Self Consistent solution of a multi-band k.p Hamiltonian and Poisson's Equation using a Plane Wave Expansion Method

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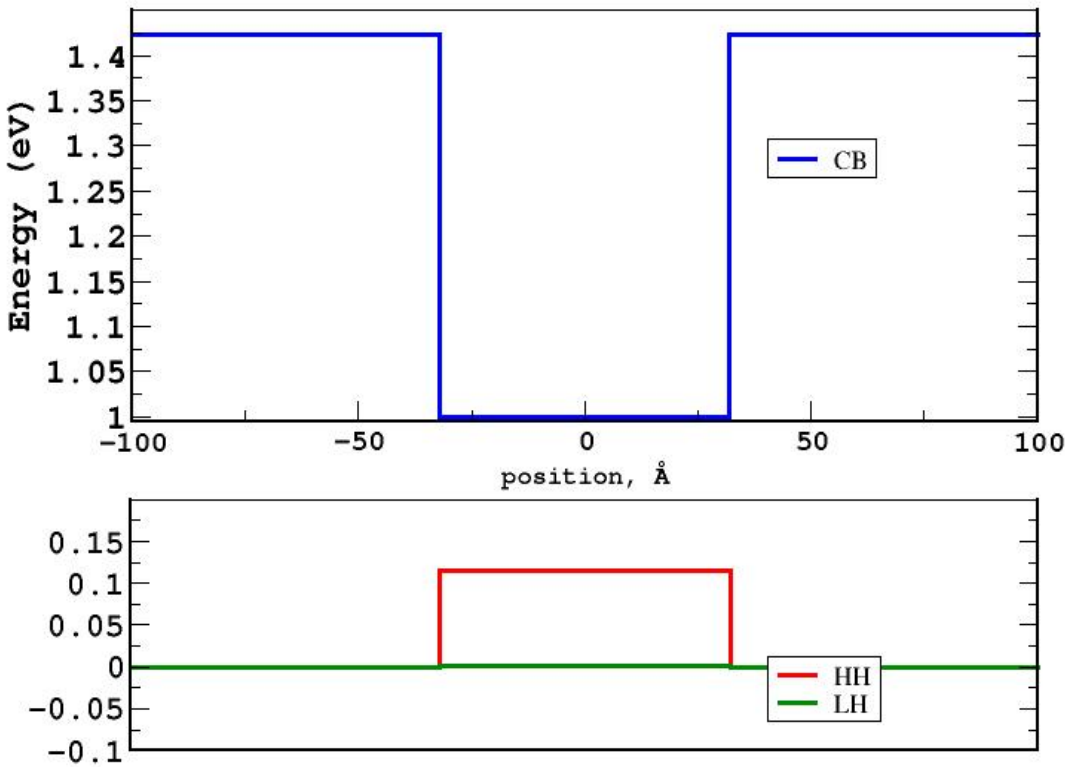
NDP NATIONAL DEVELOPMENT PLAN

Outline

- Necessity of electrostatic effects?
- An efficient self consistent algorithm.
- Application to 1300 nm GaInNAs systems.
- Conclusions

1300nm $In_{0.34}Ga_{0.36}As_{0.983}N_{0.017}$ QWs

- Large conduction band offset ~400meV
- Increased localisation of wavefunction due to dilute nitride.
- Small-medium valence band HH offset: ~4kT at RT?
- Lasers exhibit unexpected temperature sensitivity, why?
- Hole leakage significant or not?



