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Optical Gain Analysis of Strain Compensated InGaN-AlGaN Quantum Well Active Region for Lasers Emitting at 460-500 nm

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Numerical Simulation of Optoelectronic Devices
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Outline

- **Motivation**
  - The challenge of conventional InGaN QW
  - **Strain Compensated QW** for improve gain media
- **Theoretical Formulation of 6-band *k·p* method for III-Nitride**
  - Incorporate SO-coupling and valence band mixing
  - Incorporate strain effect
  - Incorporate spontaneous and piezoelectric field
- **Spontaneous emission and optical gain properties**
  - 460-nm
  - 500-nm

  } **Conventional Vs. Strain Compensated QW**
- **Threshold Analysis for Laser Applications**
- **Summary**

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Characteristic of InGaN QW

The advantages of III-Nitride based QW

- Cover a wide spectral range, from near-IR (InN) to UV (GaN)
- $In_xGa_{1-x}N$ QW can cover emission from Blue, Green and Red

Major challenges preventing high performance conventional InGaN QW

- Strain misfit dislocation density from strain-mismatch InGaN/GaN
- Phase separation in high-In content InGaN QW
- The existence of electrostatic field in III-nitrides
  - ***Reduction of electron & hole wave function overlap***

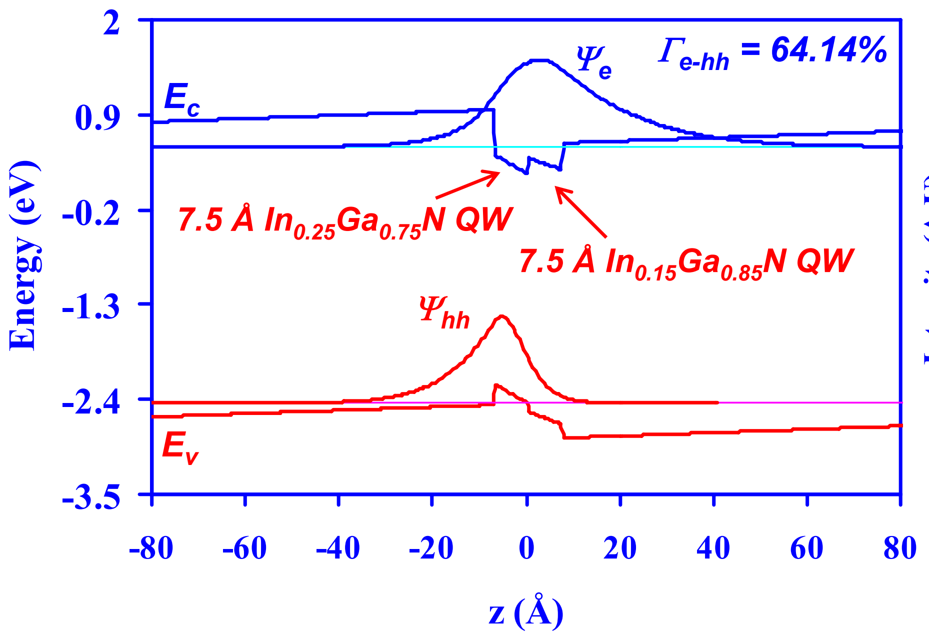
Nanostructure Engineering

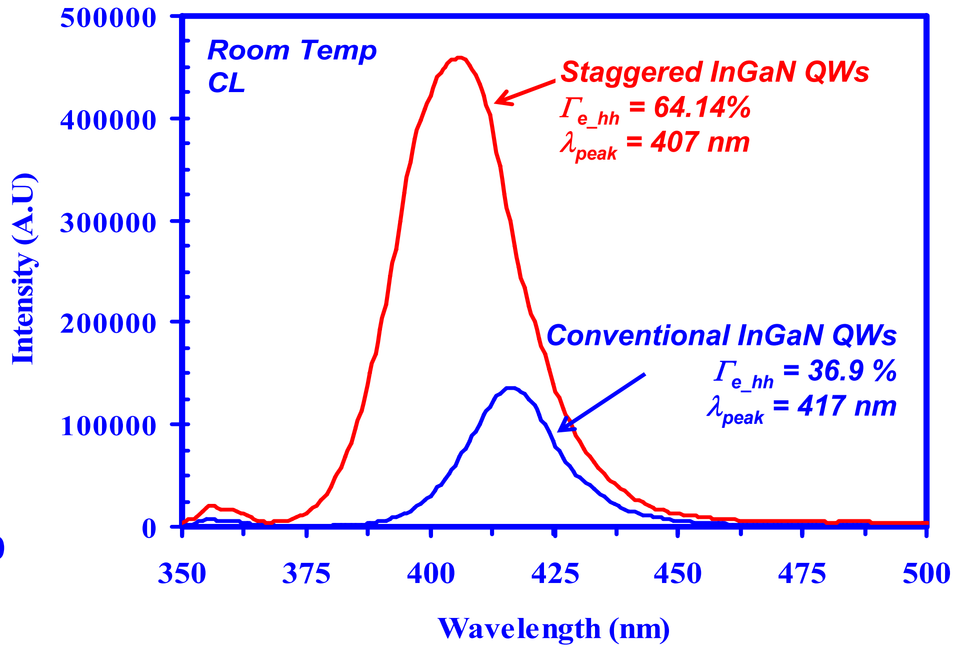
- Staggered InGaN QW [1,2]
- Type-II InGaN-GaNAs QW[3]

1. *R. A. Arif, Y. K. Ee, and N. Tansu, Appl. Phys. Lett., vol. 91 (9), Art. 091110, August 2007.*
2. *R. A. Arif, Y. K. Ee, and N. Tansu, in Proc. of the IEEE/OSA Conference on Lasers and Electro-Optics (CLEO) 2007, Baltimore, MD, May 2007;*
3. *R. A. Arif, Y. K. Ee, and N. Tansu, in Proc. of the IEEE/OSA Conference on Lasers and Electro-Optics (CLEO) 2006, Long Beach, CA, May 2006.*

