Optical properties of strain-compensated hybrid InGaN/InGaN/ZnO quantum well light-emitting diodes

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Overview

- Introduction
- Theoretical background
- Results and Discussion
- Summary

Introduction

- **Wurtzite GaN-based QW Structures**

  Potential and existing optoelectronic device applications : laser diode, traffic lights, displays, and so forth

- **Properties of (0001)-oriented WZ GaN-based QW structures: Several disadvantages, compared to conventional ZB GaAs- or InP-based QW structures**

- **Large internal field due to PZ and SP polarizations**

  ➔ Lower internal efficiency

- **Green InGaN/GaN QW LEDs show much less efficiency than that of blue InGaN/GaN QW LEDs**

  ← higher In composition and thick well width are needed to obtain longer wavelength

Hybrid InGaN/ZnO structures

- Reduce the internal field to obtain high performance short-wavelength LEDs
- By now, several methods such as using non-polar plane, inserting delta layer into InGaN well region, using ultra thin well width, and using quaternary InGaAlN barrier have been proposed to reduce the effect of the internal field due to polarizations.
- **Among them, ZnO and related oxides :**
  ← new wide band-gap semiconductors
- In particular, an alternative approach based on hybrid LED heterostructures combining p-doped GaN and n-doped ZnO epitaxial materials has been demonstrated by several

Hybrid InGaN/ZnO structures

- **With the current progress in the hybrid LED structures, the internal field engineering in the hybrid InGaN/InGaN/ZnO QW structures grown on ZnO substrate become very important for the realization of high efficiency green LEDs.**
- **Strain-compensated structure is possible.**

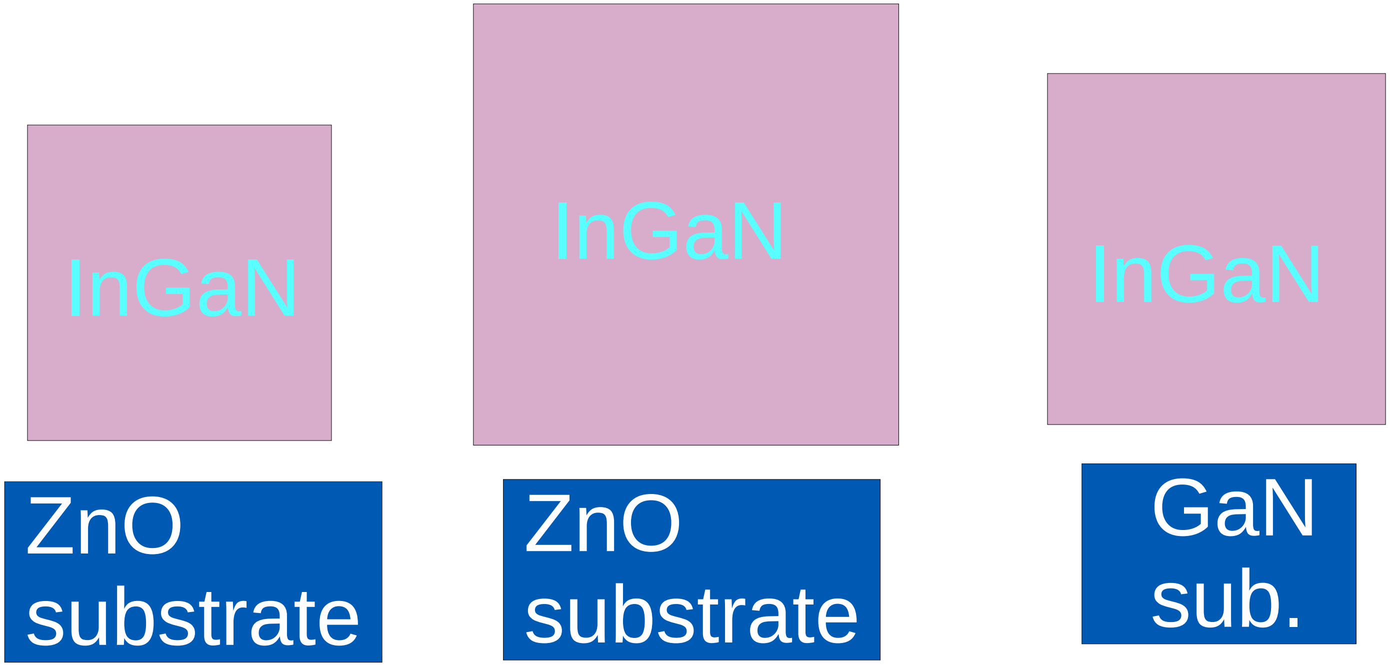
Electronic and optical properties of 530 nm hybrid InGaN/InGaN/ZnO QW structures