Infineon 1300 nm
$In_{0.34}Ga_{0.36}As_{0.983}N_{0.017}$/GaAs QW

InGaAsP-electron leakage

IEEE JOURNAL OF QUANTUM ELECTRONICS, VOL. 30, NO. 2, FEBRUARY 1994

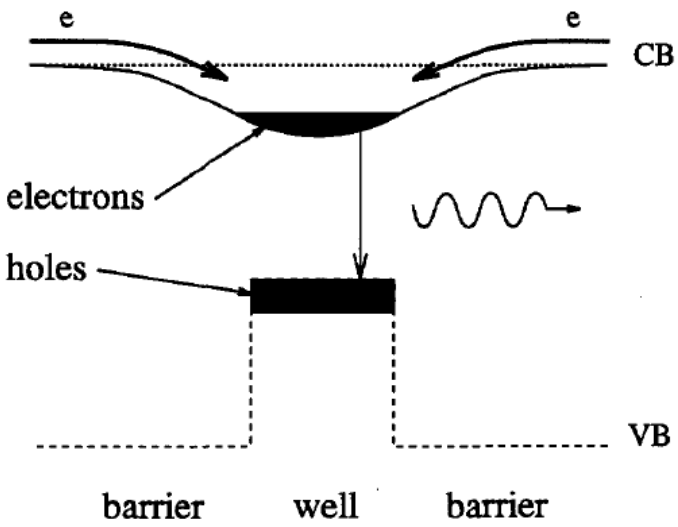


Fig. 2. For a structure with zero conduction band offset (dotted line) the electrons will see no confining barrier. However, the strong confinement of the holes (dashed line) and the need for charge neutrality throughout the structure will generate an elecrostatic well (solid line) which confines the electrons within the vicinity of the well. The valence band potential edge will experience the same change in potential but this will have comparatively little effect on the hole distribution.

M. Silver and E. P. O'Reilly

- **Previous work on effects of electrostatic confinement on CB levels shows induced potential deepens CB QW with increased carrier density, enabling lasing in 1500 nm InGaAsP.**
- **CB well can be deepened by 50-100 meV at transparency.**
- **Valence band confinement is 150-200meV, holes are substantially unaffected by induced potential.**

Approach

- 10 band k.p Bandstructure, momentum matrix elements, absorption and gain already developed using plane wave expansion method. Fourier coefficients of envelope function readily available.
- Poisson's equation *easily solvable* in Fourier space.
- Idea: identify an expression for the carrier density in Fourier space from the coefficients in the envelope function expansion, and remove the necessity to calculate the wave function in real space, (common practice in density functional theory).
- Method relies on fermi dirac statistics to provide a good approximation to the carrier densities and hence the induced mean field potential.

Deriving the Potential in Fourier Space

- **Wavefunction**

$$\psi_n(k_{||}, z) = \frac{1}{\sqrt{2L}} \sum_{k_z \beta} A_{n\beta}^{k_z}(k_{||}) exp[ik_z z] \phi_\beta(z) \tag{1}$$