Staggered / Graded InGaN QW [1,2]

for Enhanced Radiative Recombination Rate

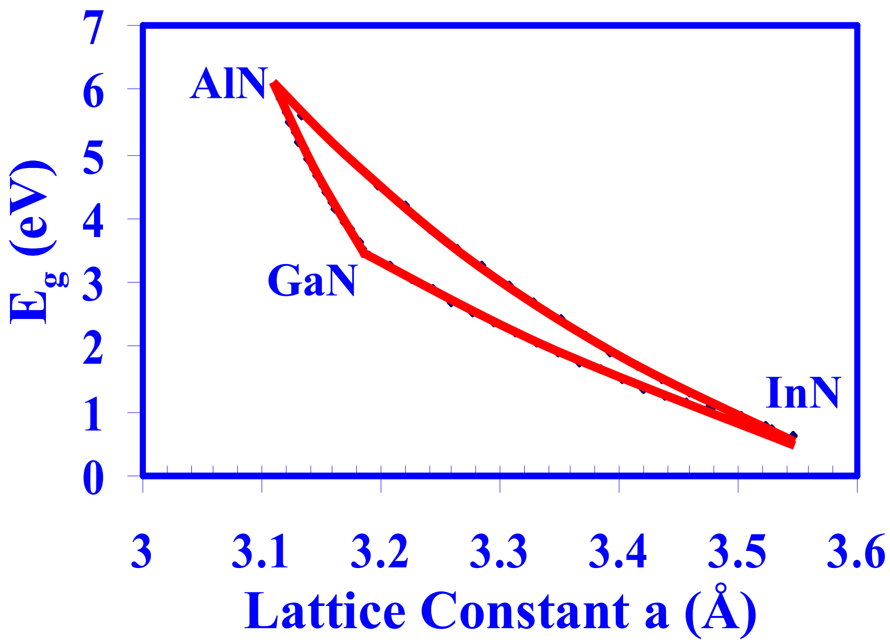




- **Staggered InGaN QW with improved Γ_{e_hh} ~ 64%**
  - **→ Conventional QW with Γ_{e_hh} ~ 36%**
- **Electrical Injected Staggered InGaN QW LEDs [1,2] (grown by MOCVD)**
  - **→ Experiments (CL, PL, devices) show good agreement with theory**

1. *R. A. Arif, Y. K. Ee, and N. Tansu, Appl. Phys. Lett., vol. 91 (9), Art. 091110, August 2007.*
2. *R. A. Arif, Y. K. Ee, and N. Tansu, Conference on Lasers and Electro-Optics 2007, Baltimore, MD, May 2007.*

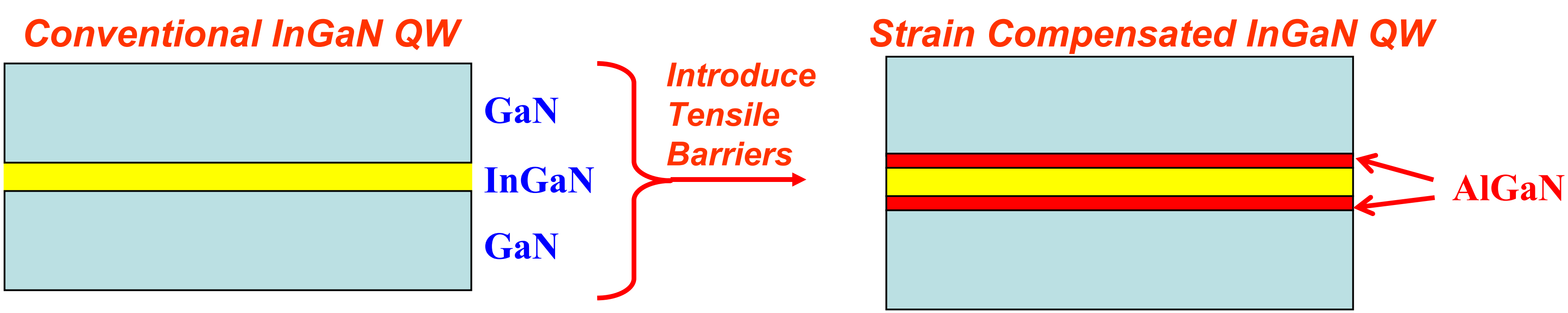
Strain compensated InGaN QW[1]



a_InN=3.545 Å
a_GaN=3.189 Å
a_AlN=3.112 Å

a_InGaN >a_GaN → Compressive Strain

a_AlGaN <a_GaN → Tensile Strain



6 x 6 Hamiltonian matrix

for valence band

$$H = \begin{bmatrix} F & -K^* & -H^* & 0 & 0 & 0 \\ -K & G & H & 0 & 0 & \Delta \\ -H & H^* & \lambda & 0 & \Delta & 0 \\ 0 & 0 & 0 & F & -K & H \\ 0 & 0 & \Delta & -K^* & G & -H^* \\ 0 & \Delta & 0 & H^* & -H & \lambda \end{bmatrix} \begin{matrix} |u_1\rangle \\ |u_2\rangle \\ |u_3\rangle \\ |u_4\rangle \\ |u_5\rangle \\ |u_6\rangle \end{matrix}$$

$$F = \Delta_1 + \Delta_2 + \lambda + \theta$$

$$\lambda = \frac{\hbar^2}{2m_0}\left[A_1 k_z^2 + A_2(k_x^2 + k_y^2)\right] + \lambda_\varepsilon$$

$$\lambda_\varepsilon = D_1 \varepsilon_{zz} + D_2(\varepsilon_{xx} + \varepsilon_{yy})$$

$$\theta = \frac{\hbar^2}{2m_0}\left[A_3 k_z^2 + A_4(k_x^2 + k_y^2)\right] + \theta_\varepsilon$$

$$\theta_\varepsilon = D_3 \varepsilon_{zz} + D_4(\varepsilon_{xx} + \varepsilon_{yy})$$

$$G = \Delta_1 - \Delta_2 + \lambda + \theta$$

$$K = \frac{\hbar^2}{2m_0} A_5 (k_x + i k_y)^2 + D_5 \varepsilon_+$$

$$H = \frac{\hbar^2}{2m_0} A_6 (k_x + i k_y) k_z + D_6 \varepsilon_{z+}$$

$$\Delta = \sqrt{2}\Delta_3$$

$$\varepsilon_\pm = \varepsilon_{xx} \pm 2i\varepsilon_{xy} - \varepsilon_{yy}$$

$$\varepsilon_{z\pm} = \varepsilon_{zx} \pm i\varepsilon_{yz}$$

1 *Chuang S L and Chang C S, Physical Review B, 54 2491, 1996*

Polarization in III-Nitride Semiconductors

- **Two types of Polarization existed in wurtzite crystals**
  - Spontaneous Polarization (SP)
  - Piezoelectric Polarization (PZ) → Strain induced
- **Calculation of PZ**

$$P_{PZ}^{i} = 2d_{31}^{i}(C_{11}^{i} + C_{12}^{i} - \frac{2C_{13}^{i}{}^{2}}{C_{33}^{i}})\varepsilon'^{i(3)}_{xx}$$