→ Compare with those of conventional InGaN/GaN QW structures

ZnO substrate :
Strain-compensated structure

a(InN)=3.53 A
a(GaN)=3.1892 A

a(ZnO)=3.2505 A



InGaN

ZnO substrate

InGaN

ZnO substrate

InGaN

GaN sub.

(a) Tensile
In < 0.18

(b) Compressvie
In > 0.18

(c) Always compressive

Valence band structure: (0001)-oriented Hamiltonian

$$H(\mathbf{k},\epsilon) = \begin{pmatrix} F & -K^* & -H^* & 0 & 0 & 0 \\ -K & G & H & 0 & 0 & \Delta \\ -H & H^* & \lambda & 0 & \Delta & 0 \\ 0 & 0 & 0 & F & -K & H \\ 0 & 0 & \Delta & -K^* & G & -H^* \\ 0 & \Delta & 0 & H^* & -H & \lambda \end{pmatrix} \begin{matrix} |U_1\rangle \\ |U_2\rangle \\ |U_3\rangle \\ |U_4\rangle \\ |U_5\rangle \\ |U_6\rangle \end{matrix},$$

Bases

$$\begin{aligned} |U_1\rangle &= -\frac{1}{\sqrt{2}}|(X+iY)\uparrow\rangle, \\ |U_2\rangle &= \frac{1}{\sqrt{2}}|(X-iY)\uparrow\rangle, \\ |U_3\rangle &= |Z\uparrow\rangle, \\ |U_4\rangle &= \frac{1}{\sqrt{2}}|(X-iY)\downarrow\rangle, \\ |U_5\rangle &= -\frac{1}{\sqrt{2}}|(X+iY)\downarrow\rangle, \\ |U_6\rangle &= |Z\downarrow\rangle. \end{aligned}$$

$$\begin{aligned} F &= \Delta_1 + \Delta_2 + \lambda + \theta, \\ G &= \Delta_1 - \Delta_2 + \lambda + \theta, \\ \lambda &= \frac{\hbar^2}{2m_o}[A_1 k_z{}^2 + A_2(k_x{}^2 + k_y{}^2)] + \lambda_\epsilon, \\ \theta &= \frac{\hbar^2}{2m_o}[A_3 k_z{}^2 + A_4(k_x{}^2 + k_y{}^2)] + \theta_\epsilon, \\ K &= \frac{\hbar^2}{2m_o}A_5(k_x + ik_y)^2 + D_5\epsilon_+, \\ H &= \frac{\hbar^2}{2m_o}A_6(k_x + ik_y)(k_z) + D_6\epsilon_{z+}, \\ \lambda_\epsilon &= D_1(\epsilon_{zz}) + D_2(\epsilon_{xx} + \epsilon_{yy}), \\ \theta_\epsilon &= D_3(\epsilon_{zz}) + D_4(\epsilon_{xx} + \epsilon_{yy}), \\ \epsilon_+ &= \epsilon_{xx} - \epsilon_{yy} + 2i\epsilon_{xy}, \\ \epsilon_{z+} &= \epsilon_{xz} + i\epsilon_{yz}, \\ \Delta &= \sqrt{2}\Delta_3. \end{aligned}$$

Self-consistent solution with screening effect

The self-consistent (SC) band structures and wave functions are obtained by solving the Schrodinger equation for electrons, the 6x6 Hamiltonian for holes, and Poisson's equation iteratively.