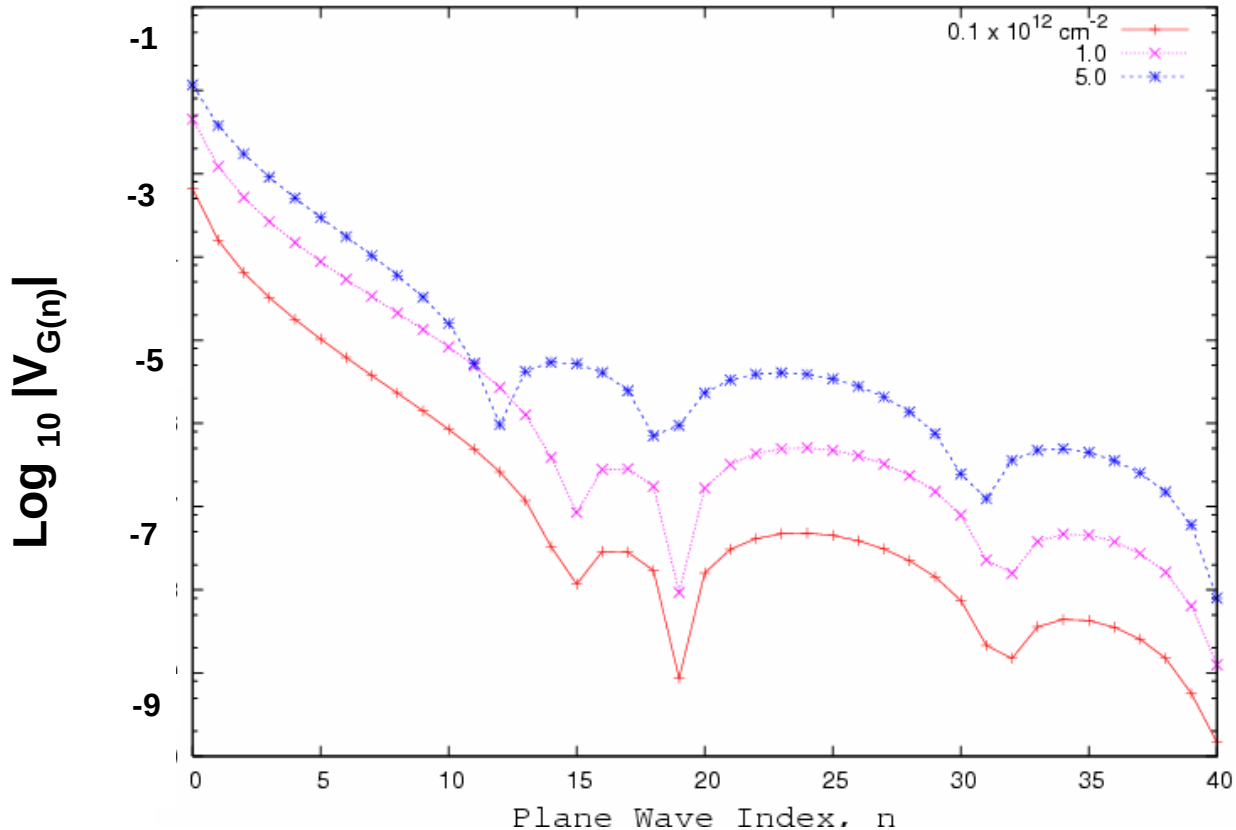
- **Carrier density**

$$n(z) = \int \frac{k_{||} dk_{||}}{2\pi} \sum_n \left(\psi_n(k_{||}, z) \psi_n^*(k_{||}, z) f_e(E_{cn}, \mu_c) \right) \tag{2}$$

- **Potential in Fourier Space**

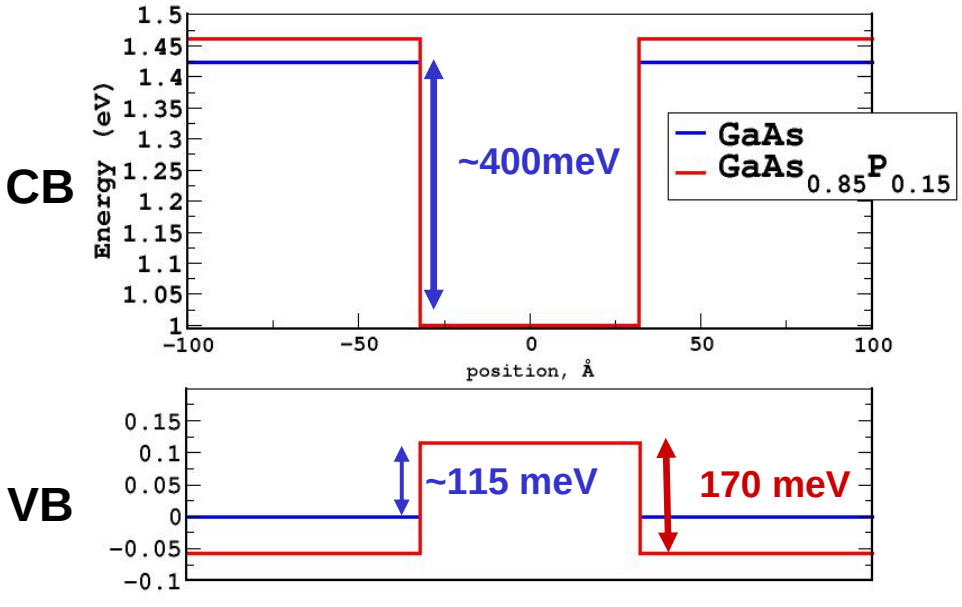
$$\tilde{V}_G = \frac{e^2}{\epsilon} \frac{1}{G^2} \int \frac{k_{||} dk_{||}}{4\pi L} \sum_{n\beta k_z} \left(A_{n\beta}^{k_z}(k_{||}) A_{n\beta}^{*k_z+G}(k_{||}) f_e - h.t. \right) \tag{3}$$

