Many-body optical gain in ZnO- and GaN-based quantum well lasers

Seoung-Hwan Park[1] and Doyeol Ahn[2]

[1]*Catholic University of Daegu*,[2]*University of Seoul, South Korea*

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Overview

- Introduction
- Theory
- Results and Discussion
  - ✓ (0001)-oriented QW structures
  - ✓ Crystal orientation effects
- Summary

Introduction

- **Wurtzite GaN-based QW Laser**

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

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

1) GaN : significantly larger effective mass
2) Biaxial strain : does not effectively reduce effective mass
3) Large internal field : PZ and SP polarizations

➔ Higher threshold current density for lasing

[Control the internal field and the effective mass]

Main Goals of the Approach

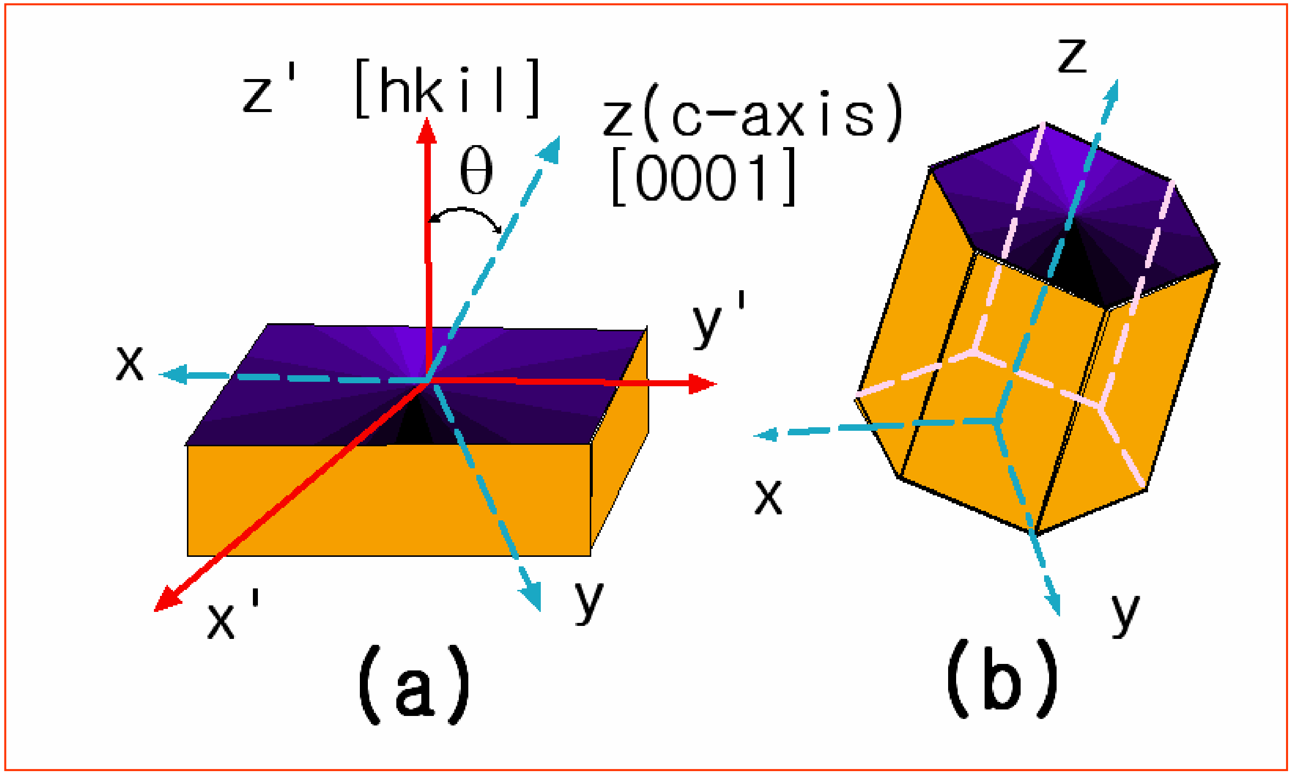
- **The crystal orientation effects : a new parameter in the band structure engineering**
  ← by controlling the internal field and the effective masses
- **Recently, ZnO and related oxides :**
  ← new wide band-gap semiconductors

1) Growth temperature of ZnO : around 500 ^{o}C (GaN: 1000 ^{o}C)
2) The internal field is expected to be much smaller than that in GaN-related systems.

Electronic and optical properties of ZnO/MgZnO QW structures and Crystal orientation effects

→ Compare with those of GaN-based QW structures

Theoretical background



Wurtzite
primitive cell

Only θ dependence due to hexagonal symmetry (ϕ=0)
$\theta=0$: (0001), $\theta=\pi/2$: $(10\bar{1}0)$

Valence band structure

(0001)-oriented Hamiltonian

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

Bases

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

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

Rotation matrix

$$U = \begin{pmatrix} \cos\theta\cos\phi & \cos\theta\sin\phi & -\sin\theta \\ -\sin\phi & \cos\phi & 0 \\ \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \end{pmatrix}$$

Hamitonian for (0001)-oriented WZ crystal

$(k_i, \varepsilon_{ij}(\theta=0))$

Hamiltonian for general crystal orientation

$(k'_i, \varepsilon_{ij}(\theta))$

$$k'_i = \sum_{i\alpha} U_{i\alpha}\, k_\alpha$$

$\varepsilon_{ij}(\theta)$ <= **Minimization of strain energy**

Strain tensors in general coordinate

$$\epsilon_{xx} = \epsilon_{xx}^{(0)} + \epsilon_{xz}\frac{\sin\theta}{\cos\theta},$$

$$\epsilon_{yy} = \epsilon_{xx}^{(0)},$$

$$\epsilon_{zz} = \epsilon_{xz}\frac{\cos\theta}{\sin\theta} + \epsilon_{zz}^{(0)},$$

$$\epsilon_{xy} = \epsilon_{yz} = 0,$$

$$\epsilon_{xx}^{(0)} = (a_s - a_e)/a_e \text{ and } \epsilon_{zz}^{(0)} = (c_s - c_e)/c_e$$

Subscripts s and e denote the substrate and epilayer, respectively.

$$\epsilon_{xz} = -\frac{[(c_{11}+c_{12}+c_{13}\epsilon_{zz}^{(0)}/\epsilon_{xx}^{(0)})\sin^2\theta + (2c_{13}+c_{33}\epsilon_{zz}^{(0)}/\epsilon_{xx}^{(0)})\cos^2\theta]\epsilon_{xx}^{(0)}\cos\theta\sin\theta}{c_{11}\sin^4\theta + 2(c_{13}+2c_{44})\sin^2\theta\cos^2\theta + c_{33}\cos^4\theta}$$

Hamiltonian for general crystal orientation ← Vectors and tensors

PZ and SP polarizations for general crystal orientation
: Function of θ

$$P_{PZ} = P_x \sin\theta + P_z \cos\theta,$$

$$P_{SP} = P_{SP}^{(0001)} \cos\theta$$

$$P_x = 2d_{15}c_{44}\epsilon_{xz},$$

$$P_z = [d_{31}(c_{11} + c_{12}) + d_{33}c_{13}](\epsilon_{xx} + \epsilon_{yy}) + [2d_{31}c_{13} + d_{33}c_{33}]\epsilon_{zz}$$

$P_x = 0$ for $\theta = \pi/2$
($\varepsilon_{xz}=0$)

$(10\bar{1}0)$ Crystal orientation
$[\theta = \pi/2]$

→ $P_{PZ} = 0$ and $P_{SP} = 0$

Non-Markovian gain model with many-body effects

$$g(\omega) = \sqrt{\frac{\mu_o}{\epsilon}} \left(\frac{e^2}{m_o^2 \omega}\right) \int_0^{2\pi} d\Phi \int_0^{\infty} dk_{||} \frac{2k_{||}}{(2\pi)^2 L_w} |M_{nm}(k_{||},\Phi)|^2 [f_n^c(k_{||},\Phi) - f_m^v(k_{||},\Phi)] L(\omega, k_{||},\Phi)$$

$$L(\omega, k_{||}, \Phi) = \frac{(1 - \mathrm{Re}Q(k_{||},\hbar\omega))\mathrm{Re}\Xi(E_{lm}(k_{||},\hbar\omega)) - \mathrm{Im}Q(k_{||},\hbar\omega)\mathrm{Im}\Xi(E_{lm}(k_{||},\hbar\omega))}{(1 - \mathrm{Re}Q(k_{||},\hbar\omega))^2 + (\mathrm{Im}Q(k_{||},\hbar\omega))^2}$$

$$\begin{aligned}\mathrm{Re}\Xi(E_{lm}(k_{||},\hbar\omega)) &= \sqrt{\frac{\pi\tau_{co}}{2\hbar\Gamma_{cv}(k_{||},\hbar\omega)}} \\ &\times \exp\left(-\frac{\tau_{co}}{2\hbar\Gamma_{cv}(k_{||},\hbar\omega)} E_{lm}^2(k_{||},\hbar\omega)\right)\end{aligned}$$

$$\begin{aligned}\mathrm{Im}\Xi(E_{lm}(k_{||},\hbar\omega)) &= \frac{\tau_{co}}{\hbar}\int_0^{\infty} \exp\left(-\frac{\Gamma_{cv}(k_{||},\hbar\omega)\tau_{co}}{2\hbar} t^2\right) \\ &\times \sin\left(\frac{\tau_{co}E_{lm}(k_{||},\hbar\omega)}{\hbar} t\right) dt.\end{aligned}$$