- **Electric Field due to polarization in QW**

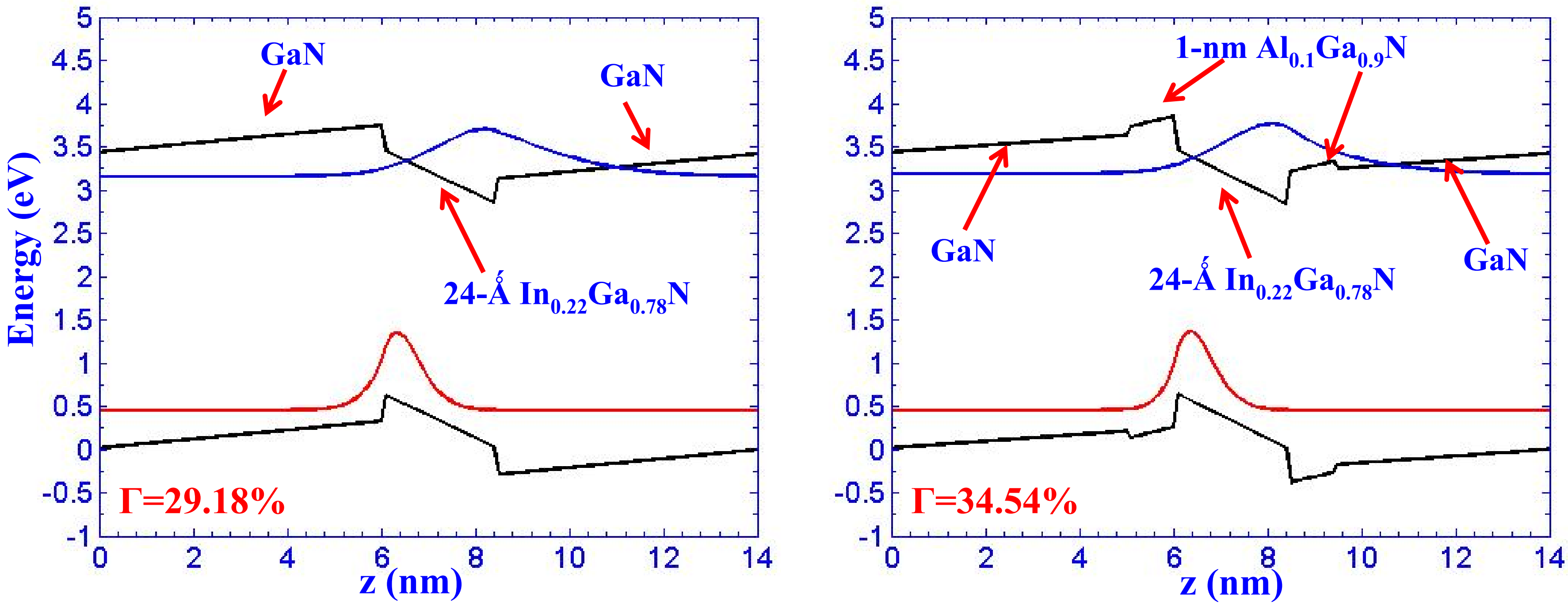
$$E_{z'} = \frac{(P_{SP}^{b} + P_{PZ}^{b} - P_{SP}^{w} - P_{PZ}^{w})L^{b}}{L^{b}\varepsilon^{w} + L^{w}\varepsilon^{b}}$$

- **Hamiltonian incorporating with polarization**

$$\sum_{\upsilon'}[H_{\upsilon\upsilon'} + qE_{z'}z'\delta_{\upsilon\upsilon'}]g_{\upsilon} = E'g_{\upsilon}$$

1 F. Bernardini and V. Fiorentini, phys. stat. sol. (b), 216, 391 (1999).

Strain-Compensated InGaN-AlGaN QW

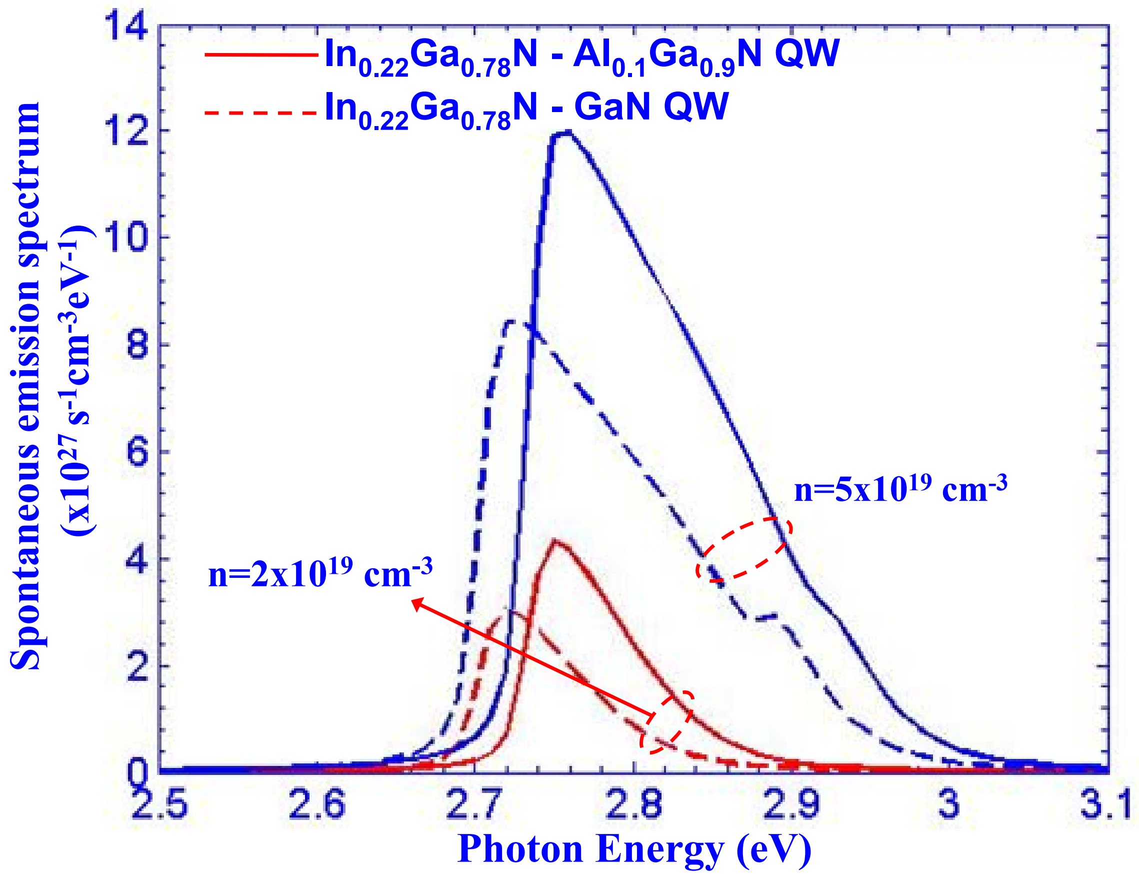


Strain-Compensated InGaN-AlGaN QW

- **Allows a strain-balanced structure**
  - **reduction in the strain energy**
  - **reduction in strain-misfit dislocation density**
- **Larger ΔE_c and ΔE_v improve carrier confinement in QW**
  - **advantageous for high temperature operation**

