Successful Application of the 8-band ***k•p*** Framework to Optical Properties of Highly Strained In(Ga)As/InGaAs Quantum Wells with Strong Conduction-Valence Band Coupling

T. Fujisawa, T. Sato, M. Mitsuhara, T. Kakitsuka, T. Yamanaka, Y. Kondo, and F. Kano
NTT Photonics Laboratories, Japan
e-mail:fujisawa@aecl.ntt.co.jp

NUSOD ThA5, Sep. 2008

Outline

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2. ***k*** **·** ***p*** theory
3. Purpose
4. Analytical methods
5. Numerical and experimental results
6. Conclusion

1. Background – Highly strained quantum wells (QWs)

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Infrared light source for measuring environmental gases

Single mode lasing, mW output power, and wavelength tunability

→ Bandgap tuning of QW laser for conventional optical fiber communication

→ Larger compressive strain in well layer

Semiconductor lasers with highly strained In(Ga)As QWs on InP substrates			
	Well	Strain [%]	Lasing wavelength [μm]
1	InGaAs	1.65	2.07
2	InGaAs	1.85	2.103
3	InGaAs	1.94	2.13
4	InAs	3.2	2.33

1. M. Mitsuhara *et al*., APL, vol. 72, pp.3106, 1998.
2. T. Sato *et al*., APL, vol. 87, 211903, 2005.
3. T. Sato *et al*., JSTQE, vol. 13, pp.1079, 2007.
4. T. Sato *et al*., EL, vol. 43, pp. 1143, 2007.

2. ***k* · *p*** theory

k* · *p theory — Band structure analysis of semiconductors

- Gain (Absorption), Scattering rate, Photoluminescence (PL) spectra

Total Hamiltonian of unstrained system

$$H_{total} = H_{k \cdot p} + H_{s.o.}$$

Transformation to strained system

- Coordinate transformation
- Expansion up to first order of strain

Total Hamiltonian of strained system

$$H_{total} = H_{k \cdot p} + H_{s.o.} + D_{k \cdot p} + D_{s.o.}$$
$$\approx H_{k \cdot p} + H_{s.o.} + D_{k \cdot p}$$

$D_{s.o.}$ is usually neglected in conventional ***k* · *p*** analysis

	Hamiltonian originating from
H_{total}	Total system
$H_{k \cdot p}$	***k* · *p*** perturbation
$H_{s.o.}$	Spin-orbit coupling
$D_{k \cdot p}$	Strain and $H_{k \cdot p}$
$D_{s.o.}$	Strain and $H_{s.o.}$

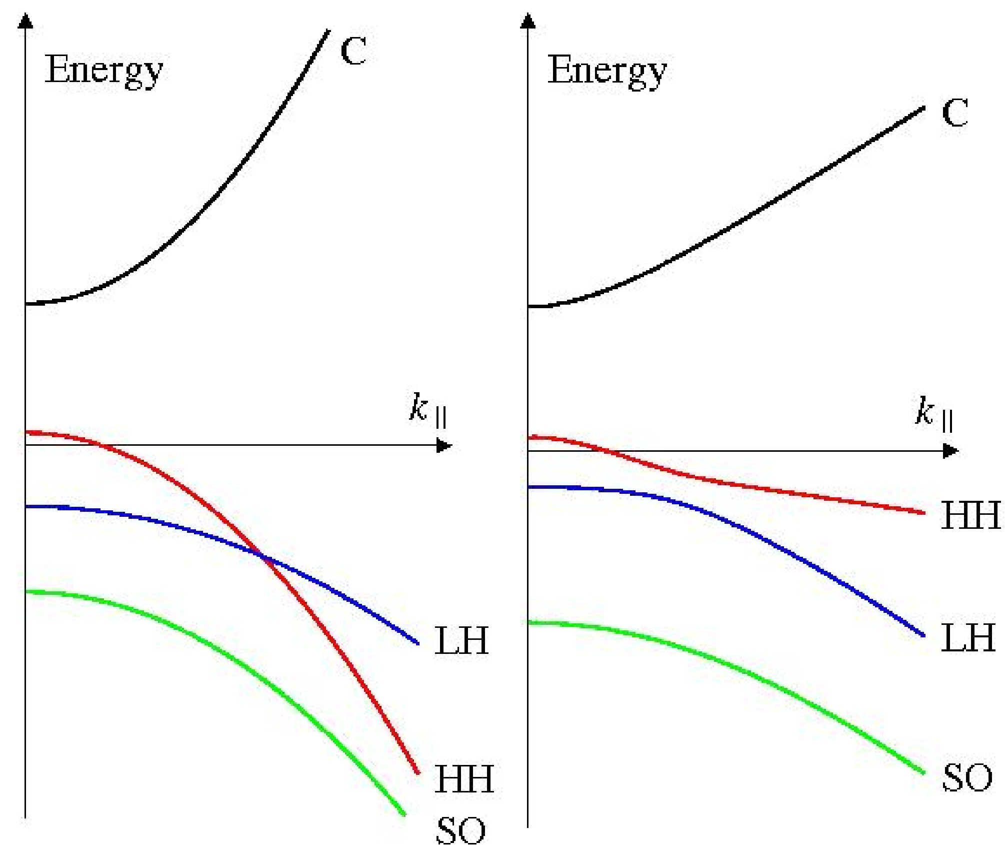
2-1. Effective-mass approximation

Band	Parabolic	4-band
C	$m_{C,eff}$	$m_{C,eff}$
HH	$m_{HH,eff}$	Coupling
LH	$m_{LH,eff}$	
SO	$m_{SO,eff}$	$m_{SO,eff}$
Band	**6-band**	**8-band**
C	$m_{C,eff}$	Coupling
HH	Coupling	
LH		
SO		

C: Conduction band
HH: Heavy-hole band
LH: Light-hole band
SO: Spin-orbit split-off band

Band structures of bulk InAs on InP

Parabolic | 8-band



2-2. 6- and 8-band model

Block-diagonalized Hamiltonian (QW, $k_t = 0$)