$|M|^2$: Momentum matrix element

f_n and f_m : Fermi functions

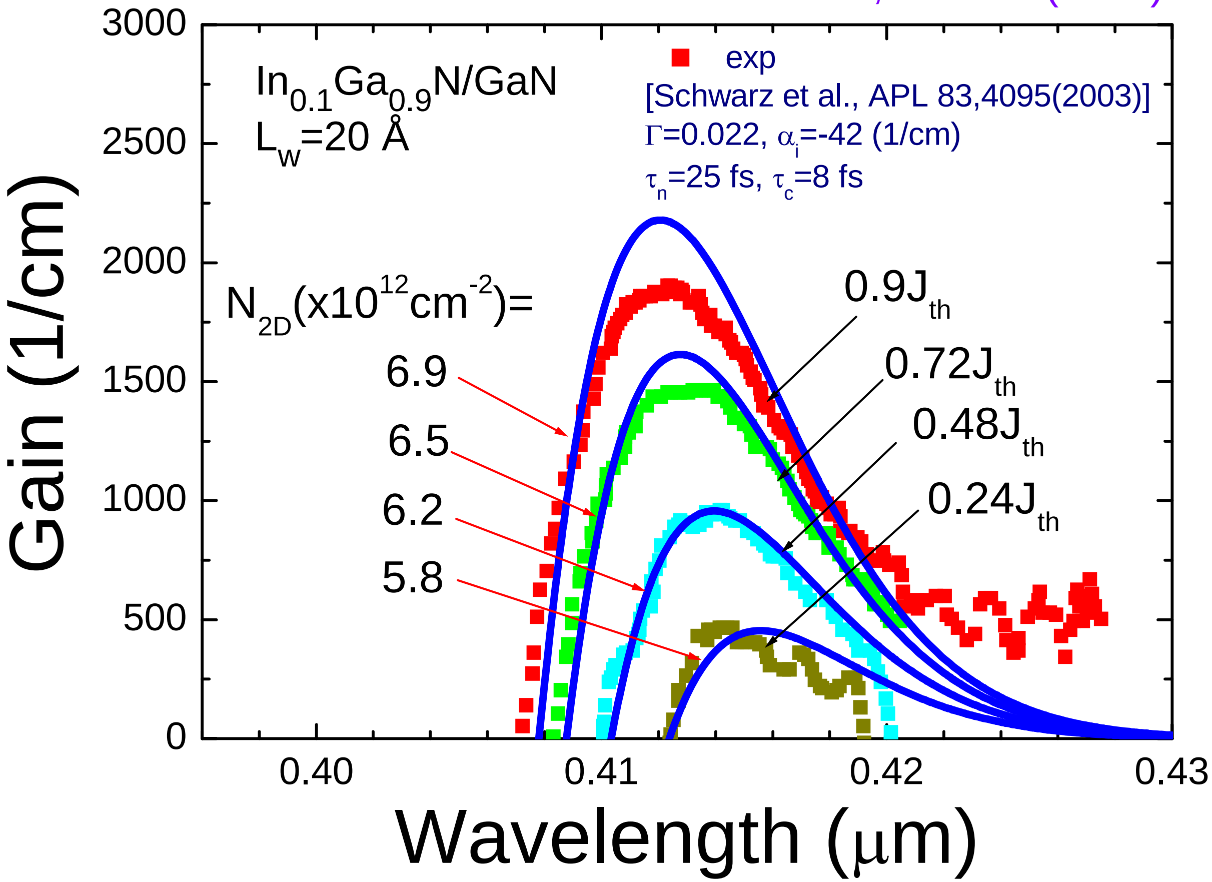
L : Gaussian line shape function renormalized with many-body effects

Q : CE many-body effect

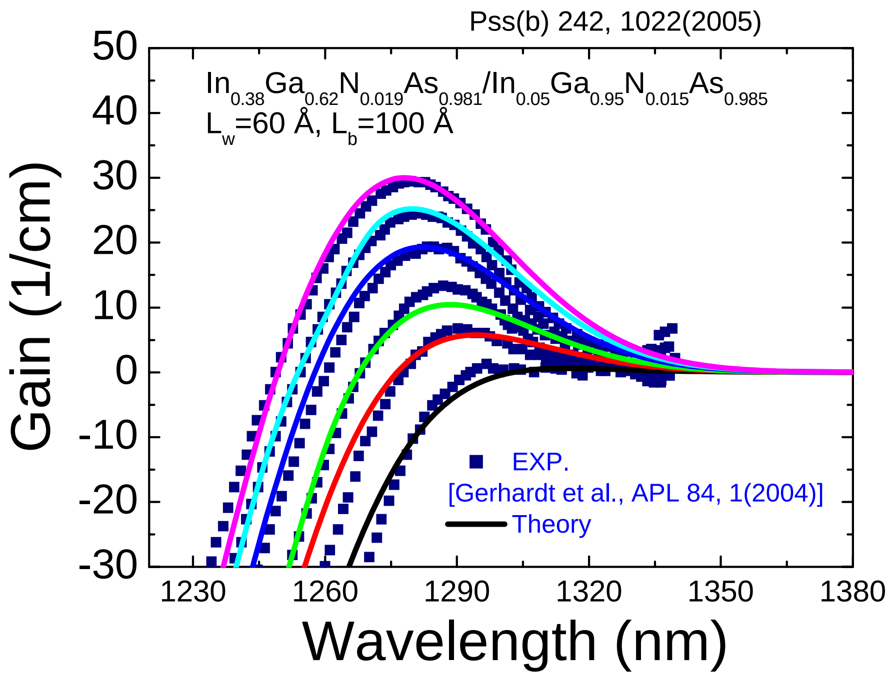
Φ : Angle between kx' and ky' wavevectors

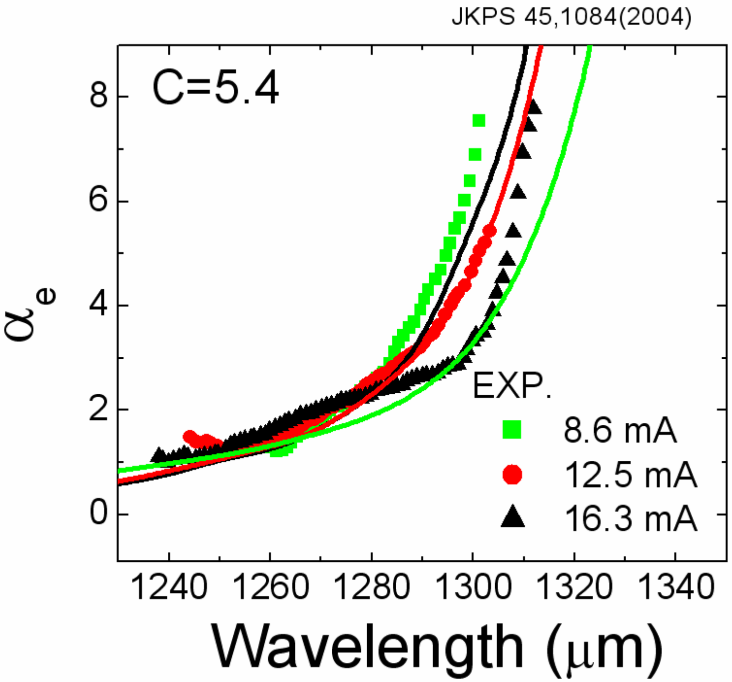
InGaN/GaN QW Structure

APL 87, 044103 (2005)