Leads to Improved Optical Gain

Spontaneous Emission Spectrum



$$g_{sp}^{e}(\hbar\omega)=\frac{2q^{2}\pi}{n_{r}c\varepsilon_{0}m_{0}^{2}\omega L_{w}}\sum_{\sigma=U,L}\sum_{n,m}\int\frac{k_{t}dk_{t}}{2\pi}\left|(M_{e})_{nm}^{\sigma}(k_{t})\right|^{2}\frac{f_{n}^{c}(k_{t})(1-f_{\sigma m}^{v}(k_{t}))(\gamma/\pi)}{(E_{\sigma,nm}^{cv}(k_{t})-\hbar\omega)^{2}+\gamma^{2}}$$

➡ **Strain-compensated InGaN-AlGaN QW exhibit increase in spontaneous emission rate**

Material Gain properties of InGaN QW

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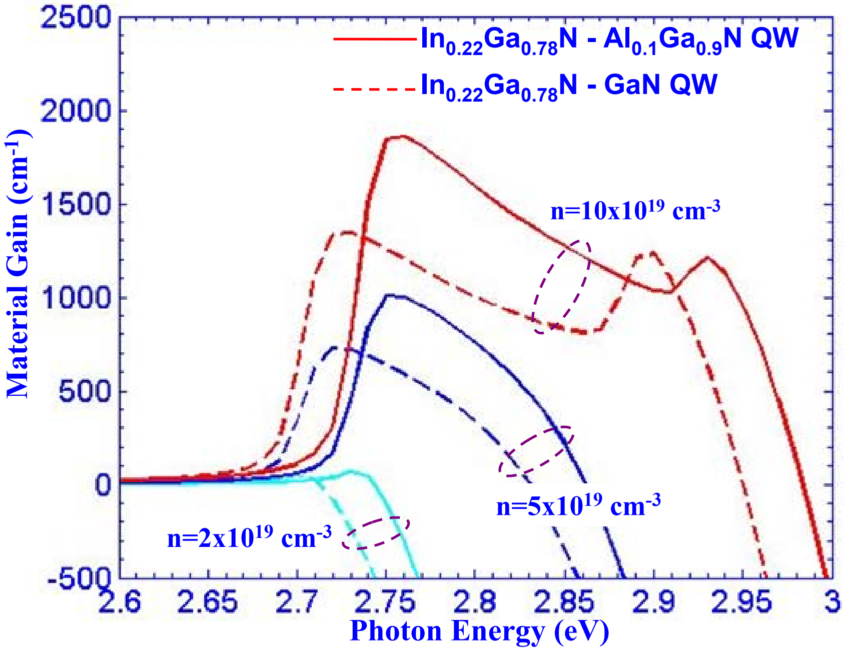
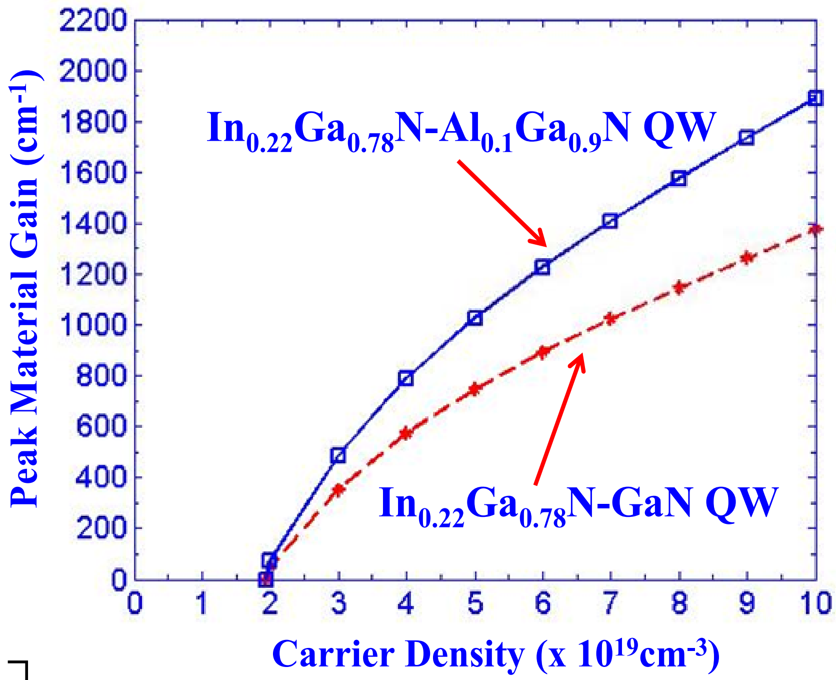
Conventional Vs. Strain Compensated InGaN QW