Total potential profile for electron and hole

$$\begin{aligned} V_c(z) &= V_{cw}(z) - |e|\phi(z), \\ V_v(z) &= V_{vw}(z) - |e|\phi(z), \end{aligned}$$

where Vw=square-well potential

Poisson equation

$$\frac{d}{dz}\left(\epsilon(z)\frac{d}{dz}\right)\phi(z) = -|e|[p(z) - n(z)],$$

Electron and hole concentrations

$$n(z) = \frac{kTm_e}{\pi\hbar^2}\sum_n |f_n(z)|^2 \ln\left(1 + e^{[E_{fc}-E_{cn}(0)]/kT}\right)$$

$$p(z) = \sum_{\sigma=U,L}\sum_m \int dk_{||}\frac{k_{||}}{2\pi}\sum_\nu |g^{\sigma(\nu)}_{mk_{||}}(z)|^2\left(\frac{1}{1 + e^{[E_{fv}-E_{vm}(k_{||})]/kT}}\right),$$

Potential

$$\phi(z) = -\int_{-L/2}^{z} E(z')dz',$$

where

$$E(z) = \int_{-L/2}^{z} \frac{1}{\epsilon(z)}\rho(z')dz'.$$

Non-Markovian model with many-body effects for spontaneous emission spectrum

$$g_{sp}(\omega) = \sqrt{\frac{\mu_o}{\epsilon}} \sum_{\sigma=U,L} \sum_{l,m} \left(\frac{e^2}{m_o^2\omega}\right) \int_0^\infty dk_{||} \frac{k_{||}}{\pi L_w^{eff}} |\hat{\epsilon} \cdot \mathbf{M}_{lm}^{\sigma}(k_{||})|^2 f_l^c(k_{||})[1 - f_m^v(k_{||})] L(\omega, k_{||})$$

$$\begin{aligned}
L(\omega, k_{||}) &= \frac{(1 - \mathrm{Re}Q(k_{||}, \hbar\omega))\mathrm{Re}L(E_{lm}(k_{||}, \hbar\omega)) - \mathrm{Im}Q(k_{||}, \hbar\omega)\mathrm{Im}L(E_{lm}(k_{||}, \hbar\omega))}{(1 - \mathrm{Re}Q(k_{||}, \hbar\omega))^2 + (\mathrm{Im}Q(k_{||}, \hbar\omega))^2} \\
\mathrm{Re}[L(E_{lm}(k_{||}, \hbar\omega))] &= \sqrt{\frac{\pi\tau_{in}(k_{||}, \hbar\omega)\tau_c}{2\hbar^2}} \exp\left(-\frac{\tau_{in}(k_{||}, \hbar\omega)\tau_c}{2\hbar^2} E_{lm}^2(k_{||}, \hbar\omega)\right) \\
\mathrm{Im}[L(E_{lm}(k_{||}, \hbar\omega))] &= \frac{\tau_c}{\hbar} \int_0^\infty \exp\left(-\frac{\tau_c}{2\tau_{in}(k_{||}, \hbar\omega)} t^2\right) \sin\left(\frac{\tau_c E_{lm}(k_{||}, \hbar\omega)}{\hbar} t\right) dt.
\end{aligned}$$