$H_{k\cdot p} + H_{s.o.}$ (Hamiltonian of unstrained system)

$$
\begin{bmatrix}
E_g + \dfrac{\hbar^2 k_z^2}{2m_0} & 0 & -i\sqrt{\dfrac{2}{3}}P_0 k_z & -i\sqrt{\dfrac{1}{3}}P_0 k_z \\
0 & -\dfrac{\hbar^2}{2m_0}(\gamma_1 - 2\gamma_2)k_z^2 & 0 & 0 \\
i\sqrt{\dfrac{2}{3}}P_0 k_z & 0 & -\dfrac{\hbar^2}{2m_0}(\gamma_1 + 2\gamma_2)k_z^2 & -\dfrac{\hbar^2}{m_0}\gamma_2 k_z^2 \\
i\sqrt{\dfrac{1}{3}}P_0 k_z & 0 & -\dfrac{\hbar^2}{m_0}\gamma_2 k_z^2 & -\dfrac{\hbar^2}{2m_0}\gamma_1 k_z^2 - \Delta
\end{bmatrix}
\begin{matrix} |C\rangle \\ |HH\rangle \\ |LH\rangle \\ |SO\rangle \end{matrix}
$$

Valence band

For 6-band model, terms surrounded by **O**, are phenomenalogically incorporated into the term surrounded by **O**, as the effective mass of an electron.

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Block-diagonalized Hamiltonian (QW, $k_t = 0$)

$D_{k \cdot p}$ (Hamiltonian of strained system)

$$
\begin{bmatrix}
a_c \varepsilon & 0 & -i\sqrt{\frac{2}{3}}P_0 \frac{2c_{12}}{c_{11}} k_z \varepsilon & -i\sqrt{\frac{1}{3}}P_0 \frac{2c_{12}}{c_{11}} k_z \varepsilon \\
0 & -p-q & 0 & 0 \\
i\sqrt{\frac{2}{3}}P_0 \frac{2c_{12}}{c_{11}} k_z \varepsilon & 0 & -p+q & \sqrt{2}q \\
i\sqrt{\frac{1}{3}}P_0 \frac{2c_{12}}{c_{11}} k_z \varepsilon & 0 & \sqrt{2}q & -p
\end{bmatrix}
\begin{matrix} |C\rangle \\ |HH\rangle \\ |LH\rangle \\ |SO\rangle \end{matrix}
$$

Valence band

- Terms surrounded by ○, are NOT taken into account in 6-band model.
- Terms surrounded by ○, are linear in terms of strain, ε, and k_z.
- For QWs with larger strain, the difference between 6- and 8-band model is increased.
- The strain at which the 6-band model becomes inappropriate is unclear.

2-3. Interaction between strain and spin-orbit coupling

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Block-diagonalized Hamiltonian (QW)

$D_{s.o.}$ (Hamiltonian of strained system)

$$
\begin{bmatrix}
0 & 0 & 0 & 0 \\
0 & -\frac{2}{3}\Delta\varepsilon & 0 & 0 \\
0 & 0 & -\frac{2}{9}\Delta\left(1-\frac{4c_{12}}{c_{11}}\right)\varepsilon & -\frac{\sqrt{2}}{9}\Delta\left(1+\frac{2c_{12}}{c_{11}}\right)\varepsilon \\
0 & 0 & -\frac{\sqrt{2}}{9}\Delta\left(1+\frac{2c_{12}}{c_{11}}\right)\varepsilon & \frac{8}{9}\Delta\left(1-\frac{c_{12}}{c_{11}}\right)\varepsilon
\end{bmatrix}
\begin{matrix} |C\rangle \\ |HH\rangle \\ |LH\rangle \\ |SO\rangle \end{matrix}
$$

- Discarded in the conventional analysis
- Independent of in-plane wavenumber, k_t
- Constant energy shift of valence bands
- Larger energy shift for larger strain

⇒ Non-negligible energy shift for highly strained quantum wells

3. Purpose

For QWs with larger strain

- 6- or 8-band model?
- Effect of interaction between spin-orbit coupling and strain ($D_{s.o.}$)

↓

- Highly strained In(Ga)As/InGaAs QWs on InP
- Strain dependence of band edge optical properties
  - PL spectra
  - Absorption spectra