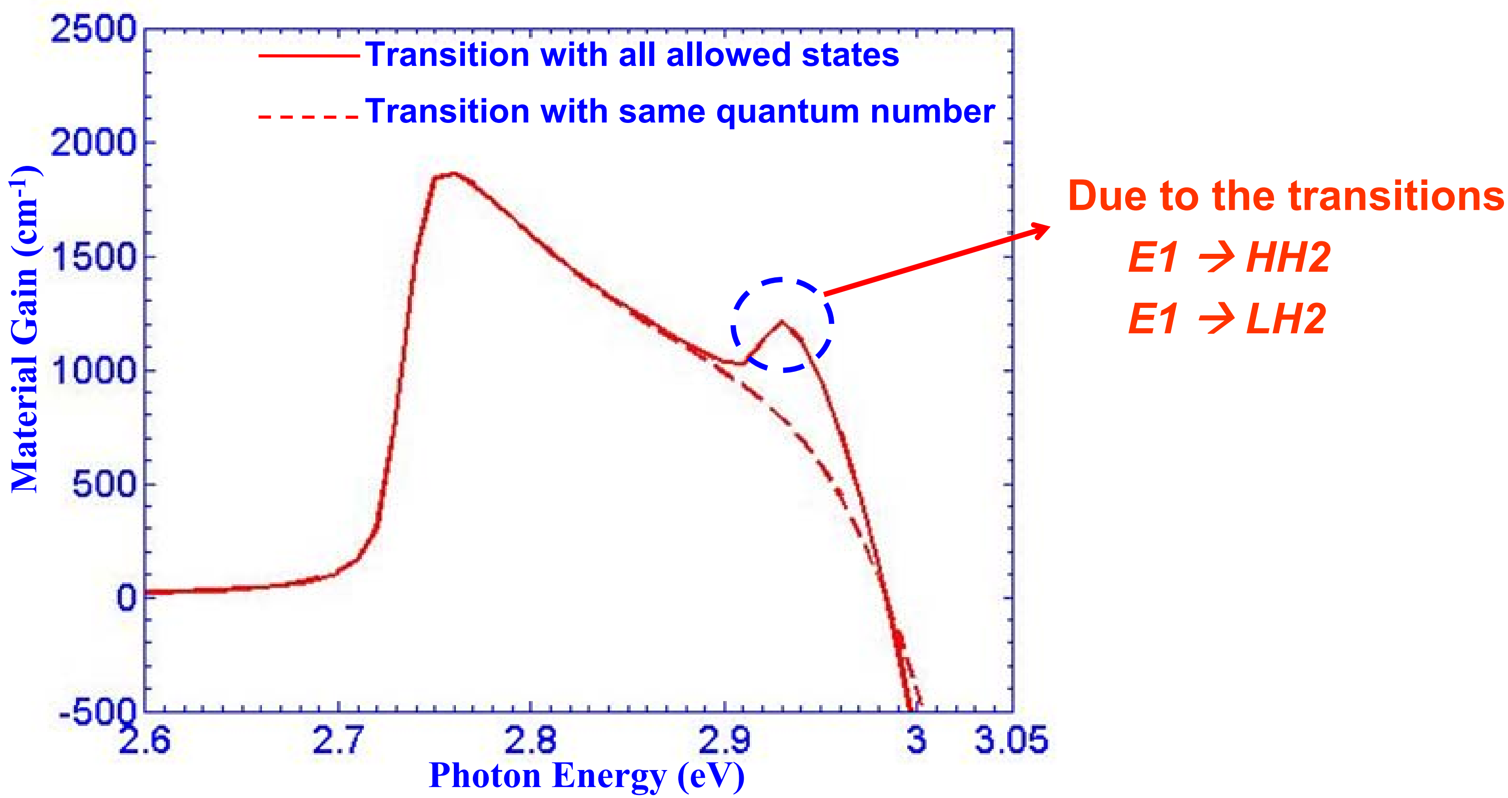


$$g(\hbar\omega) = g_{sp}^{e}(\hbar\omega)\left[1 - \exp\left(\frac{\hbar\omega - \Delta F}{k_B T}\right)\right]$$

- **λ~460 nm: ($n=10\times10^{19} cm^{-3}$)**
  - **$In_{0.22}Ga_{0.78}N$-$Al_{0.1}GaN$: $g\sim1889 cm^{-1}$**
  - **$In_{0.22}Ga_{0.78}N$-GaN: $g\sim1374 cm^{-1}$**

  } ***+48% improvement***
- **Relatively similar transparency carrier density**
  - **$n_{tr} = 1.94\text{-}1.95\times10^{19} cm^{-3}$**

Gain Characteristics *for Polar III-Nitride*



- Non-Polar → Symmetric band lineup

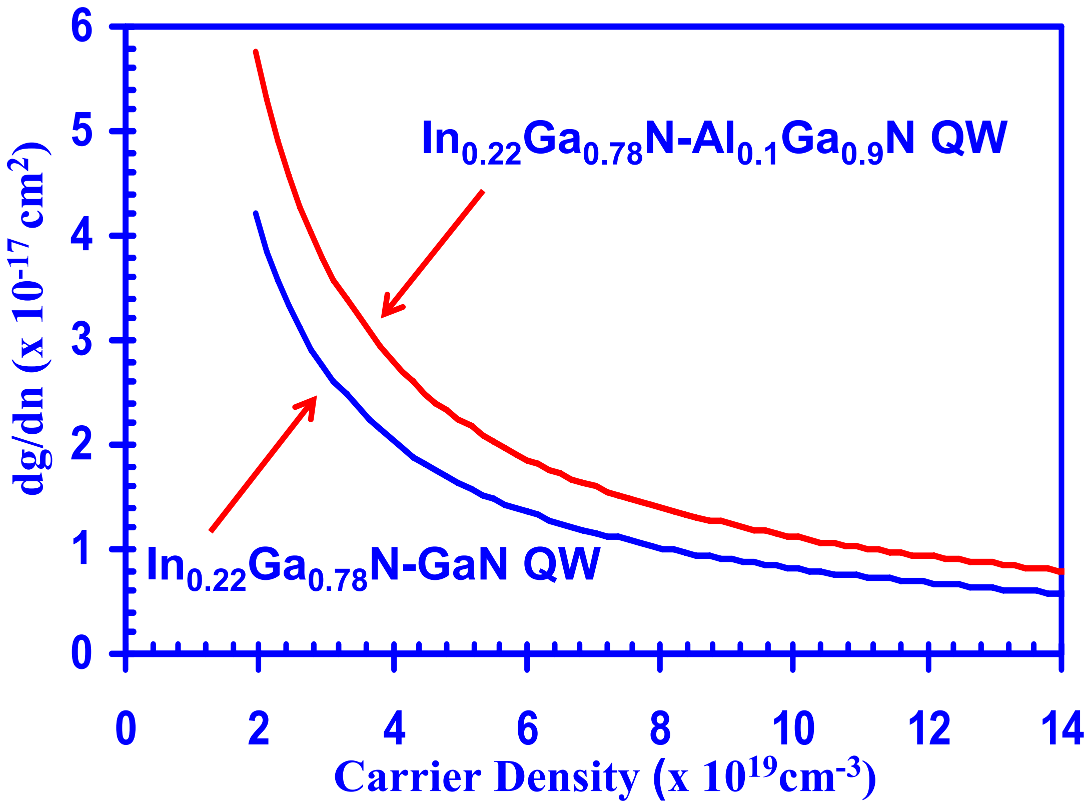
  Zero matrix element for $n_c \neq n_v$ transitions

- Polar III-Nitrides → Asymmetric band lineup

  Non-zero matrix element for all confined states transitions [1]