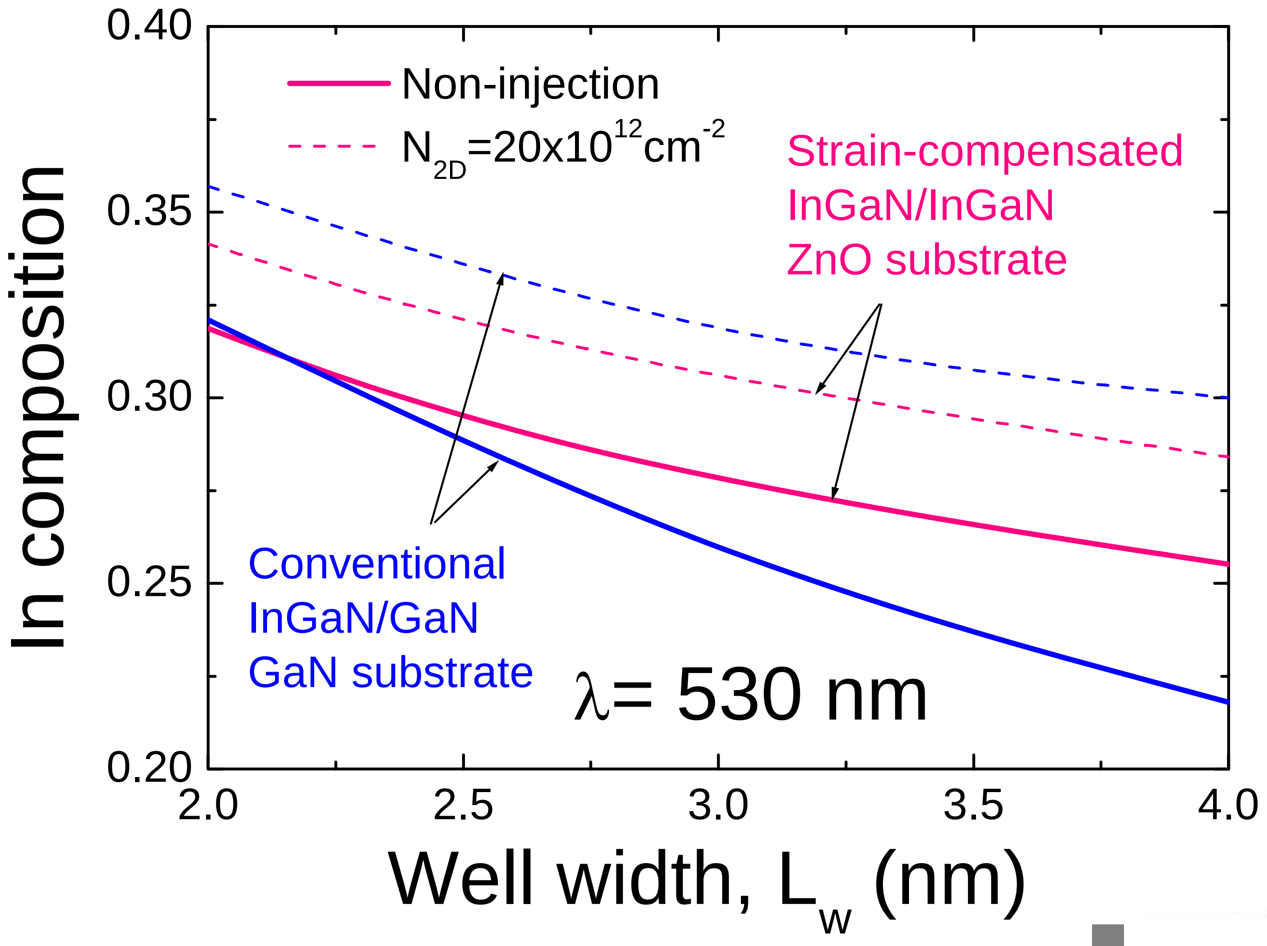
$|M|^2$: Momentum matrix element

f_n and f_m : Fermi functions