4. Analytical methods

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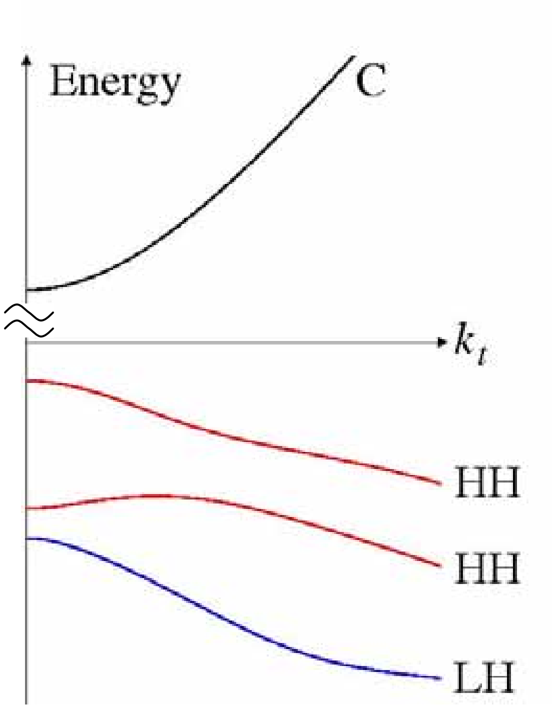
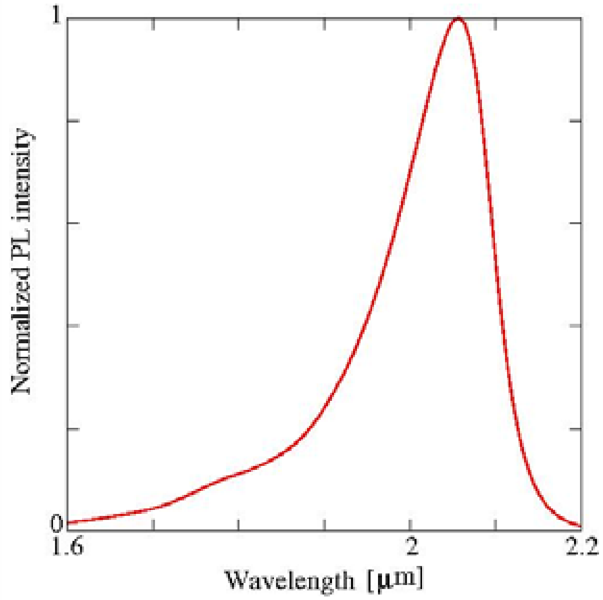
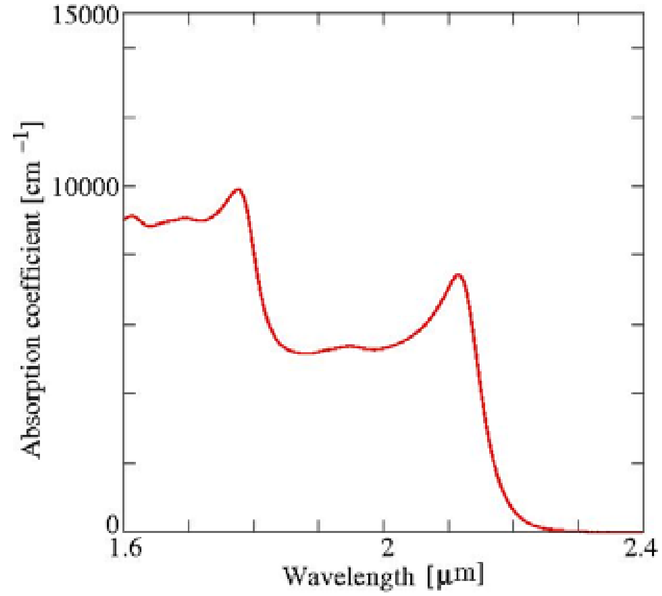
Band structure	PL spectra	Absorption







- Band structure – 8×8 ***k*** · ***p*** Hamiltonian
  – Finite-difference method
- PL spectra – Fermi's golden rule
  – sech lineshape broadening
- Absorption spectra – Non-variational approach (exciton effects)

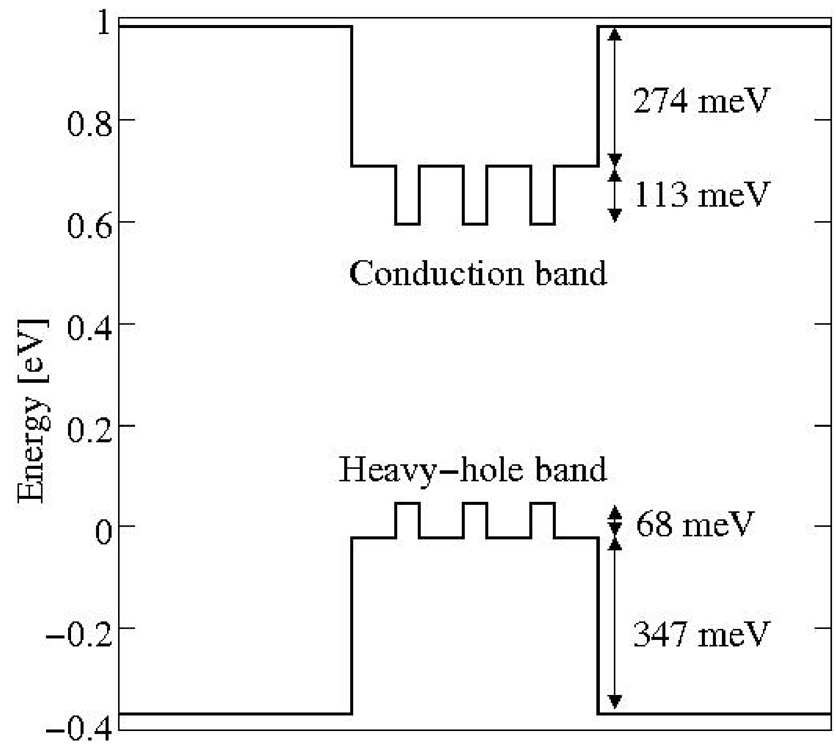
5-1. 6- or 8-band model?

Highly strained InGaAs/InGaAs QWs (L_w = 10 nm, ε = 1.65%)

Layer structure

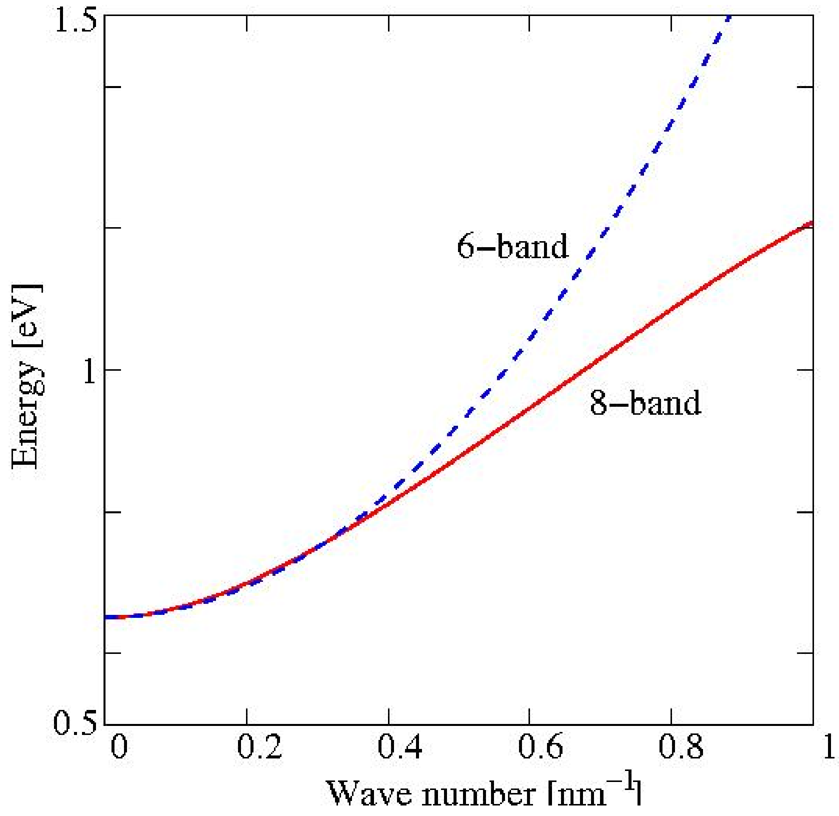
InP
InGaAs Barrier 0% 19 nm
InGaAs Well 1.65% 10 nm
InGaAs Barrier 0% 19 nm
InGaAs Well 1.65% 10 nm
InGaAs Barrier 0% 19 nm
InGaAs Well 1.65% 10 nm
InGaAs Barrier 0% 19 nm
InP