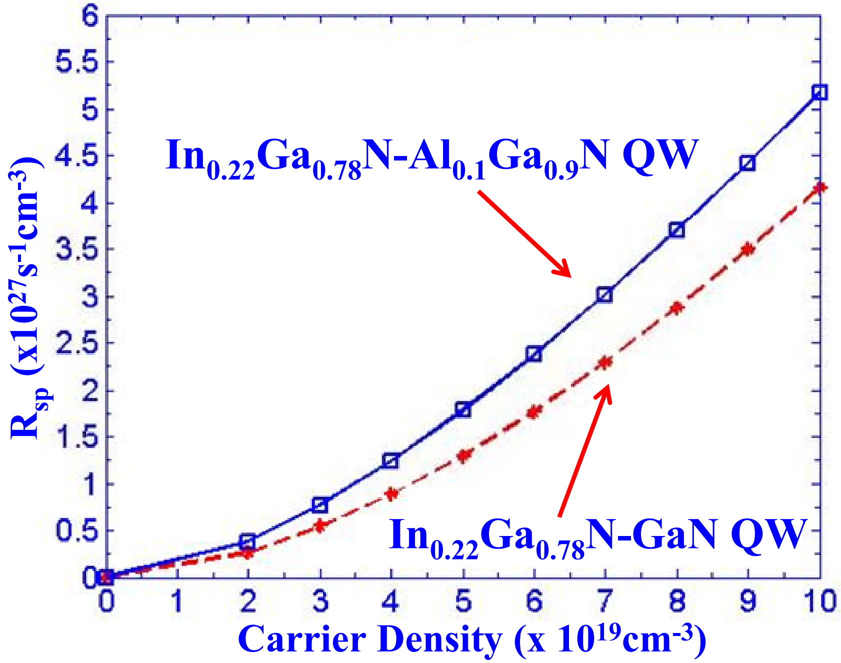
1 *Claus Klingshirn, Semiconductor Optics, Springer, 2006*

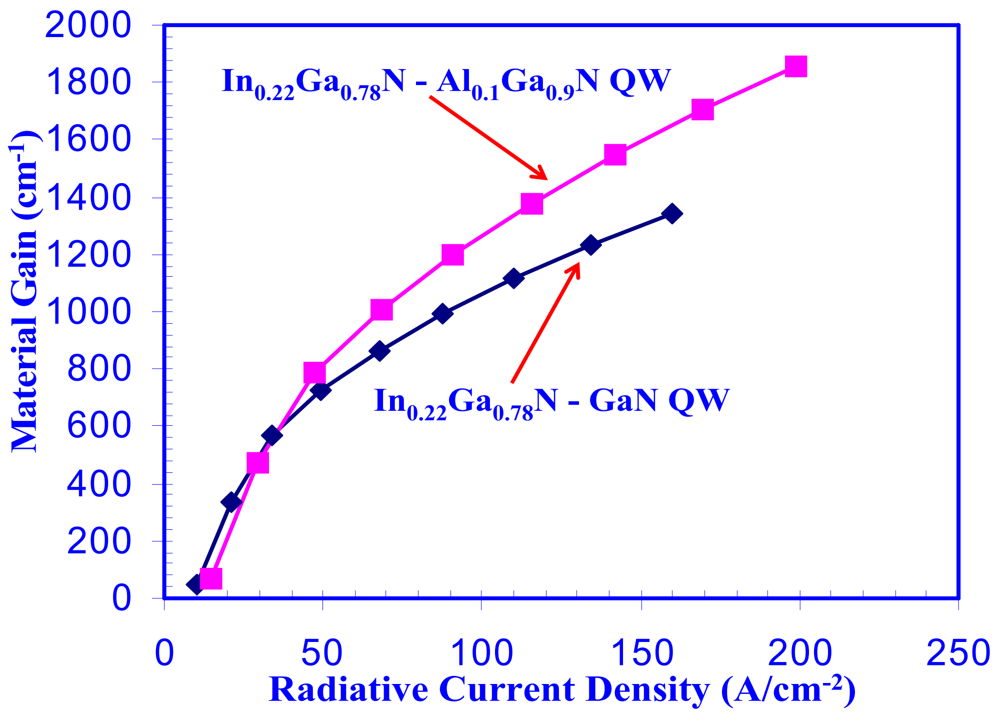
Differential Gain of InGaN QW



Differential gain near transparency
- Conventional Structure: 4.2×10^{-17} cm²
- Strain-compensated structure: 5.8×10^{-17} cm²

R_{sp} and Radiative Current Density for InGaN QW

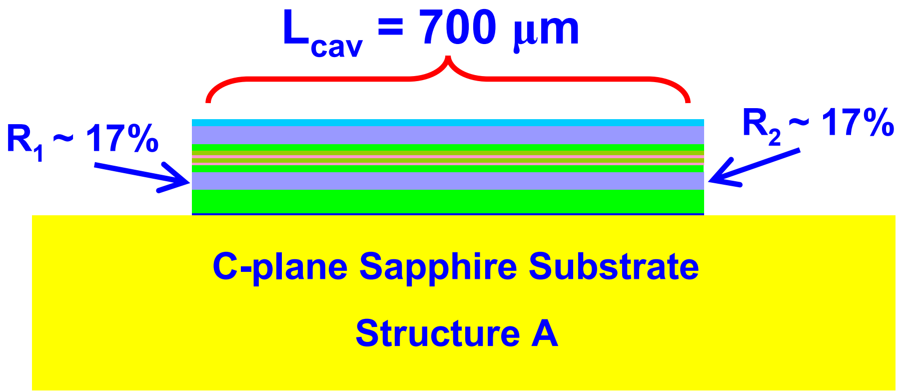




- 25%-40% improvement of spontaneous emission rate for InGaN-AlGaN structure at different carrier density
- $J_{rad}=qdR_{sp}$ → Reduction of radiative current density for strain-compensated structure