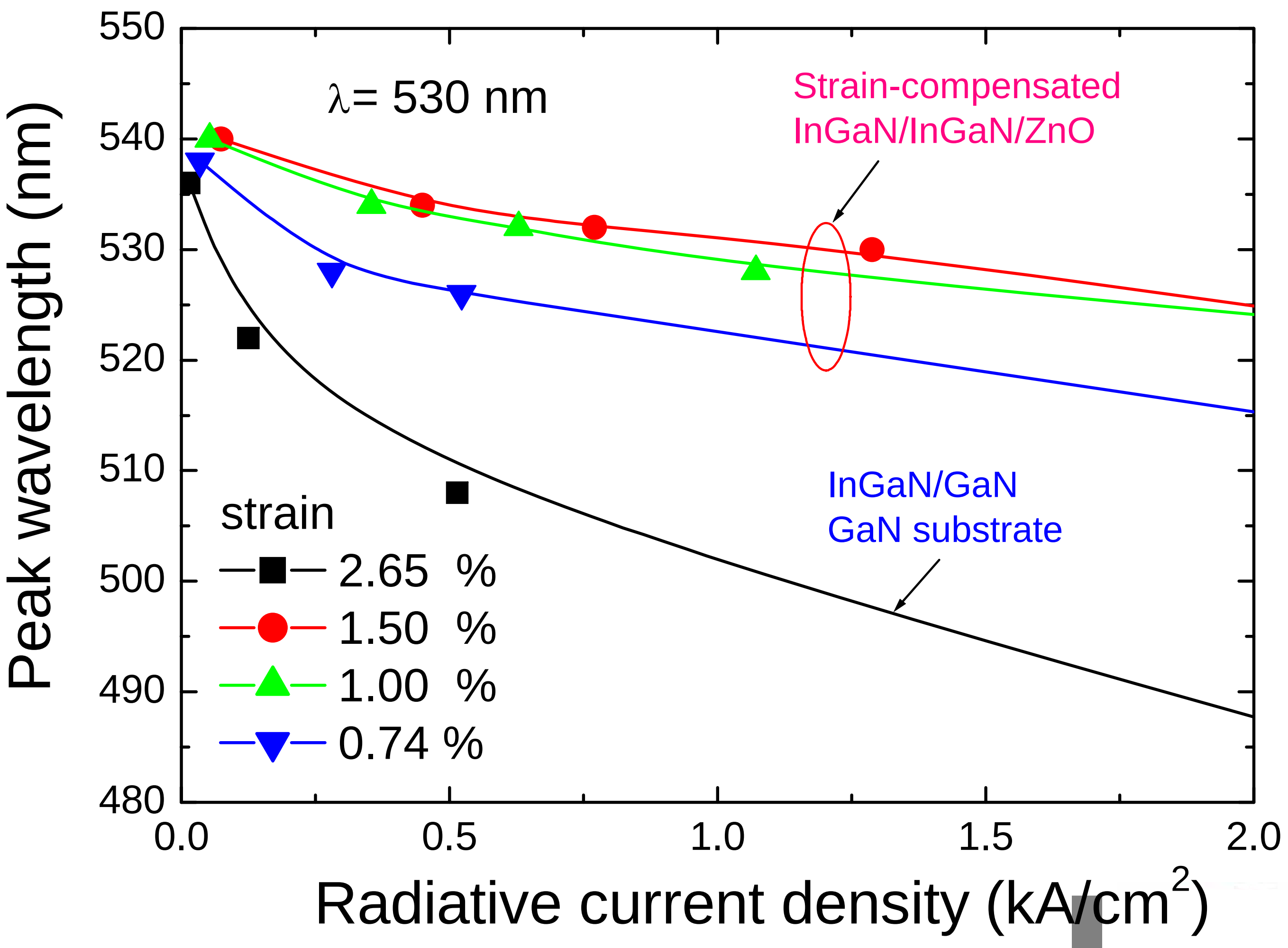
L : Gaussian line shape function renormalized with many-body effects