Fourier Series convergence of the potential

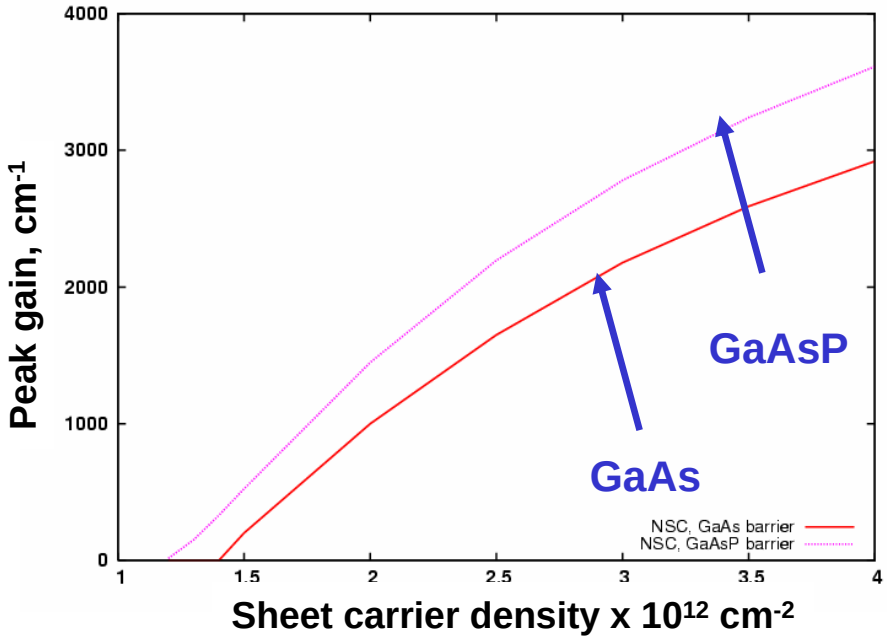


$\frac{1}{G^2}$ Term brings rapid convergence of potential with number of plane waves for all carrier densities.