Threshold Analysis for InGaN QW Lasers

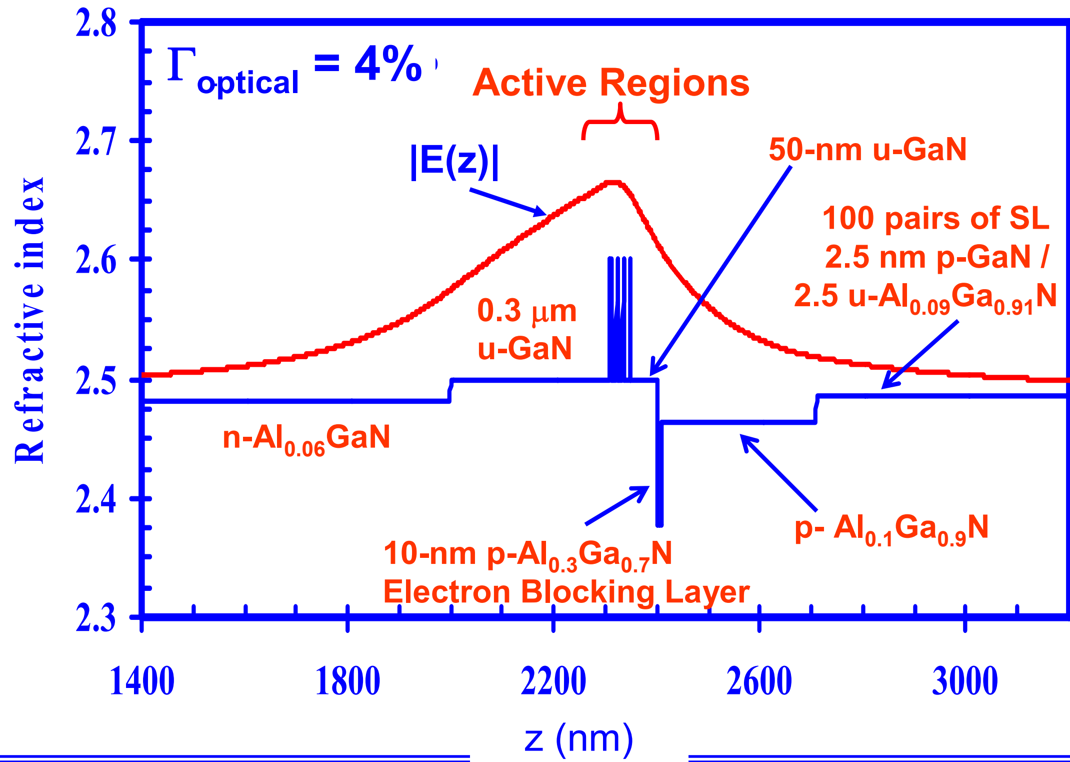
Mirror Loss



$$\alpha_m = \frac{1}{2l}\ln\left(\frac{1}{R_1 R_2}\right)$$

$\alpha_m \approx 25.5\ \mathrm{cm}^{-1}$

Threshold Gain



$$\Gamma g_{th} = \alpha_i + \alpha_m$$

$$\alpha_i = 26\ cm^{-1}$$

$g_{th} = 1280\ \mathrm{cm}^{-1}$ (per QW)

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Threshold Analysis for Strain-Compensated InGaN QW

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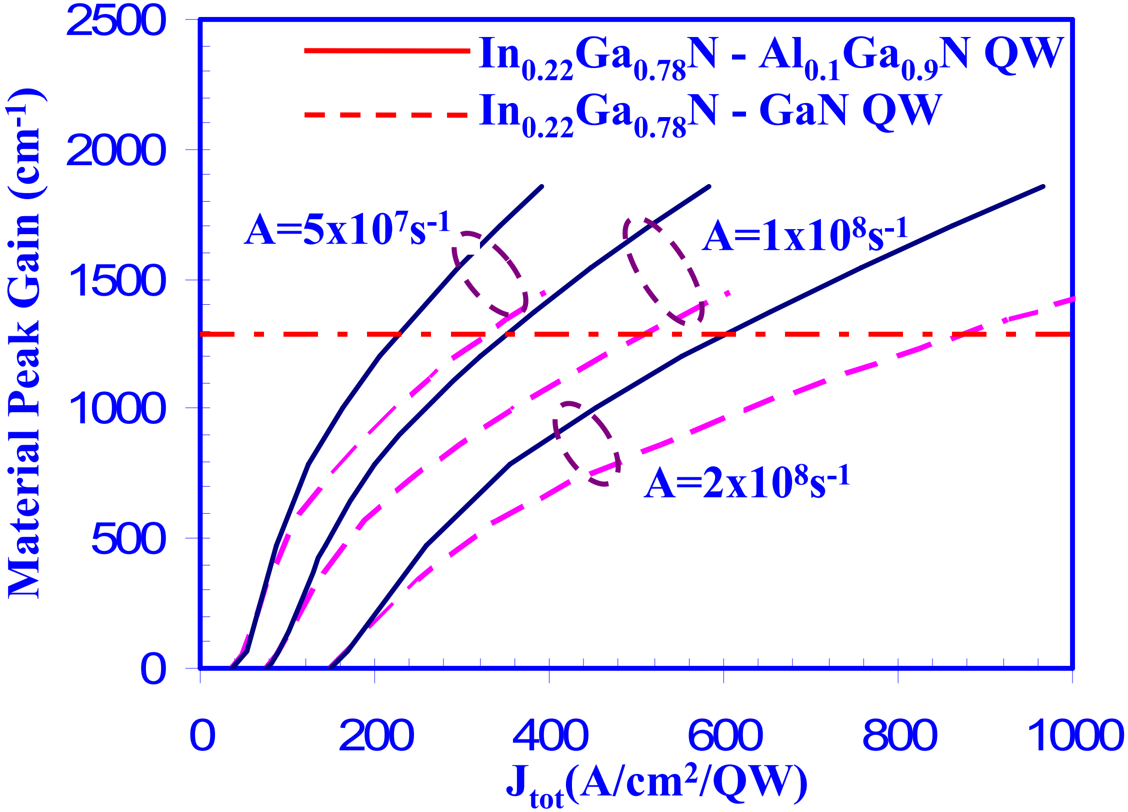

$$J_{nr}=qdR_{nr} \quad R_{nr}=An$$

$$J_{Rad}=qdR_{sp}$$

$$J_{tot}=J_{nr}+J_{rad}$$

	J_{th} for InGaN-GaN 4-QWs (A/cm^2)		J_{tot} for InGaN-AlGaN 4-QWs (A/cm^2)
$A=5x10^7 s^{-1}$	1406.4[1,2]	→	1000.3
$A=1x10^8 s^{-1}$	2174.4	→	1537.9
$A=2x10^8 s^{-1}$	3710.4	→	2613.1

1. *S. Nagahama, N. Iwasa, M. Senoh, T. Matsushita, Y. Sugimoto, H. Kiyoku, T. Kozaki, M. Sano, H. Matsumura, H. Umemoto, K. Chocho, T. Yanamoto, and T. Mukai, phys. stat. sol. (a) 188, No. 1, pp. 1–7 (2001).*
2. *S. Nagahama, Y. Sugimoto, T. Kozaki, and T. Mukai, Proc. of SPIE Photonics West, San Jose, CA, USA, January 2005.*