Potential profile

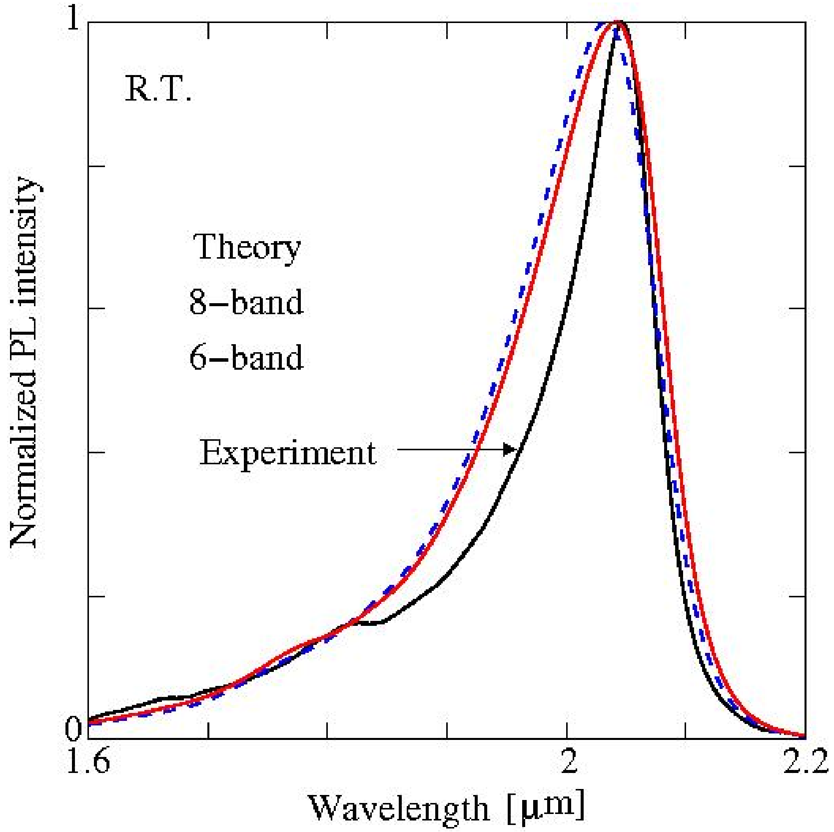


5-1. 6- or 8-band model?

Conduction band structure



PL spectra



- Around Γ point, almost the same conduction band structure for both models
- About PL spectra, good agreement with experiment for both models

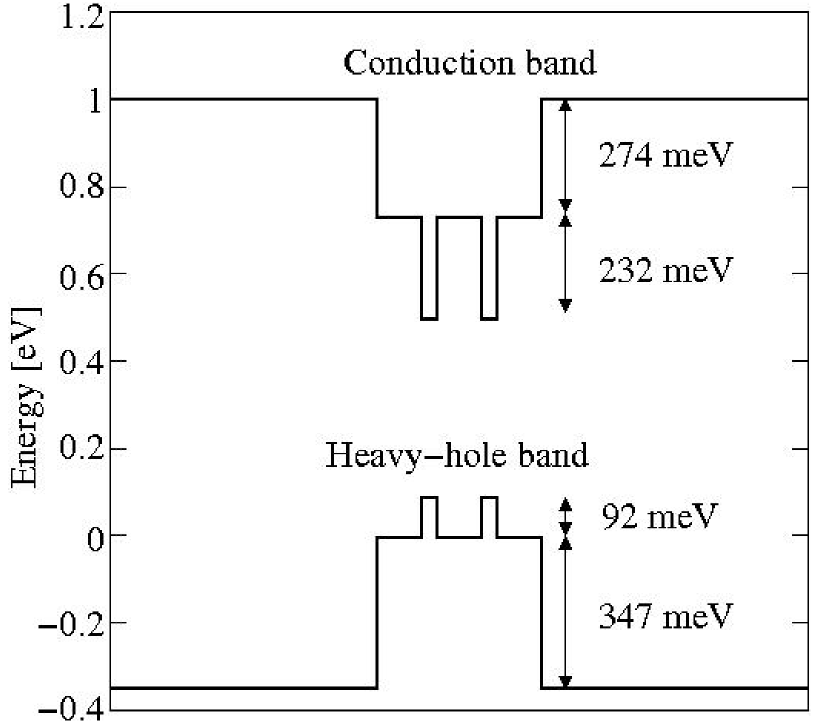
5-1. 6- or 8-band model?

