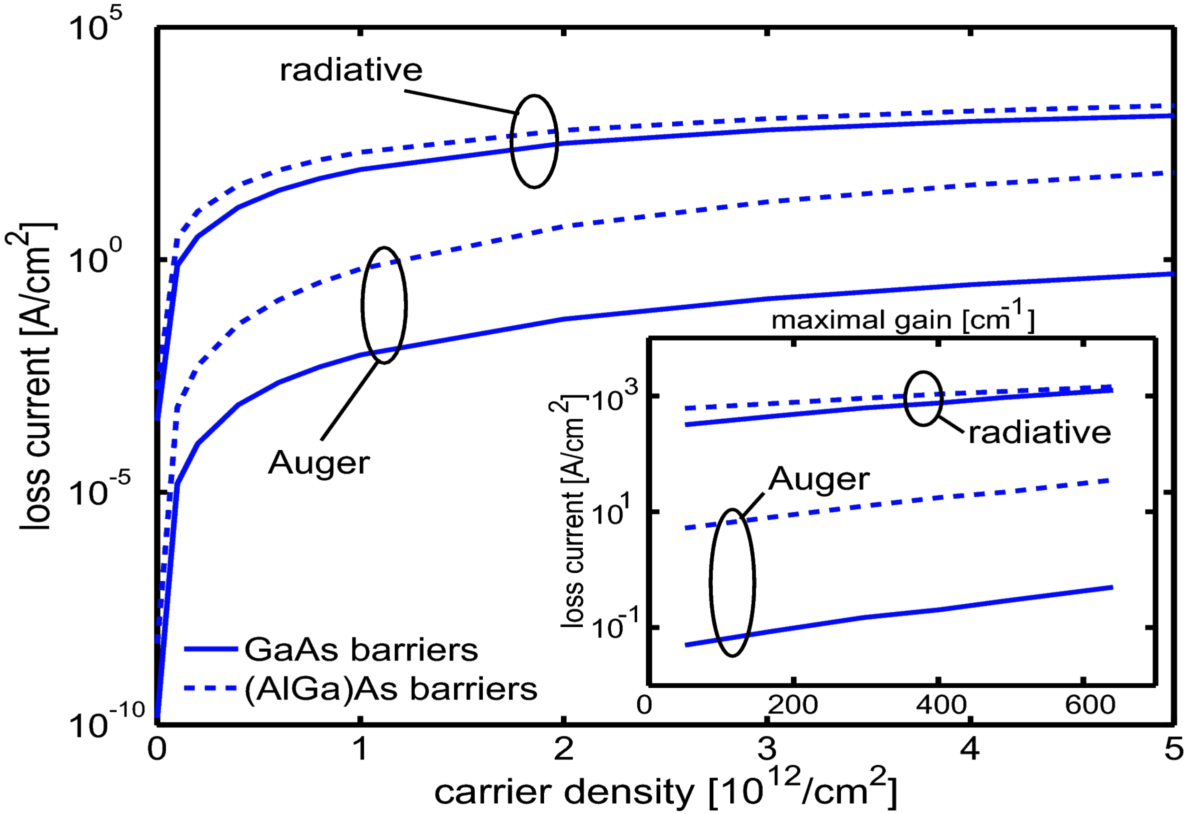
Gain Spectra of Ga(As$_{0.96}$Bi$_{0.04}$) Quantum Wells