Gain characteristics for Strain-Compensated InGaN QW at 500 nm

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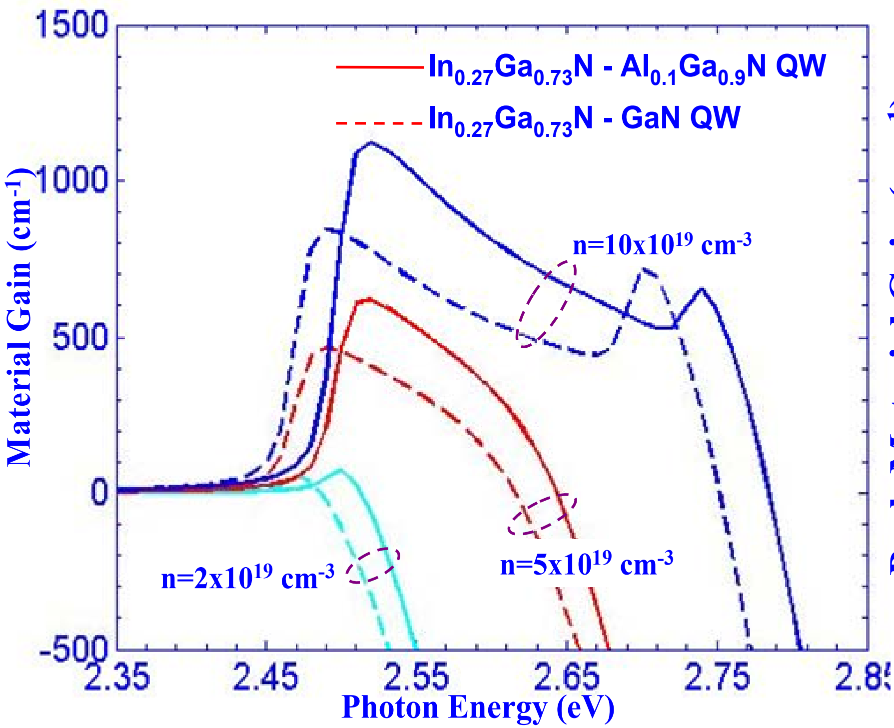

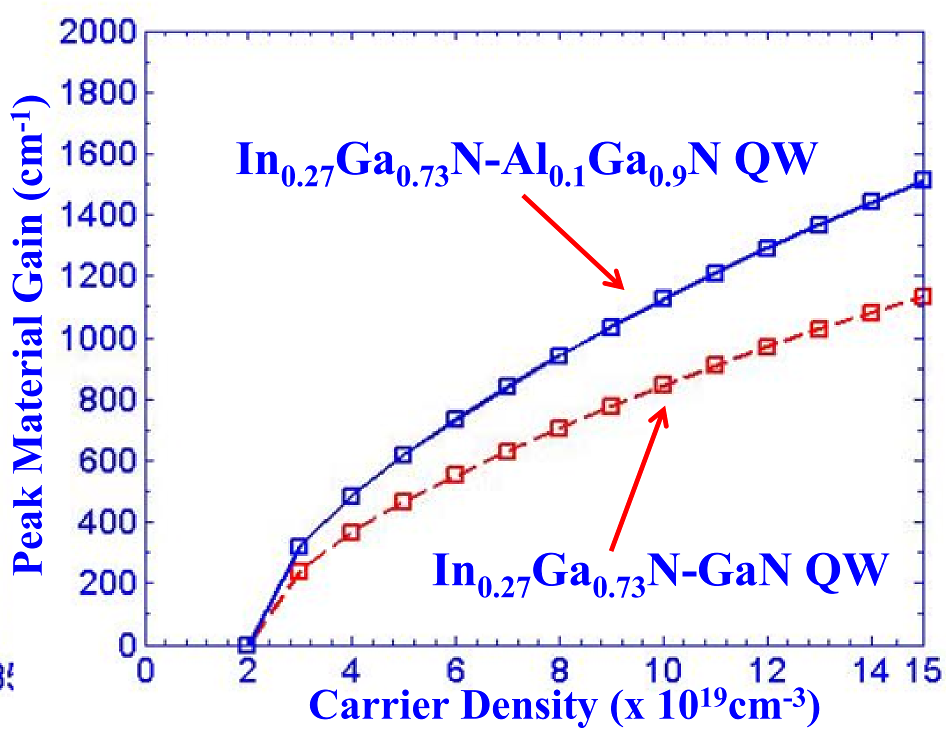

Strain-Compensated InGaN-AlGaN QW (500-nm)

- Improvement in peak optical gain by~ 30-35 %
- Reduction in the threshold carrier density (g_{th}~1280 cm^{-1})
  - Reduction of J_{nr} by ~ 42%
  - Reduction of J_{rad} by ~56%

} **Significantly reduce J_{th}**

Summary

- **Strain-compensated InGaN-AlGaN QW for improved gain media (460-nm, 500-nm)**
  - Spontaneous emission rate
  - Gain spectrum
  - Monomolecular recombination rate
  - Threshold current density

  Numerical Modeling using 6-band k.p formalism

- **Strain-compensated InGaN QW has potential for achieving:**
  - Low threshold current density lasers
  - Improved efficiency LEDs

- **Future Works**
  - Epitaxy of strain-compensated InGaN-AlGaN QW structure
  - Improving the simulation design for long wavelength emission

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Material Parameters Used in Simulations

Parameters	GaN	AlN	InN
$m_{//}^{*}/m_0$ at 300 K	0.21	0.32	0.07
$m_{\perp}^{*}/m_0$ at 300 K	0.20	0.30	0.07
A_1	-7.21	-3.86	-8.21
A_2	-0.44	-0.25	-0.68
A_3	6.68	3.58	7.57
A_4	-3.46	-1.32	-5.23
A_5	-3.40	-1.47	-5.11
A_6	-4.90	-1.64	-5.96
E_g (eV) at 300 K	3.437	6.00	0.6405
Δ_{cr} (eV)	0.010	-0.227	0.024
Δ_{so} (eV)	0.017	0.036	0.005
a_{cz} (eV)	-7.1	-3.4	-4.2
a_{ct} (eV)	-9.9	-11.8	-4.2
D_1 (eV)	-3.6	-2.9	-3.6
D_2 (eV)	1.7	4.9	1.7
D_3 (eV)	5.2	9.4	5.2
D_4 (eV)	-2.7	-4.0	-2.7
C_{13} (GPa)	106	108	92
C_{33} (GPa)	398	373	224
d_{13} (pmV^{-1})	-1.0	-2.1	-3.5
d_{33} (pmV^{-1})	1.9	5.4	7.6
P_{sp} (C/m^2)	-0.034	-0.090	-0.042

1. *J. Piprek., Nitride Semiconductor Devices: Physics and Applications, Wiley, 2007. – Chapter 2 (Meyer and Vurgaftmann)*