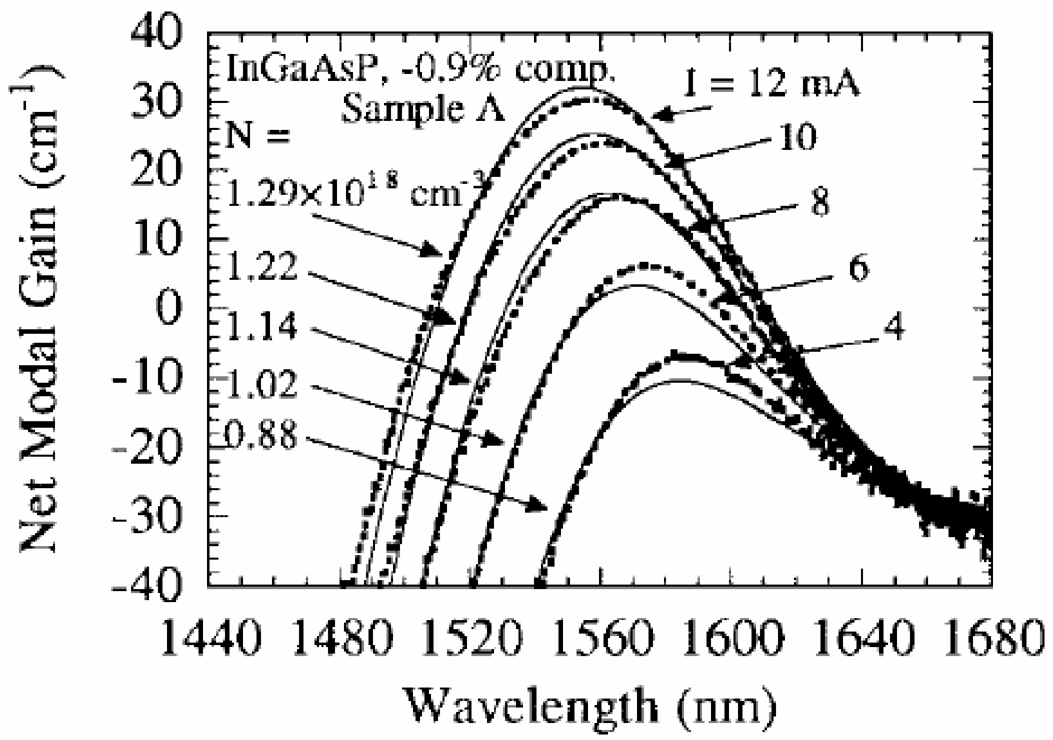


InGaNAs/GaAs QW structure



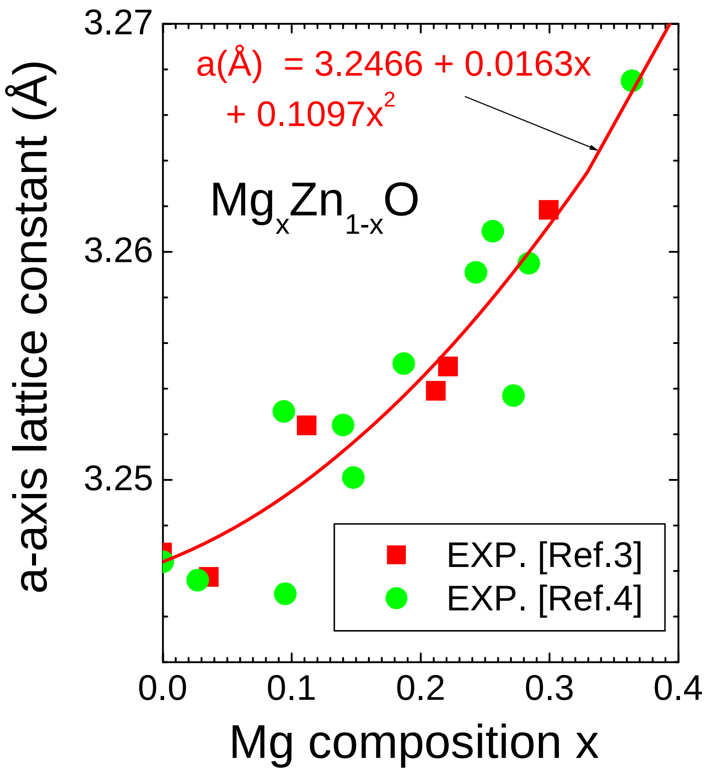


InGaAsP/InP QW structure



IEEE JQE 35, 771(1999)

Lattice constant for MgZnO

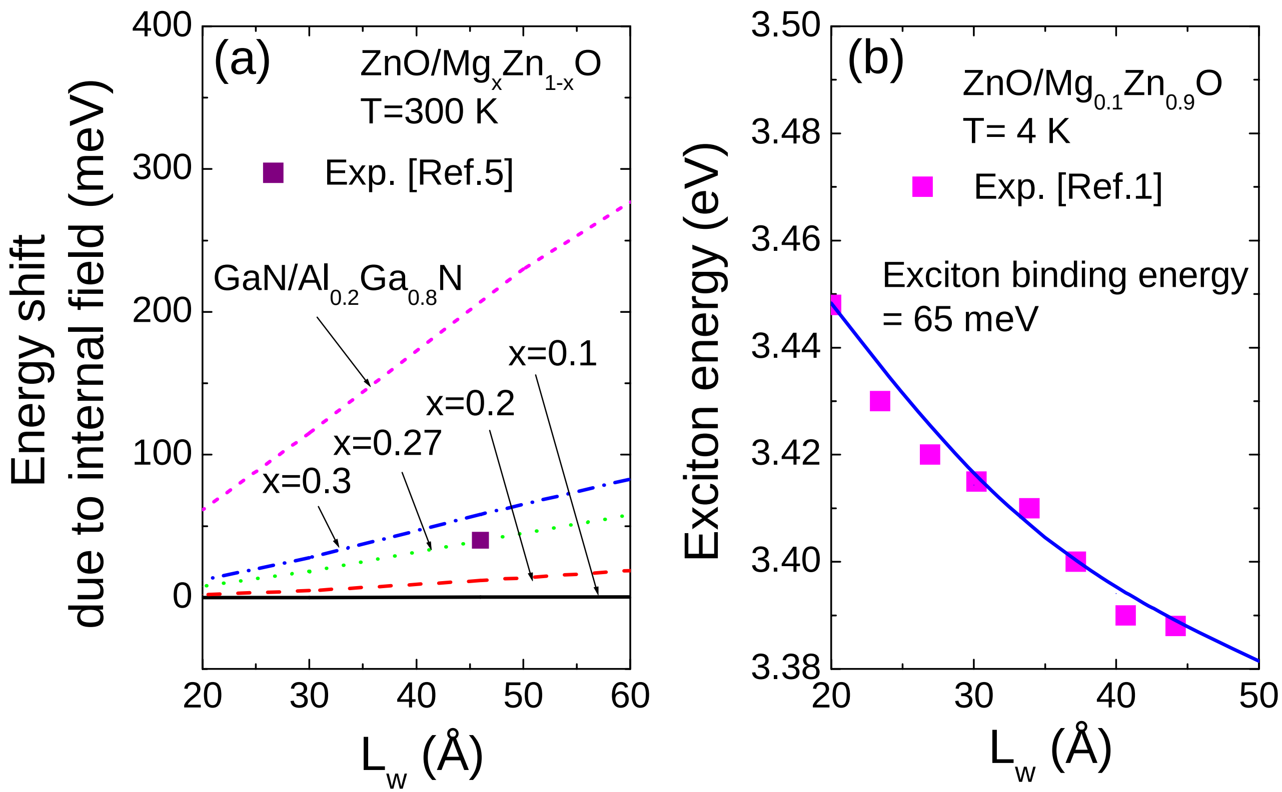


[3] T. Makino, Y. Segawa, M. Kawasaki, A. Ohtomo, R. Shiroki, K. Tamura, T. Yasuda, and H. Koinuma, Appl. Phys. Lett. **78**, 1237 (2001).
[4] A. Ohtomo and A. Tsukazaki, Semicond. Sci. Technol. **20**, S1 (2005).