better electron confinement with AlGaAs barriers

Spontaneous Recombination and Auger Losses

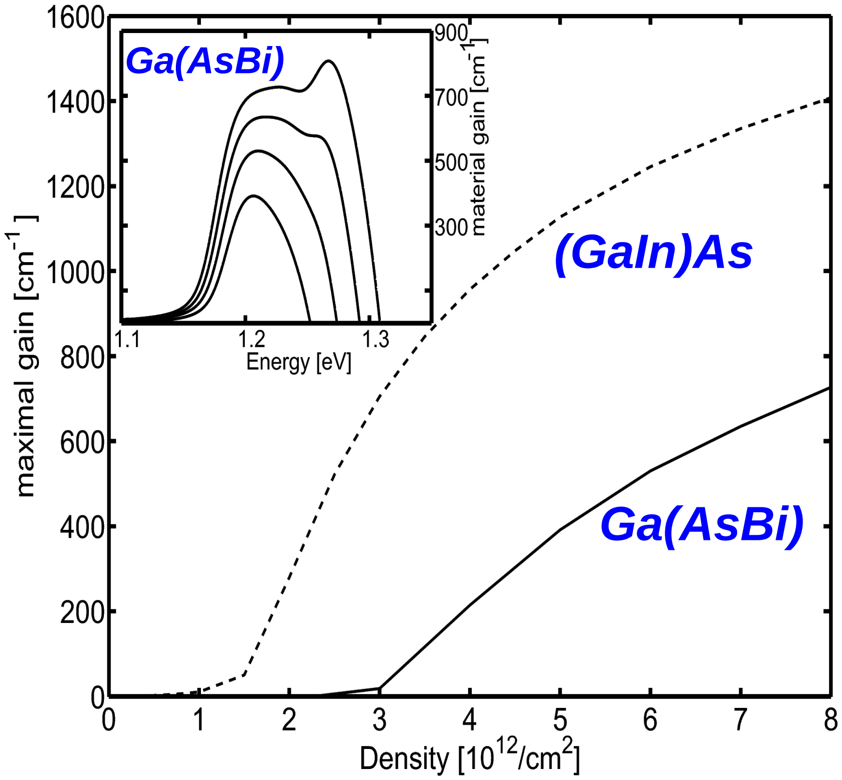
8 nm Ga($As_{0.96}Bi_{0.04}$) quantum wells, T=300K

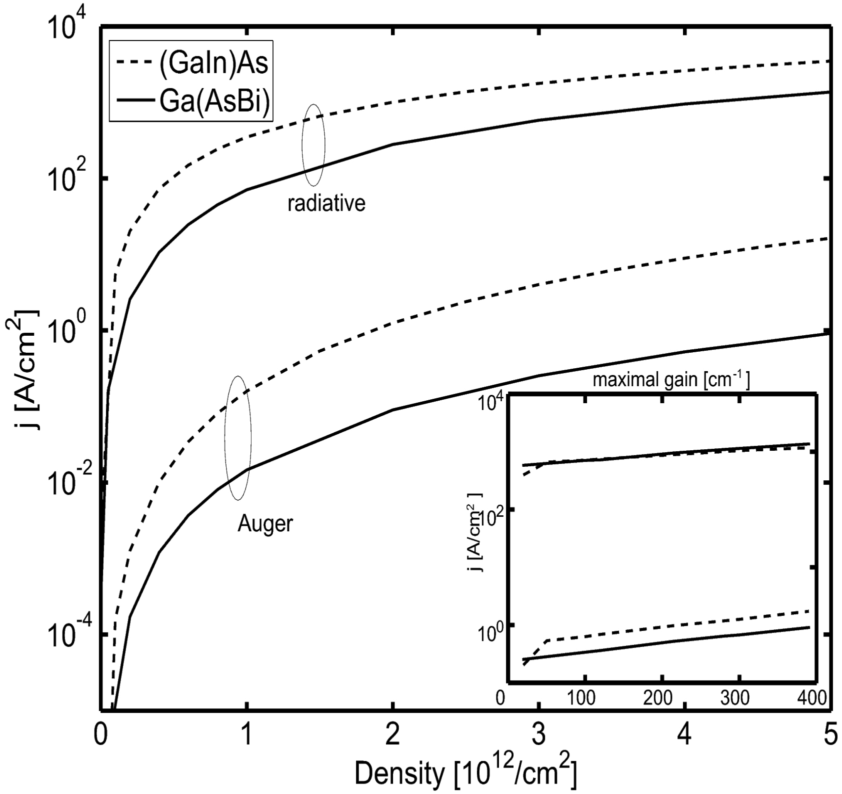


in both cases dominance of radiative losses
strong confinement due to AlGaAs barriers leads to higher Auger losses

Comparison Ga(AsBi) and (GaIn)As

both structures designed for peak gain around 1.2 eV





more gain in (GaIn)As, lower losses in Ga(AsBi)

no significant differences in losses when normalized to material gain

Summary

- predictive microscopic theory
- application to Bi containing GaAs based materials
- gain and absorption
- intrinsic losses (radiative, Auger)

To Do:

- detailed comparison with quantitative measruements of Bismides
- systematic treatment of disorder and many-body effects

Selected References:

- Haug/Koch, “Quantum Theory of the Optical and Electronic Properties of Semiconductors”, 5th ed. World Scientific Publishing (2009).

- Kira/Koch, Progress in Quantum Electronics (2007).