Q : CE many-body effect

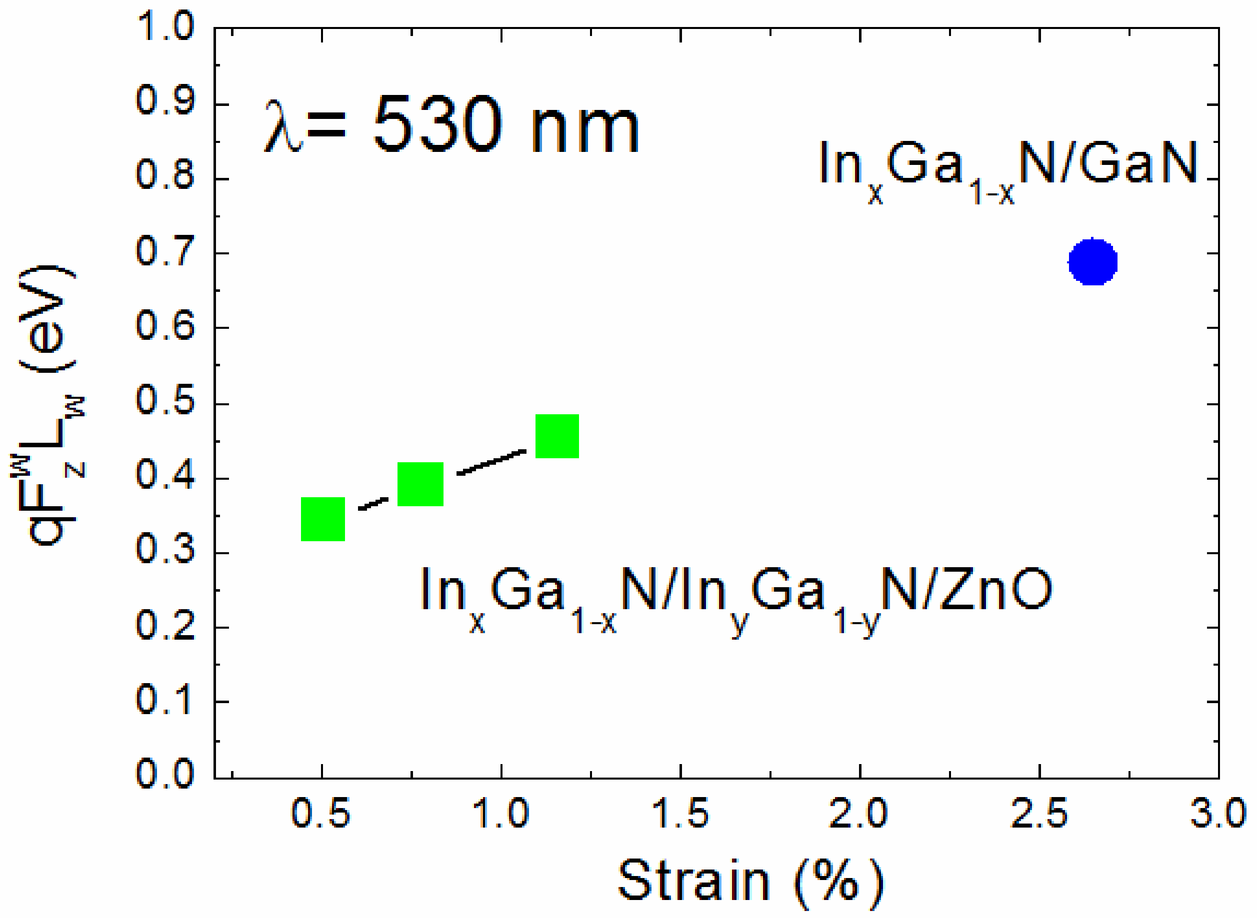
In composition as a function of well width to obtain transition wavelength of 530 nm