$$P_{SP}^{ZnO} = -0.05 C/m^2$$

Spontaneous polarization constant for MgO : a fitting parameter

Energy shift and exciton energy for ZnO/MgZnO QW structures

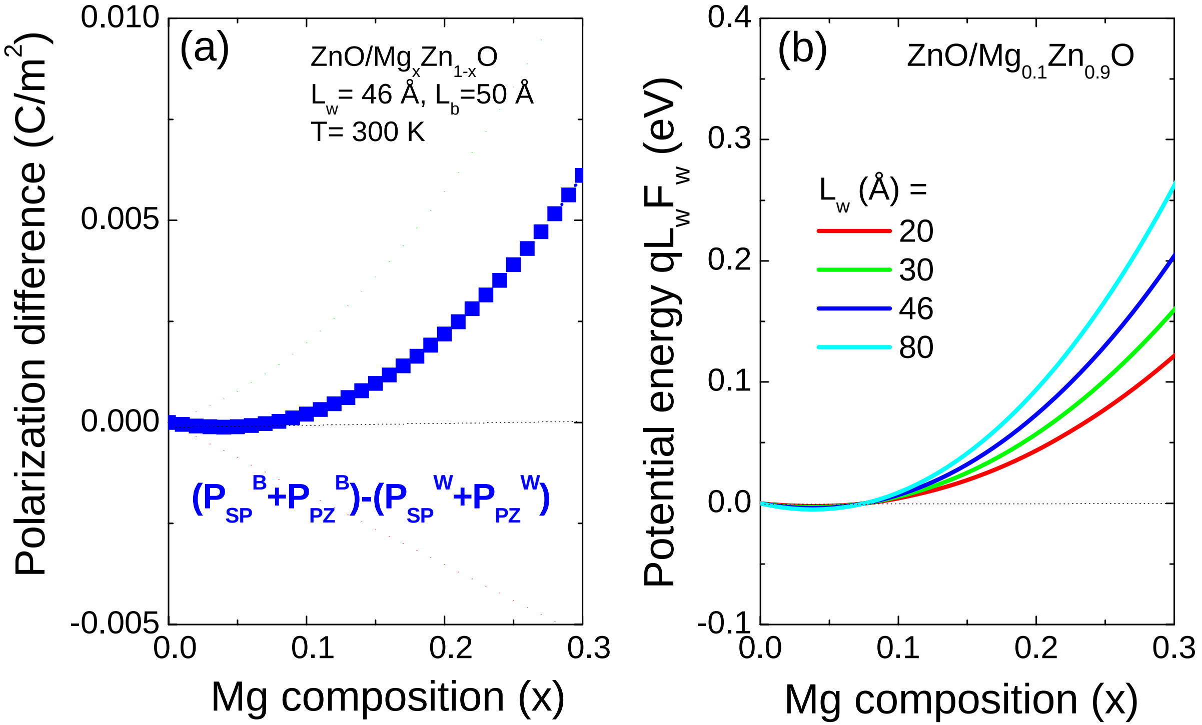


$$P_{SP}^{MgO} = -0.07\,C/m^2$$

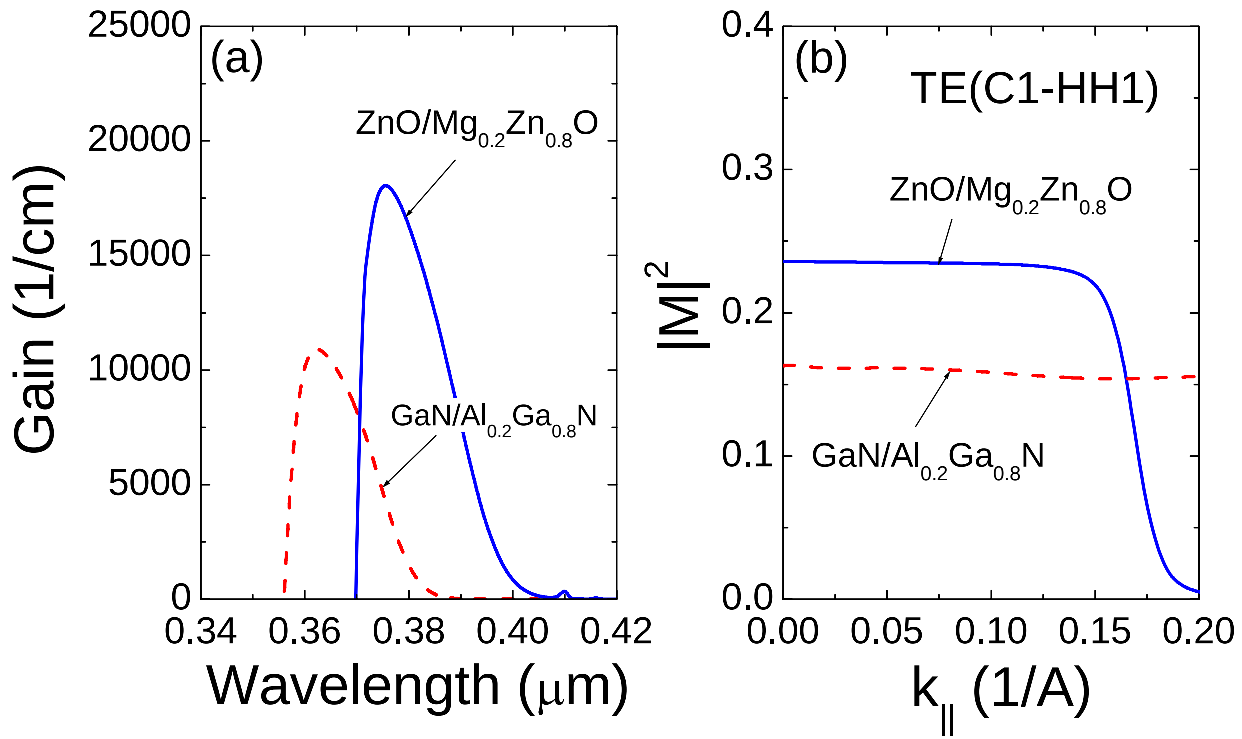
[5]T. Makino, K. Tamura, C. H. Chia, Y. Segawa, M. Kawasaki, A. Ohtomo, and H. Koinuma, Appl. Phys. Lett. **81**, 2355 (2002).

[1]B. P. Zhang, N. T. Binh, K. Wakatsuki, C. Y. Liu, Y. Segawa, and N. Usami, Appl. Phys. Lett. **86**, 032105 (2005).

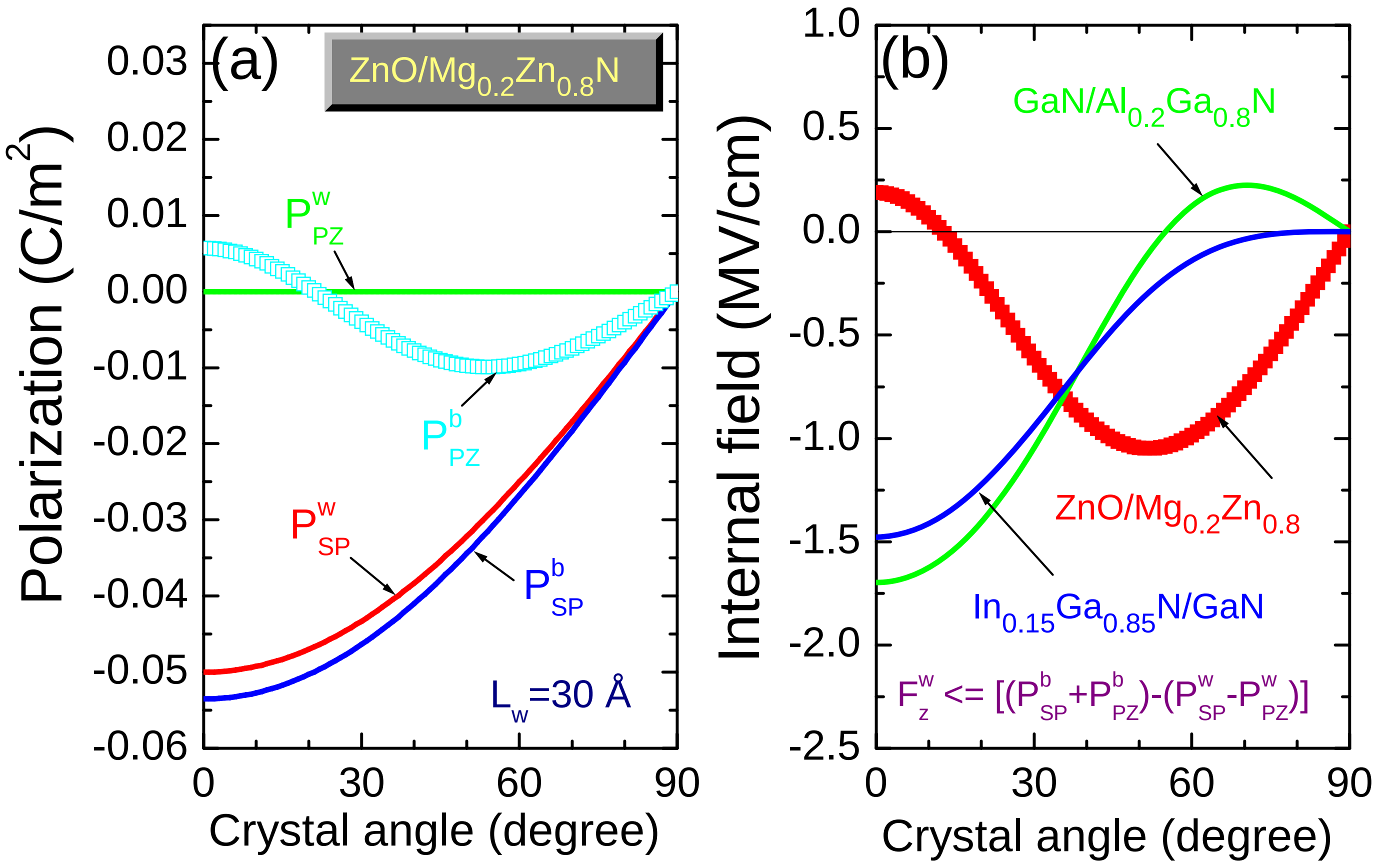
Difference between total PZ and SP polarizations and potential energy