Results - Peak Gain Vs Carrier Density, NSC

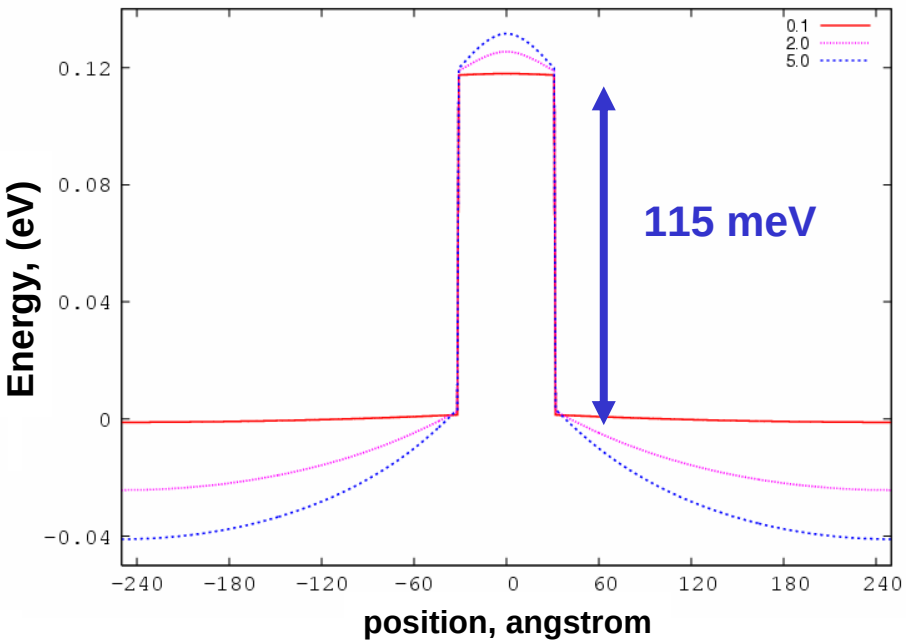


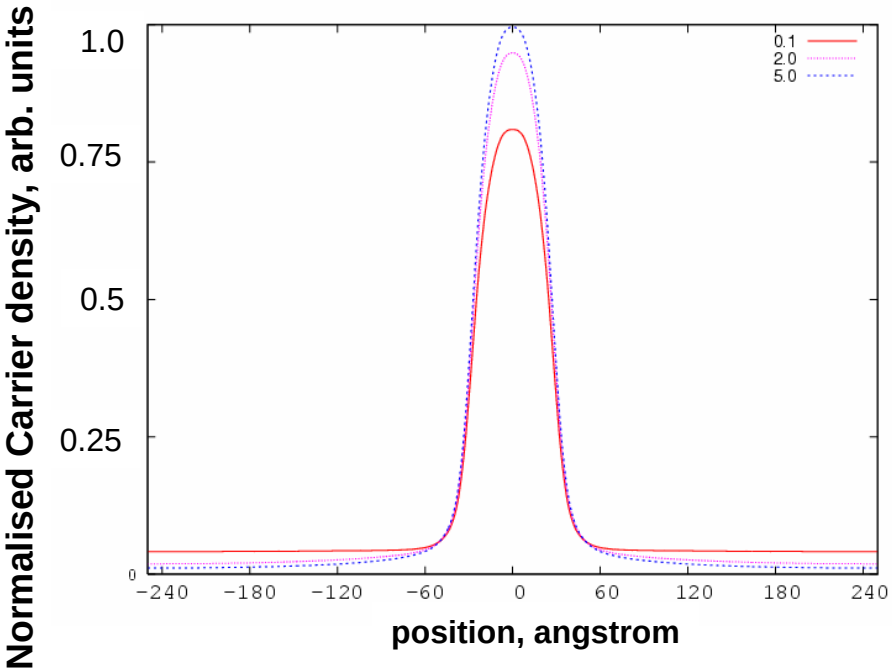
$In_{0.34}Ga_{0.36}As_{0.983}N_{0.017}$/GaAs QW



- Non self consistent results would conclude that the replacement of GaAs barriers with GaAsP has a significant effect on peak gain, consistent with previous calculations. Carrère *et al.* APL 86, 071116 (2005)
- dg/dn increases significantly with GaAsP barrier.
- Note that the barrier used is fully GaAsP in the rest of the supercell, as in the paper above.