Highly strained InAs/InGaAs QWs (L_w = 6 nm, ε = 3.2%)

Layer structure

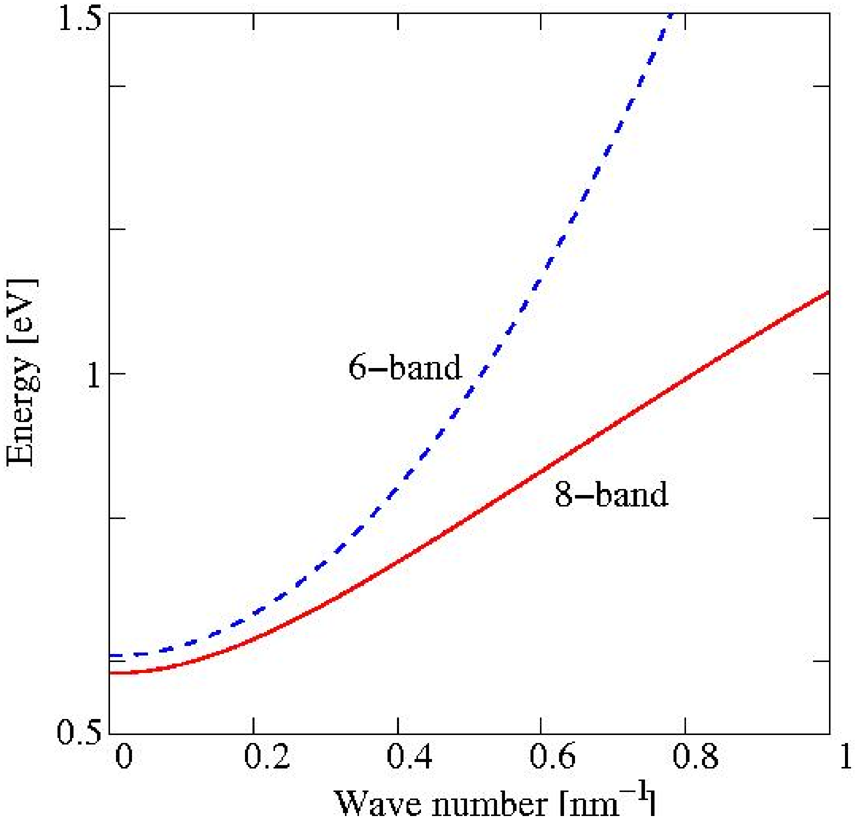
InP
InGaAs Barrier 0% 16.5 nm
InAs Well 3.2% 6 nm
InGaAs Barrier 0% 16.5 nm
InAs Well 3.2% 6 nm
InGaAs Barrier 0% 16.5 nm
InP

Potential profile

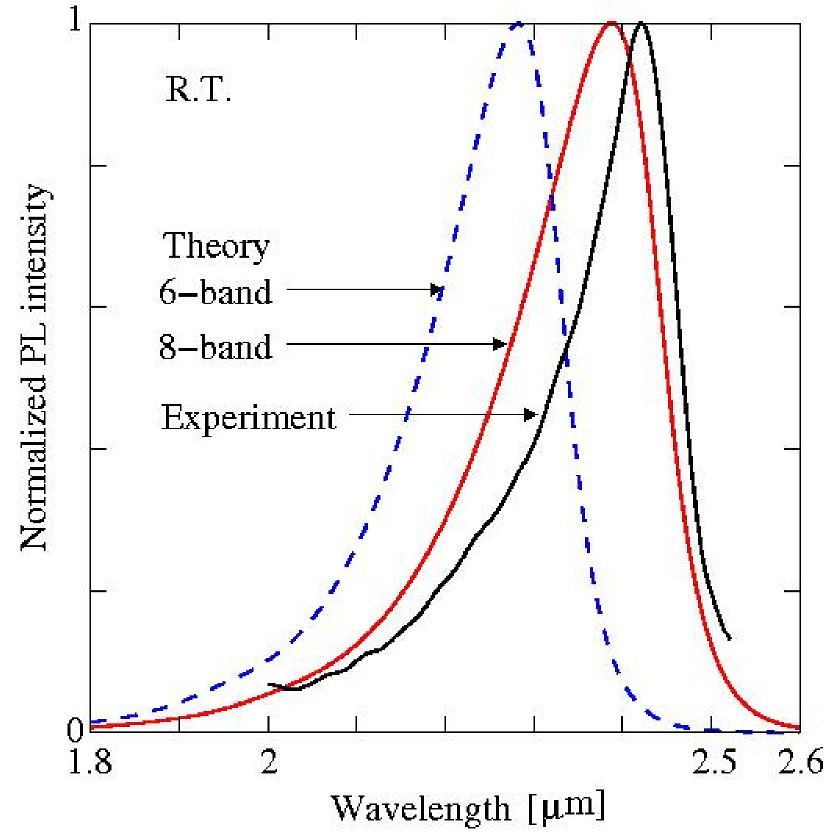


5-1. 6- or 8-band model?