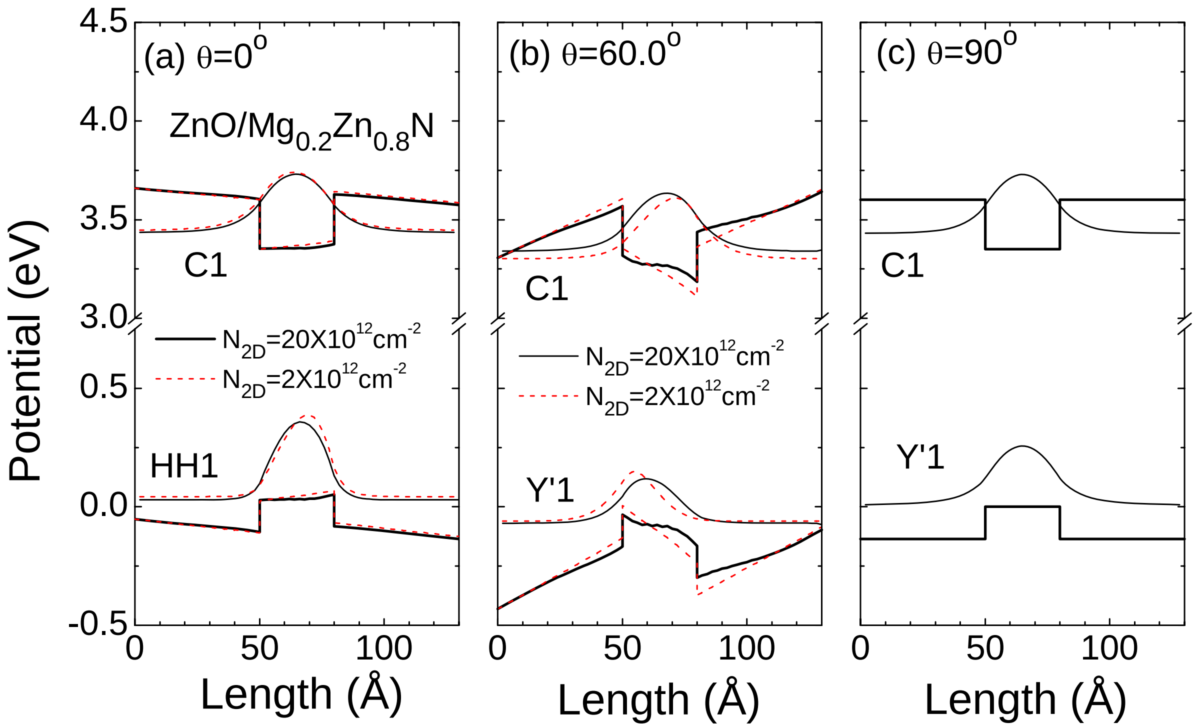
Optical gain spectra and optical matrix elements



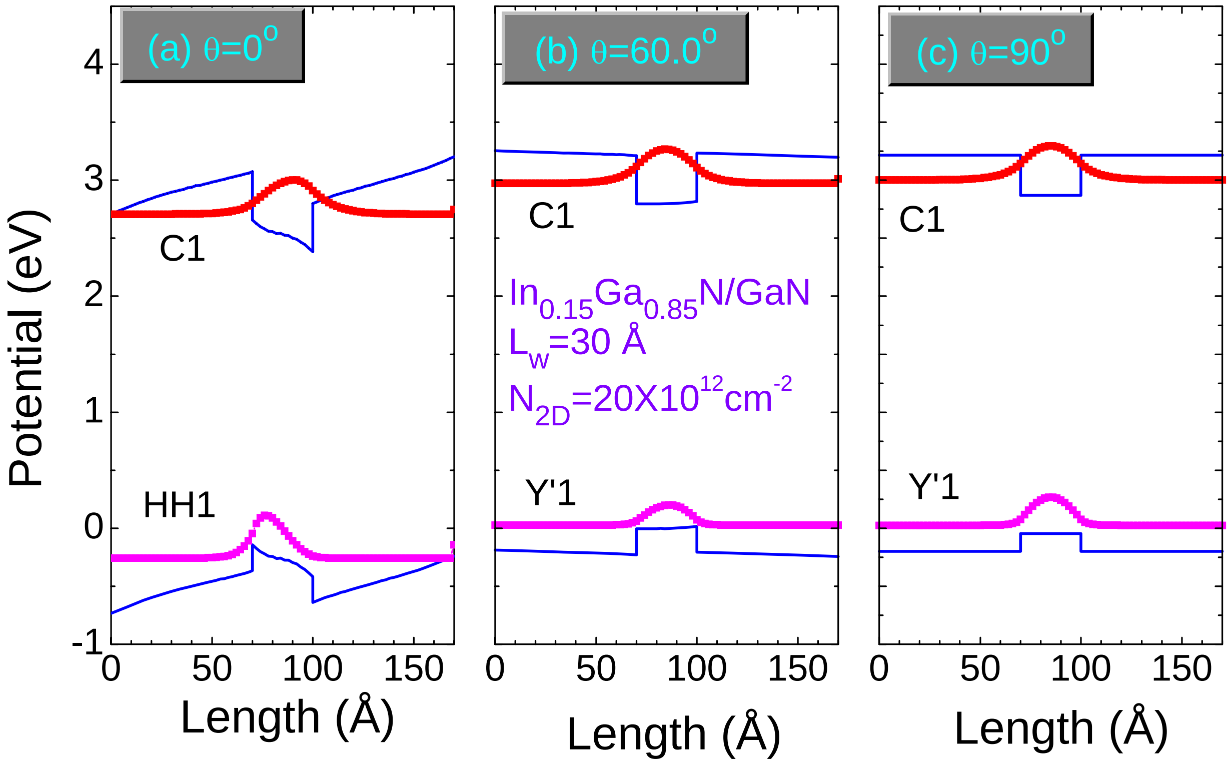
Polarization and Internal field of ZnO/MgZnO QW structures