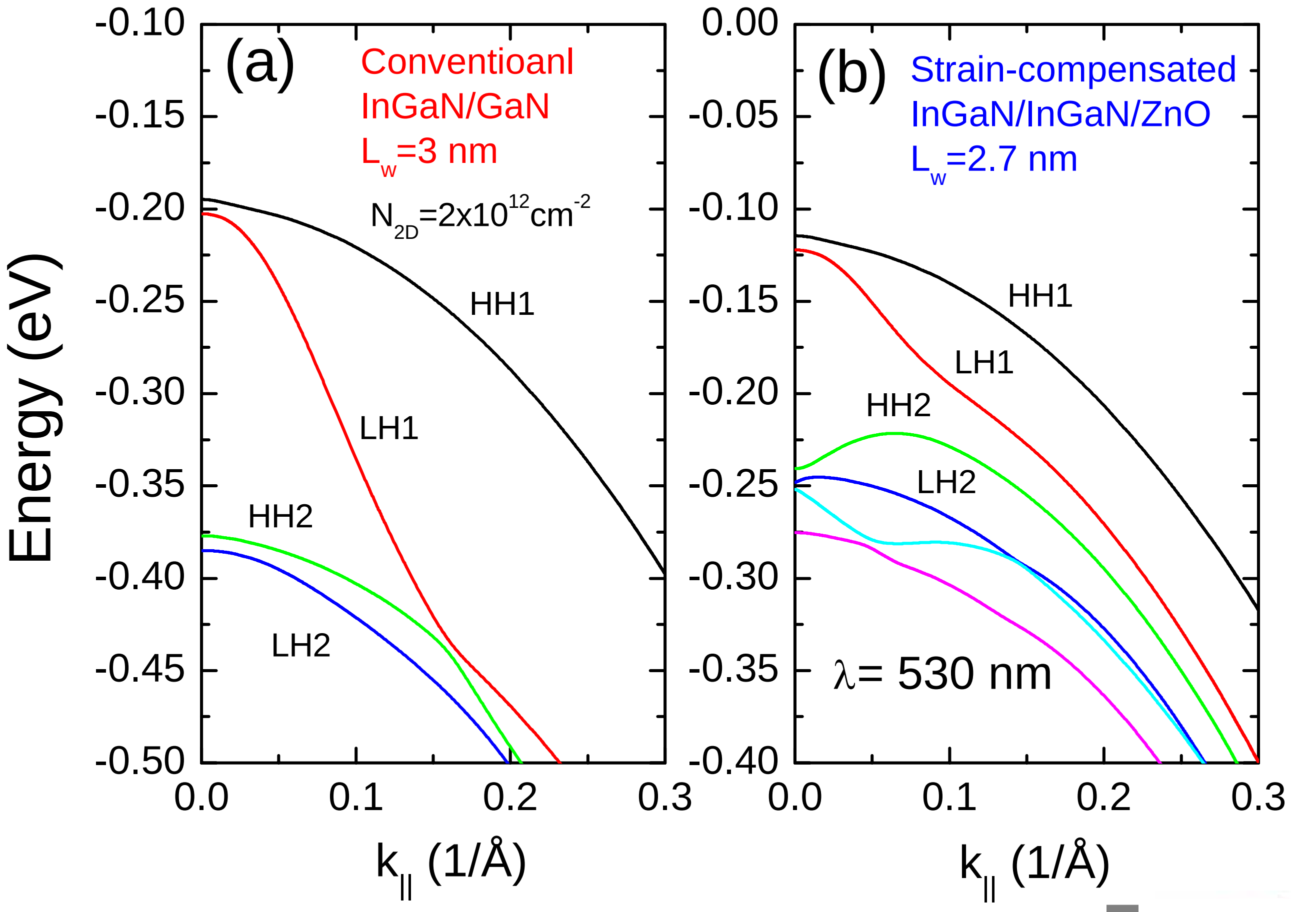
Peak wavelength as a function of radiative current density