Conduction band structure

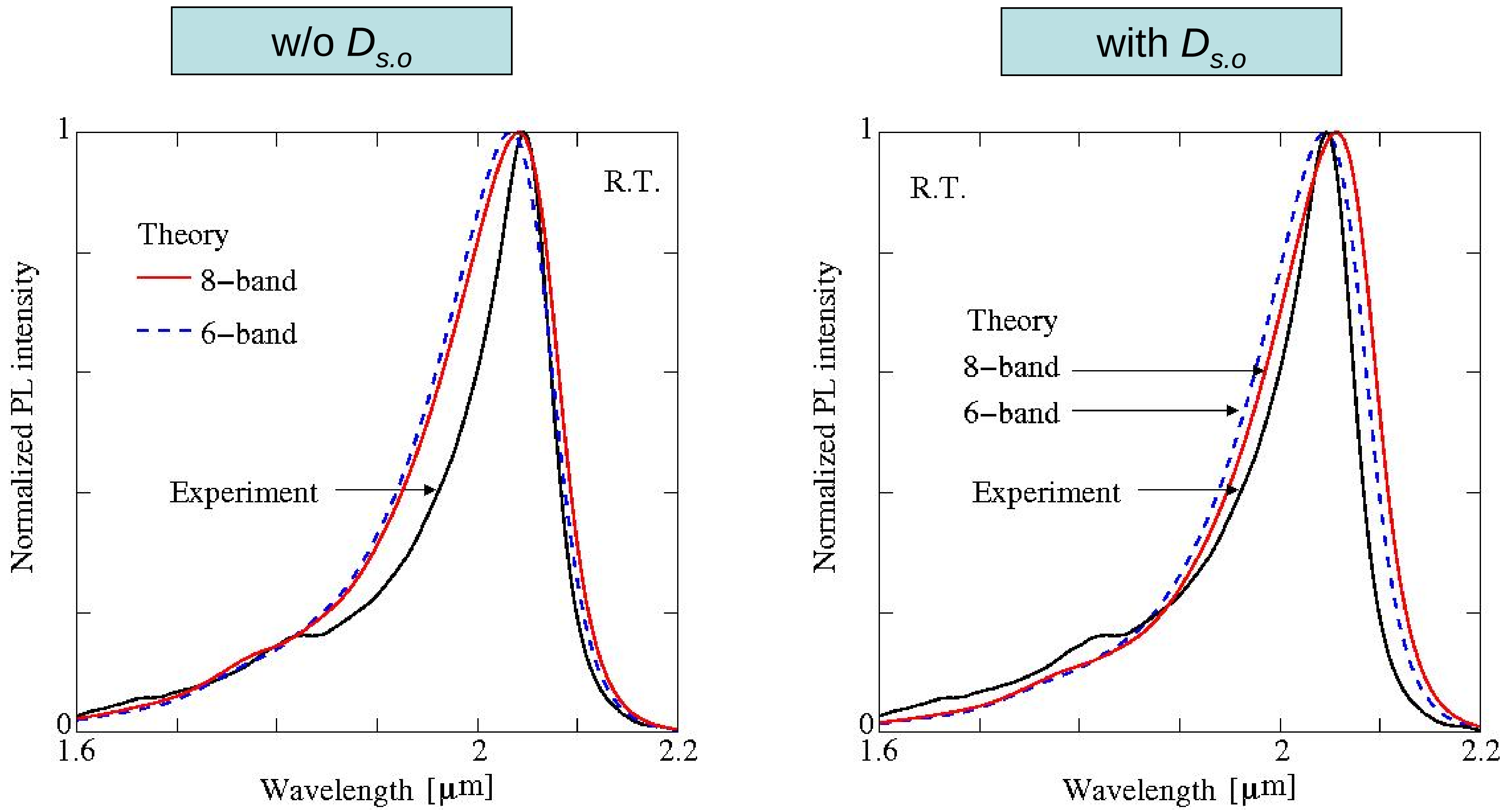


PL spectra



- Non-negligible energy shift around Γ point for 8-band model
- For 6-band model, PL peak wavelength is 150 nm too short
- About PL spectra, good agreement with experiment for 8-band model