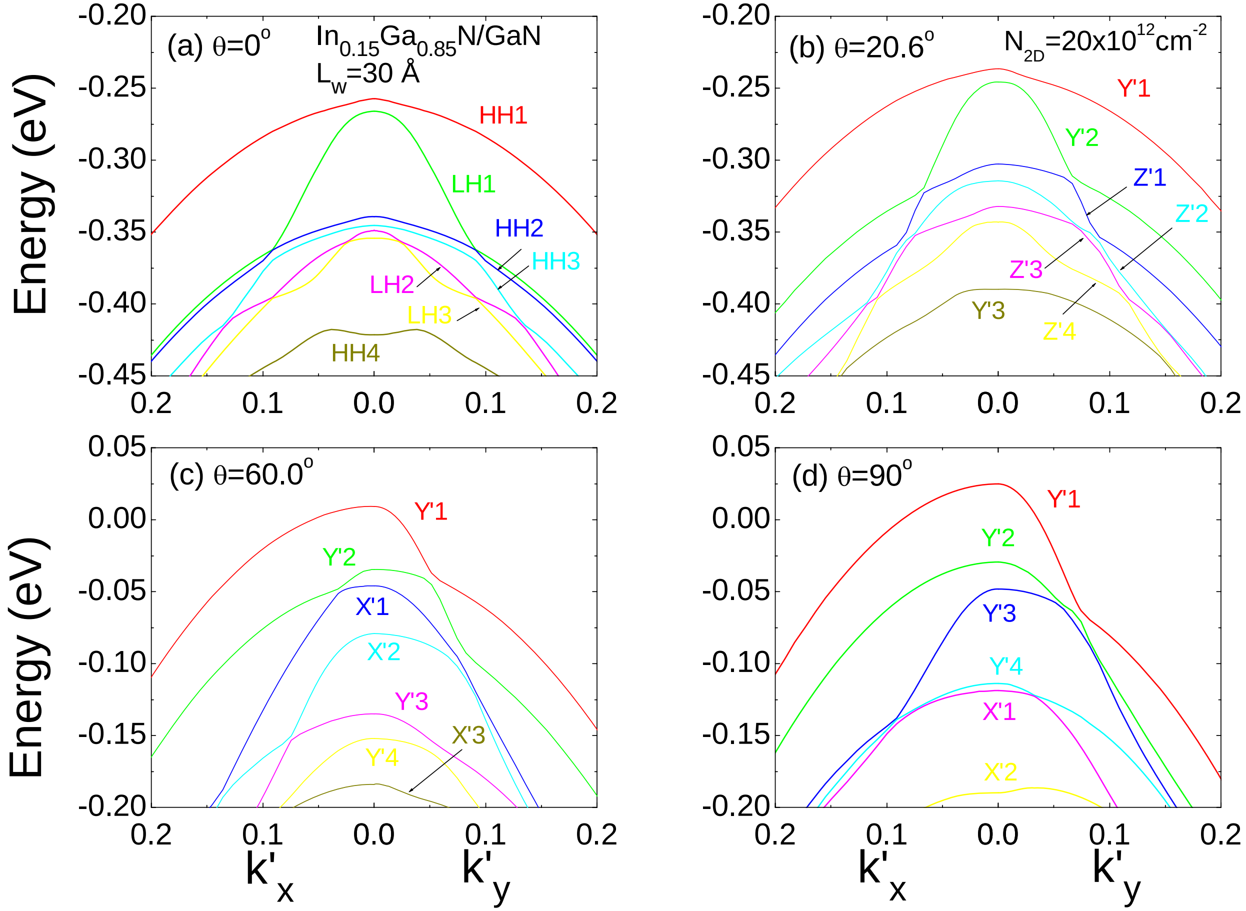
Potential profile : ZnO/MgZnO



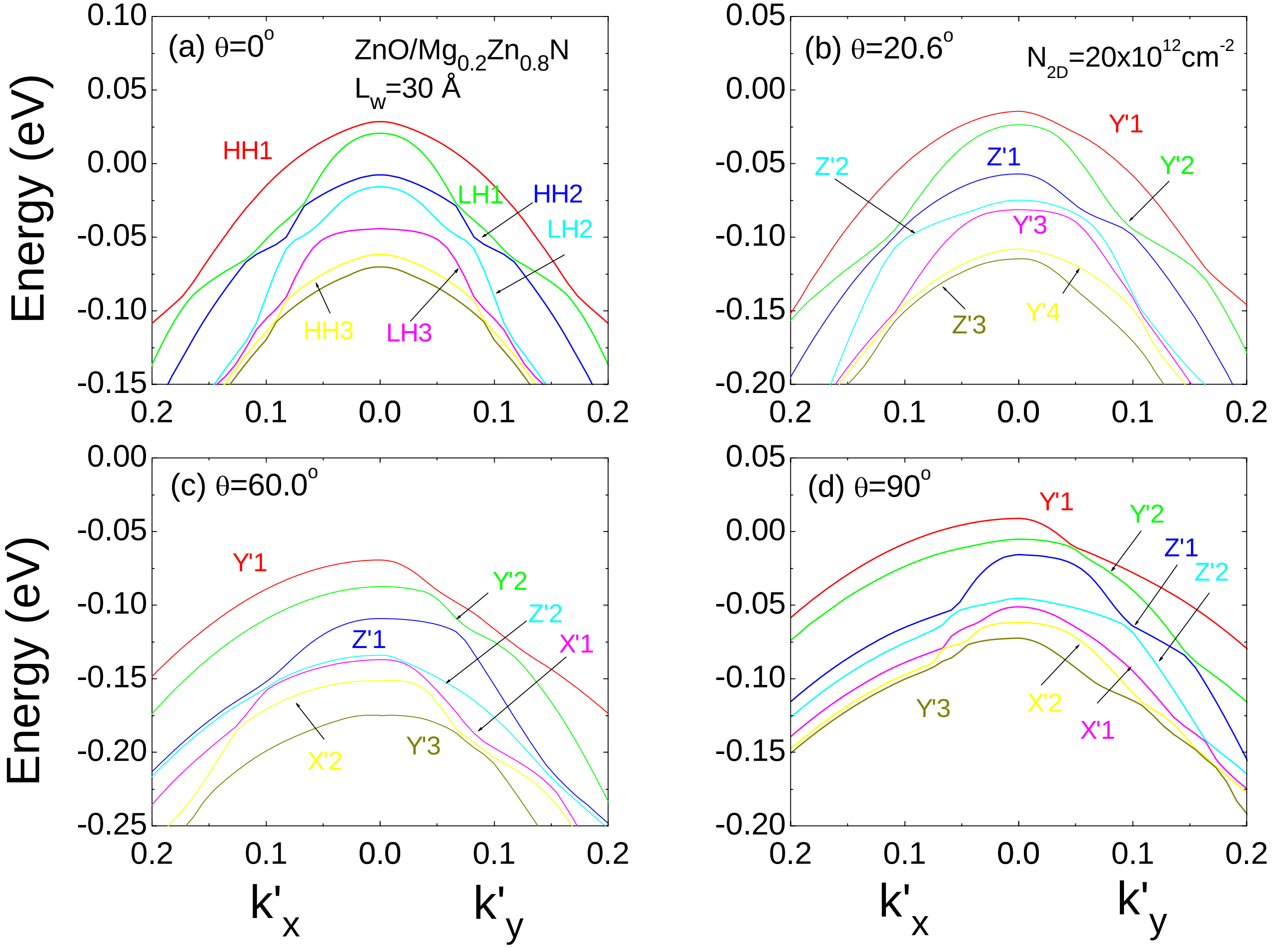
Potential profile : InGaN/GaN



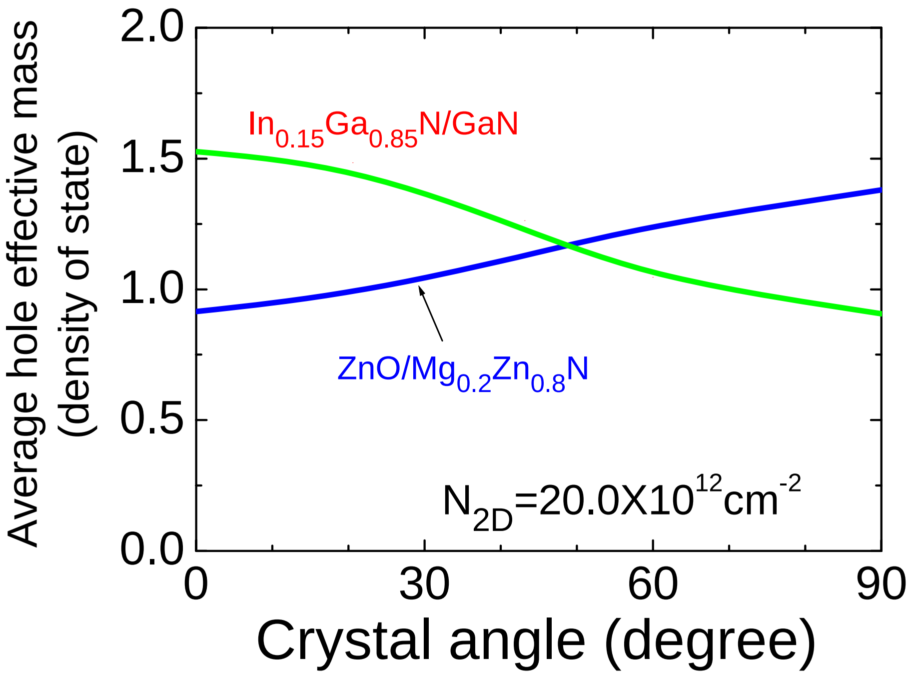
Valence band structure: InGaN/GaN

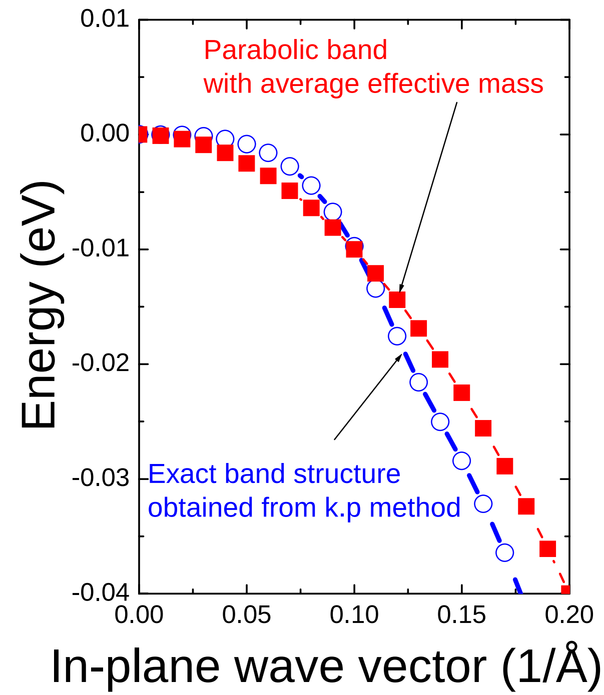


Valence band structure: ZnO/MgZnO

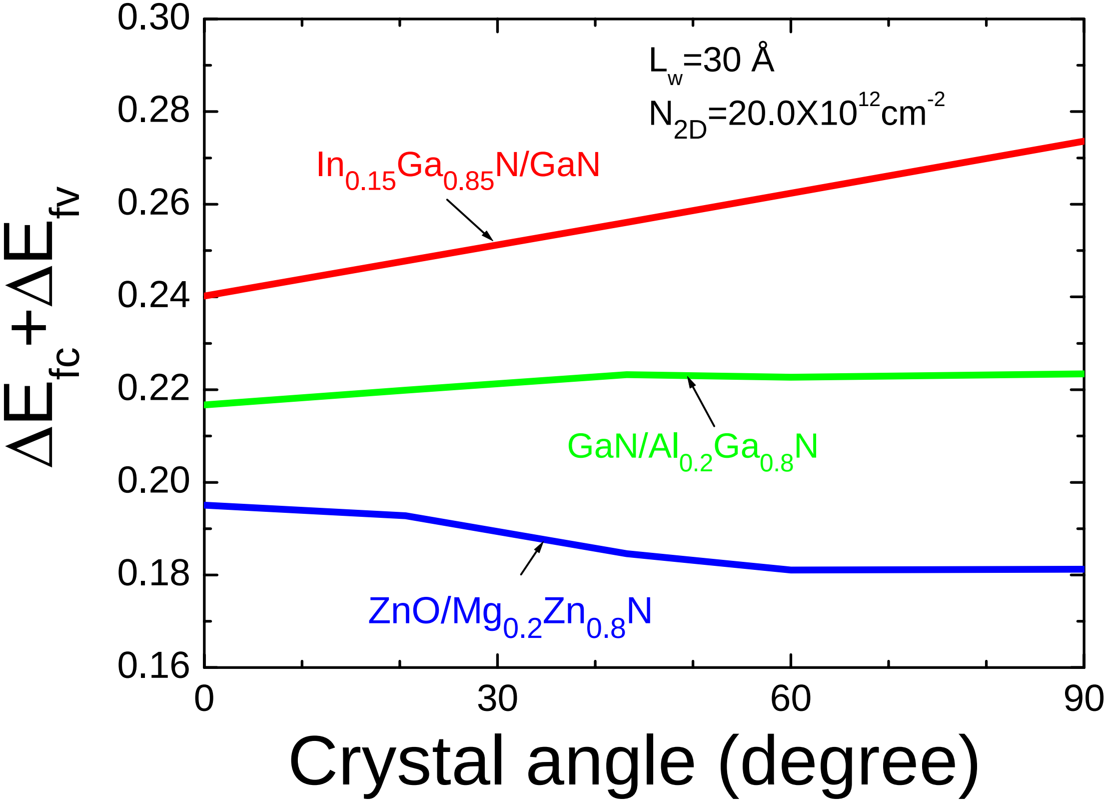


Average hole effective mass

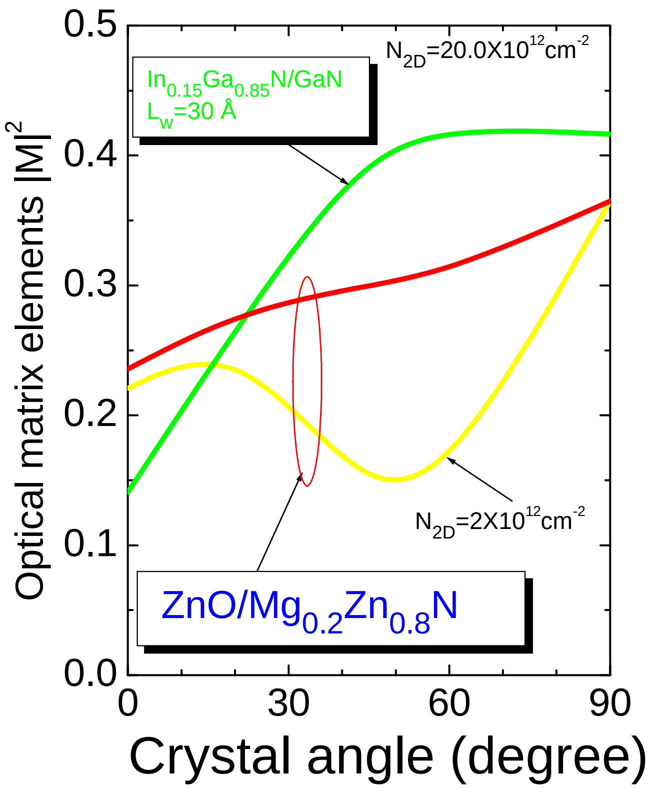




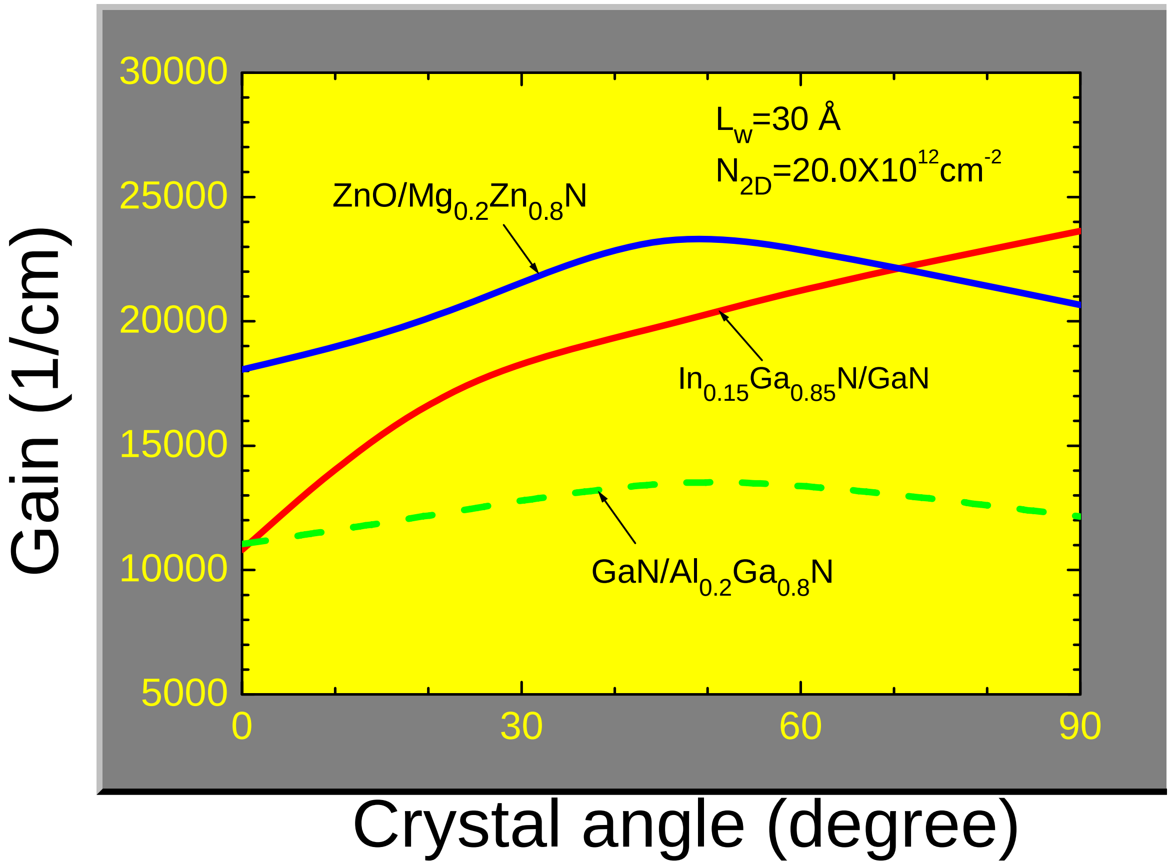
Quasi-Fermi level separation



Optical matrix elements



Optical gain



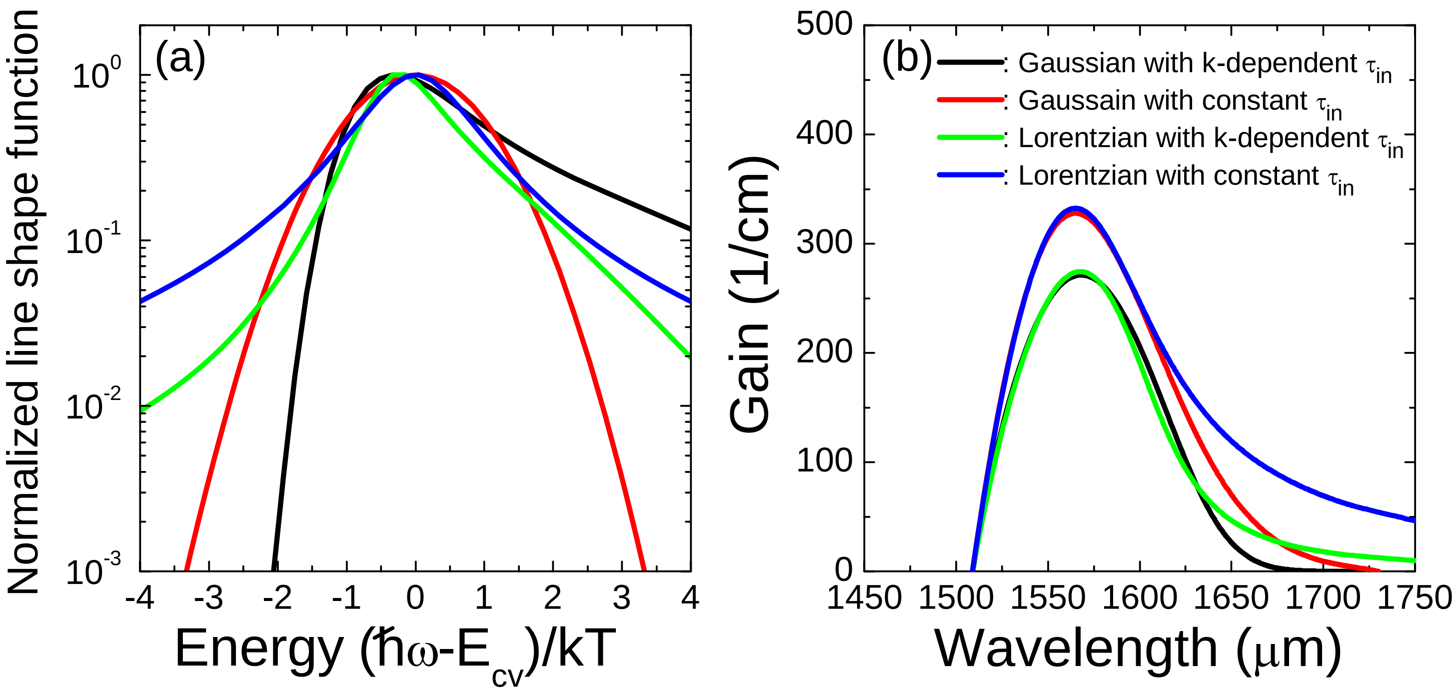