Poisson Effects on the Hole Carrier density



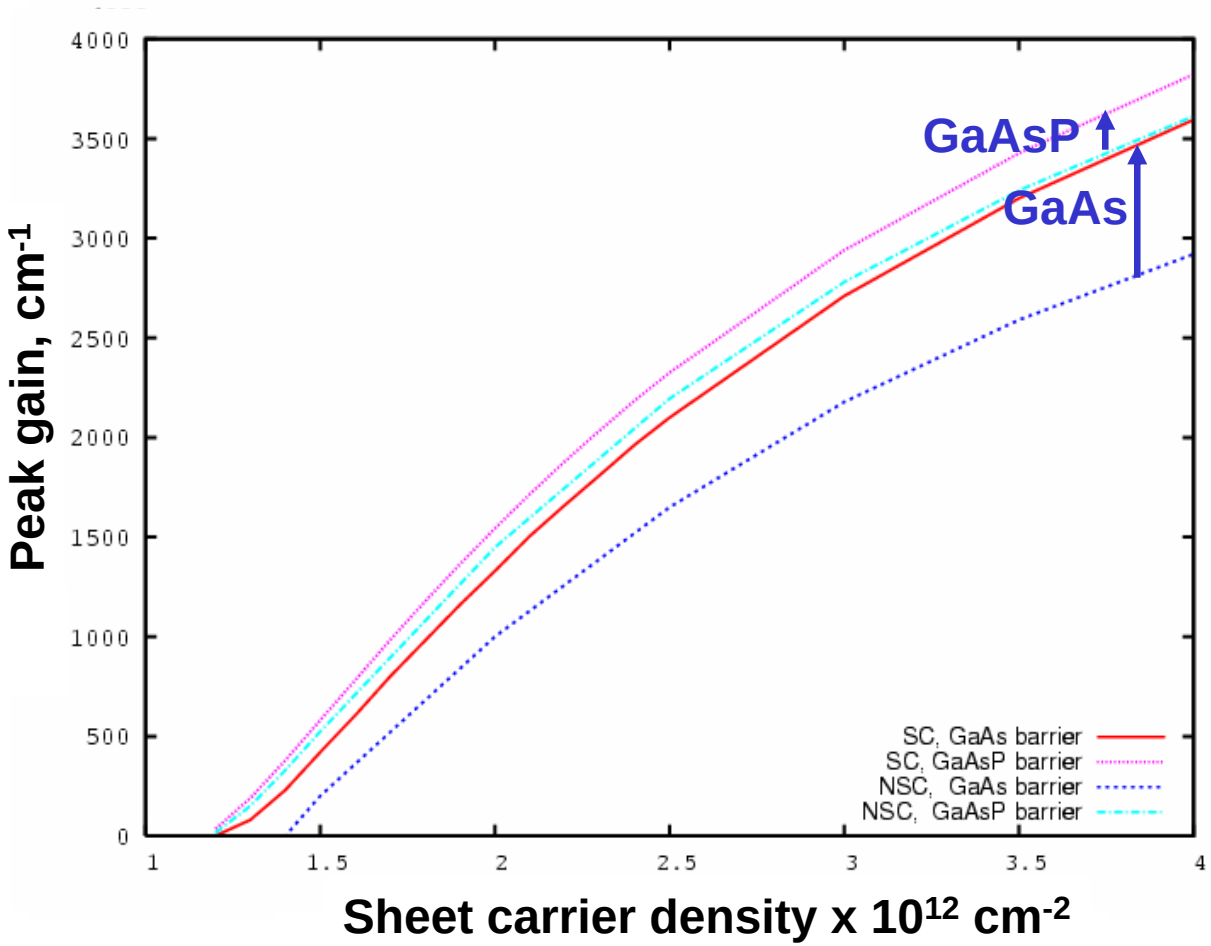


- Change in VB HH potential significant with increasing sheet carrier density
- Well deepens by ~15 meV
- Barrier increases significantly in neighbourhood of well.

- Normalised carrier distribution becomes increasingly peaked with increasing sheet carrier density
  - % carriers in barrier decreases
  - Barrier increases significantly also

Peak Gain Vs Carrier Density-SC

- Self consistent GaAs barrier reaches transparency earlier, at a similar point as the GaAsP
- Large HH mass means that a small change in potential has a large effect on dg/dn
- Increase in VB barrier height due to GaAsP has smaller effect on self consistent peak gain