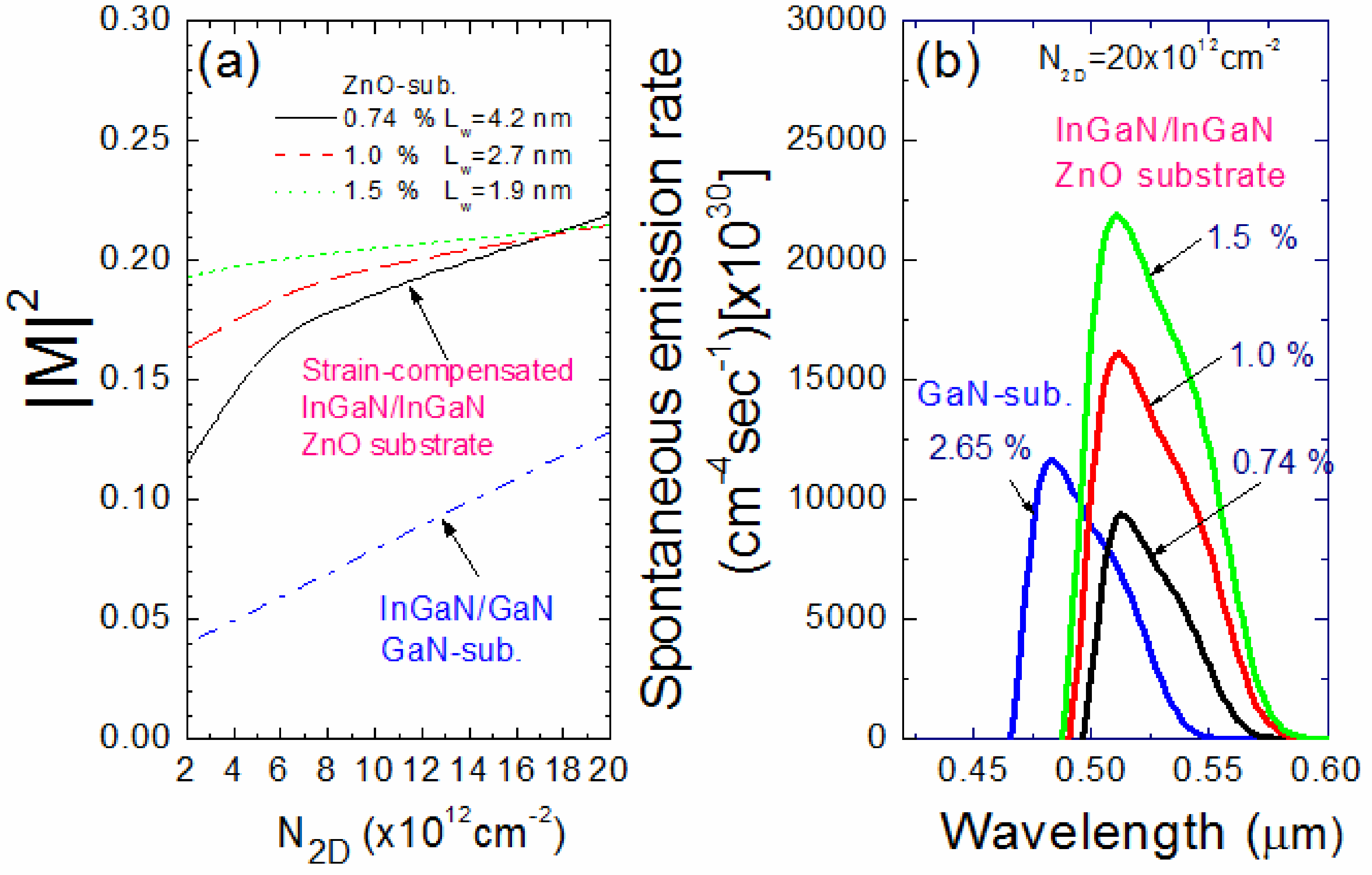
Potential energy induced by internal field



Valence band structure



Optical matrix elements and Spontaneous emission rate



Summary

- A strain-compensated QW structure with a relatively larger strain (1.5 %) is found to have much larger spontaneous emission than a InGaN/GaN QW structure, due to the reduced internal field effect.
- Also, in the case of a strain-compensated QW structure, the current density dependence of the peak wavelength is shown to be largely reduced, compared to the InGaN/GaN QW structure.