- In the case of small crystal angle, ZnO system has much larger optical gain than the GaN systems. This is because WZ ZnO/MgZnO QW structure has the larger matrix element and smaller effective mass than GaN-based QW structures near (0001) crystal orientation.
- On the other hand, in the case of the (1010) crystal orientation, InGaN/GaN QW structures show larger optical gain than ZnO/MgZnO QW structures due to the larger matrix element and the smaller effective mass.
- GaN/AlGaN : Crystal orientation effect is relatively small.

Summary

- The negligible internal field observed in the ZnO/MgZnO QW structure with small Mg compositions and thin well widths can be explained by the cancellation of total PZ and SP polarizations in the well and that in the barrier.
- In the case of (0001) crystal orientation, ZnO/MgZnO QW structure has much larger optical gain than the GaN-based QW structure.
- On the other hand, in the case of the (1010) crystal orientation, InGaN/GaN QW structure has larger optical gain than ZnO/MgZnO QW structures.
- GaN/AlGaN : Crystal orientation effect is relatively small.

Appendix

Line shape function



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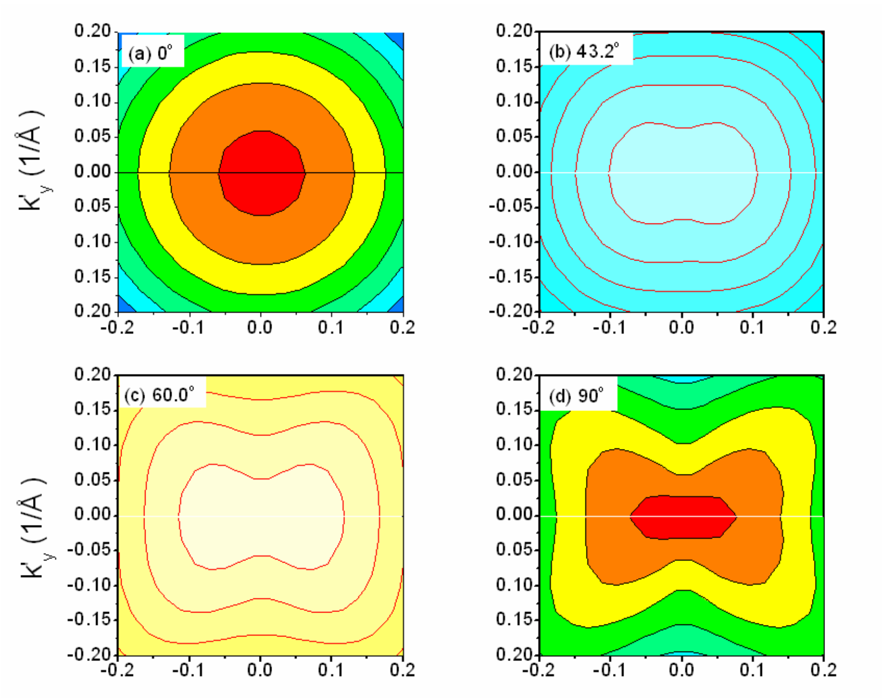
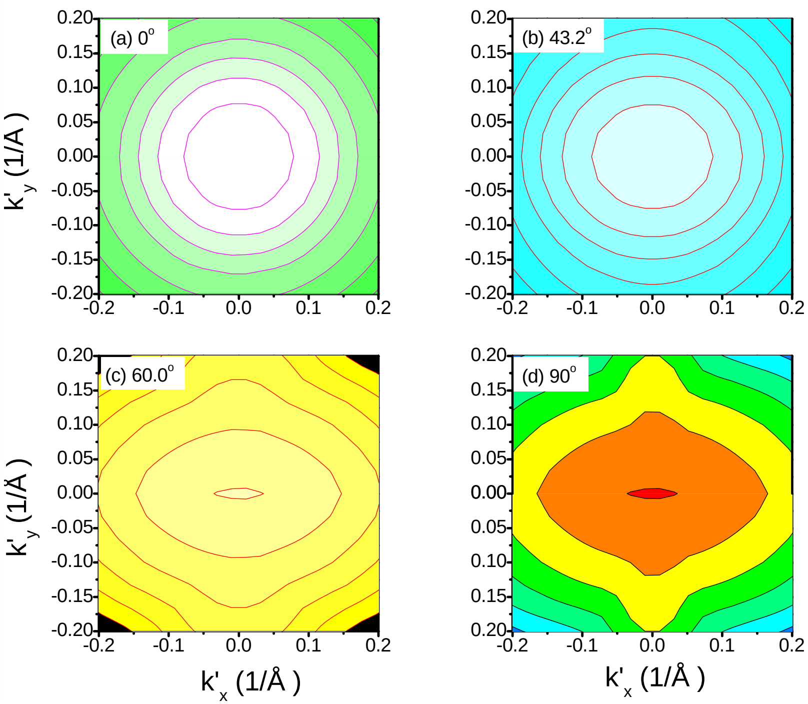
Constant energy contour



InGaN/GaN QW structure



ZnO/MgZnO QW structure

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