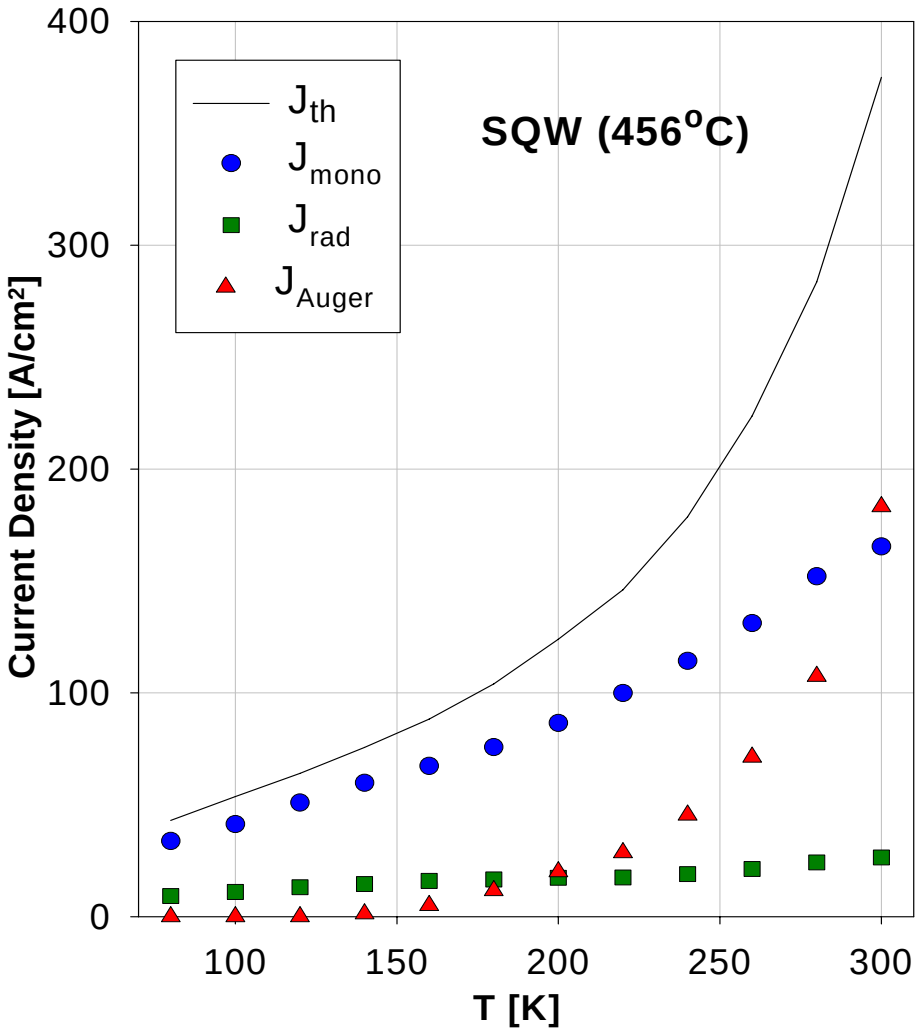


Recombination Processes in GaInNAs

- Fehse *et al* examined the role of different processes in the large increase in J_{th} with increasing temperature
- They established the significant importance of monomolecular recombination in 1300 nm dilute GaInNAs.
- It would then be expected that samples with lower nitride conc. would exhibit lower lasing threshold

$$I = eV\,(An + Bn^2 + Cn^3)$$

Fehse et al. **IEEE J. Sel. Topics in Quant. Electron., 8, 801**



Recent Experimental Results

IEEE PHOTONICS TECHNOLOGY LETTERS, VOL. 17, NO. 5, MAY 2005

Increased Monomolecular Recombination in MOCVD Grown 1.3-μm InGaAsN–GaAsP–GaAs QW Lasers From Carrier Lifetime Measurements

O. Anton, C. S. Menoni, J. Y. Yeh, L. J. Mawst, J. M. Pikal, and N. Tansu

- **Anton, Menoni *et al,* have recently shown that the carrier recombination times in InGaAsN are significantly shorter than InGaAs.**

- **They have calculated that the monomolecular recombination increases by a factor of 4, most likely due to increased numbers of defect centers in the dilute nitride alloy.**

Conclusion

- Efficient Schrödinger-Poisson technique.
- Applied to GaInNAs:
  small CB induced electrostatic potential significantly reduces likelihood of HH leakage due to large HH effective mass.
- Conclude that likely increase in J_{th} for dilute nitrides is due to large increase in monomolecular recombination.