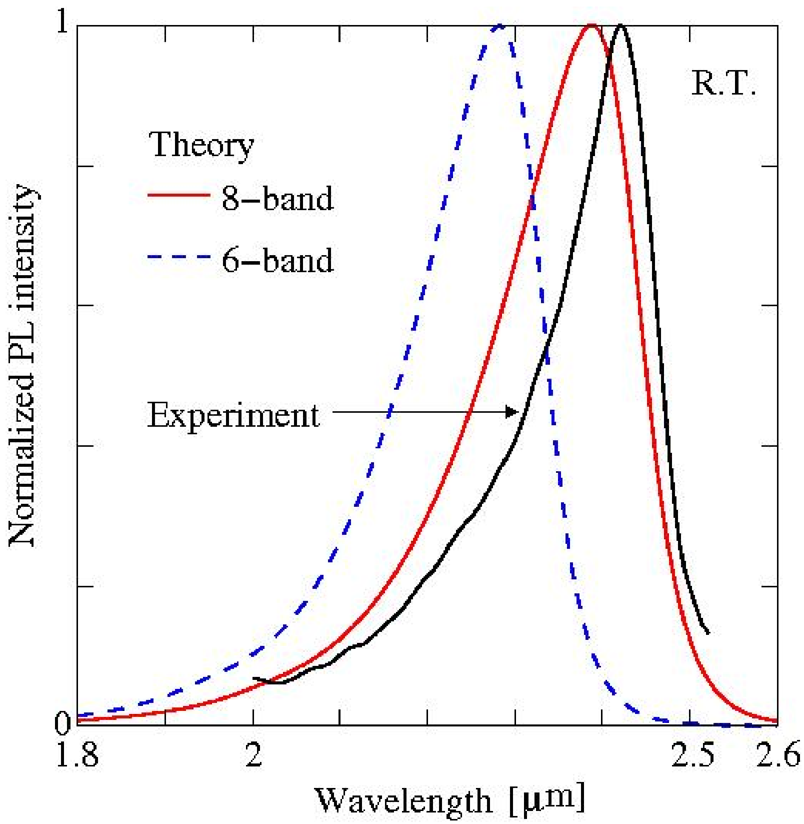
5-2. Effect of $D_{s.o.}$

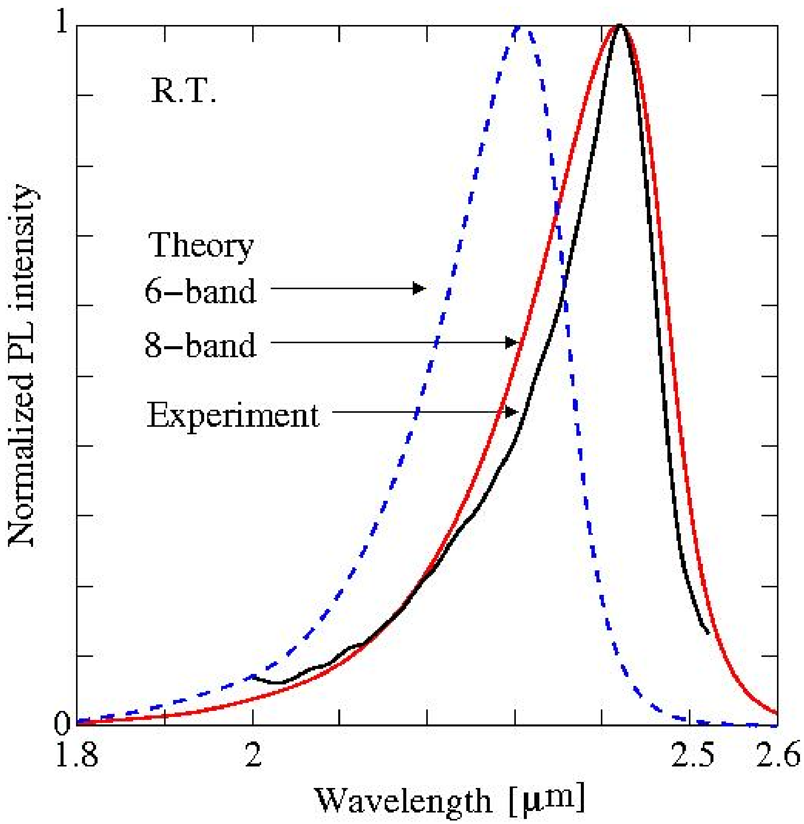


- InGaAs/InGaAs QWs (L_w = 10 nm, ε = 1.65%)
- 10-nm red shift in calculated PL spectrum

5-2. Effect of $D_{s.o.}$

w/o $D_{s.o}$	with $D_{s.o}$

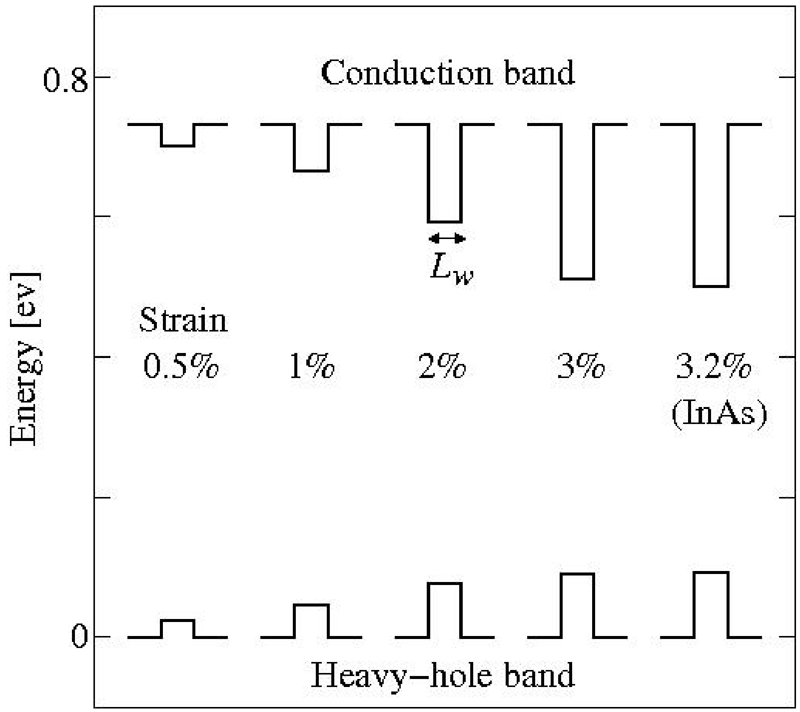




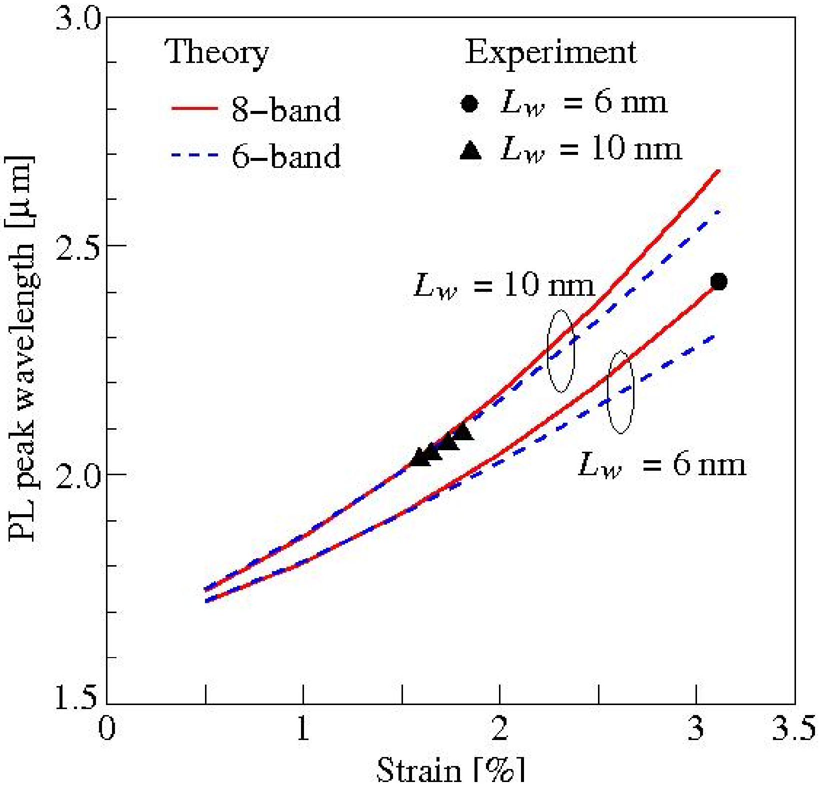
- InAs/InGaAs QWs (L_w = 6 nm, ε = 3.2%)
- 40-nm red shift in calculated PL spectrum
- Excellent agreement with experiment for 8-band model

5-3. Strain dependence of band edge optical properties

Potential profiles of In(Ga)As/InGaAs QWs



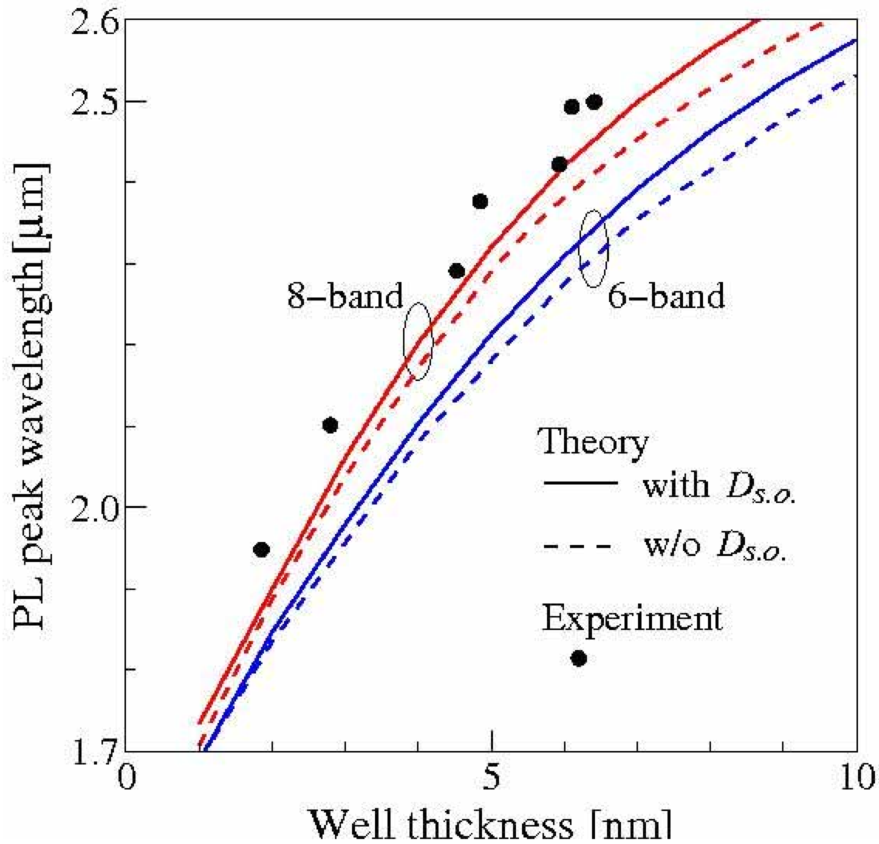
PL peak wavelength as a function of strain



- Stronger quantum confinement for larger strain
- Difference between models becomes large around a strain of 2%.

5-4. Thickness dependence of PL peak wavelength

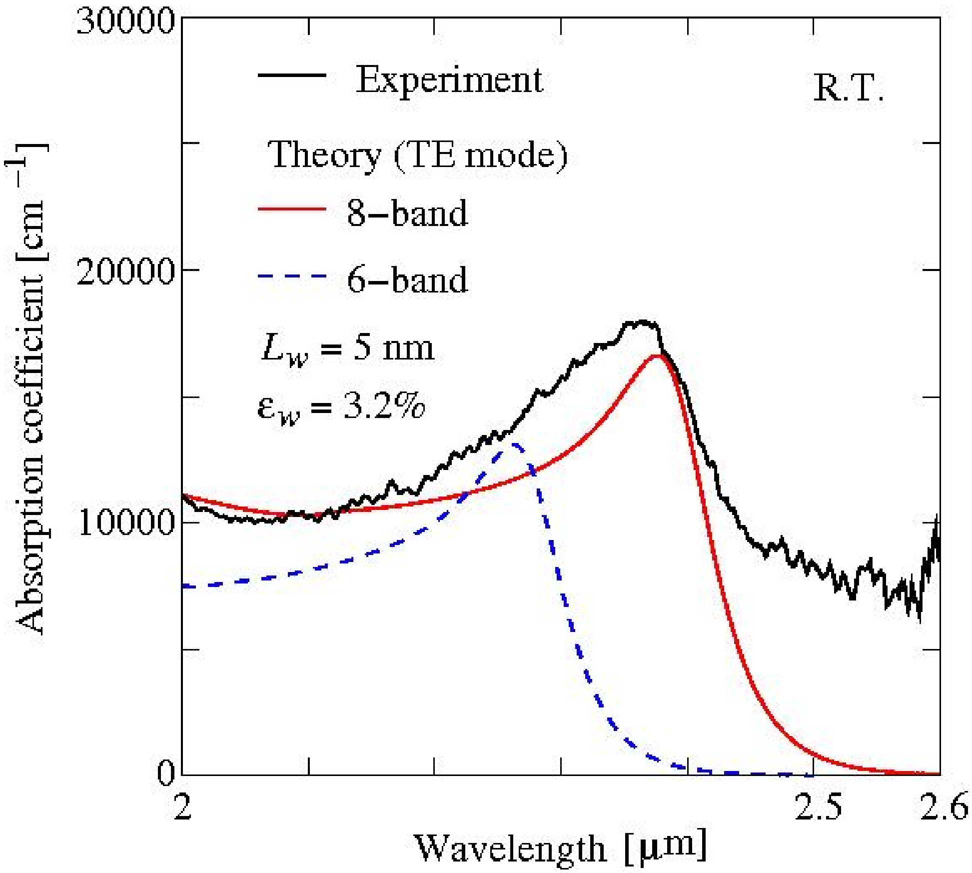
PL peak wavelength as a function of L_w



- InAs/InGaAs QWs (ε = 3.2%)
- > 100 nm too short for 6-band model
- Good agreement between experiment and 8-band model with $D_{s.o.}$

5-5. Absorption spectra

Absorption spectra



- InAs/InGaAs QWs (ε = 3.2%)
- Good agreement between experiment and 8-band model with $D_{s.o.}$

6. Conclusion

- 6- and 8-band ***k*・*p*** theory
  - Highly strained In(Ga)As/InGaAs QWs (strain up to 3.2%)
- Interaction between strain and spin-orbit coupling ($D_{s.o.}$)
  - 8-band model with $D_{s.o.}$ for InGaAs/InGaAs QWs with the strain larger than 2%