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Optical Gain of Wurtzite GaN/AlGaN Quantum Well Lasers

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Optical gain of wurtzite GaN/AlGaN quantum wells have been studied from a first-principles calculation by way of the $\mathbf{k}\cdot\mathbf{p}$ method. The most of the parameters in the $\mathbf{k}\cdot\mathbf{p}$ method were determined by fitting the band structures between the first-principles calculation and the $\mathbf{k}\cdot\mathbf{p}$ method. Owing to the small spin-orbit splitting energies of the wurtzite GaN and AlN, the optical gain has been calculated using the 6×6 Hamiltonian for the valence band. It is found that the large hole effective masses and the small spin-orbit splitting cause the higher threshold current density of wurtzite GaN/AlGaN quantum well lasers.

1. Introduction

Since high efficient short wavelength light emitting diodes (LEDs)[1] were successfully fabricated recently in terms of wurtzite GaN and related nitrides, the study of their laser diodes as the next step of the LED has been performed vigorously. Generally, most optical and transport phenomena involve only a small region of k-space centered around a particular wave number $\mathbf{k_0}$ which is an extremum. As a result, the physics of these systems is governed by the band structure in the immediate vicinity of $\mathbf{k_0}$. The $\mathbf{k}\cdot\mathbf{p}$ method is an appropriate approach not only to determine the electronic states but also to design quantum devices. The parameters in the $\mathbf{k}\cdot\mathbf{p}$ method are usually determined from measurements but the most of them for the Group-III nitrides have not been measured yet. Very recently, we have derived the unknown parameters of GaN and AlN by fitting the energy dispersions in terms of $\mathbf{k}\cdot\mathbf{p}$ method and the first-principles calculations[2]. In this paper, we have investigated the optical gain of wurtzite GaN/AlGaN quantum well structure using the $\mathbf{k}\cdot\mathbf{p}$ method with the parameters in terms of the first-principles calculation. The detail derivation of the parameters has been discussed in ref. 2. Since the spin-orbit splitting energies are less than 20 meV for AlN and GaN, we should construct the 6×6 effective Hamiltonian and have studied the valence subband structures. It is found that the large hole effective masses and the small spin-orbit splitting cause the higher threshold current density of wurtzite GaN/AlGaN quantum well laser diodes.

2. First-Principle Calculation and $\mathbf{k}\cdot\mathbf{p}$ Method

N atom has such a strong electron affinity that the valence charge of GaN and AlN tends to be localized. Therefore, conventional pseudo-potential method based on the plane wave is not adequate. Then, we have used the full-potential linearized augmented plane wave (FLAPW) method[3], within the local density functional approximation (LDA)[4]. Generally, the LDA gives reduced energy-gap,but the wavefunctions of LDA are not so changed, whether the correction is taken into account. Therefore, the mixing among the bands would be given correctly as long as the energy-gap is large. The $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian for the band edge near the Γ point of wurtzite structure is given by,

$$\mathbf{H}(\mathbf{k}) = \begin{pmatrix} \mathbf{H}_{cc} & \mathbf{H}_{cv} \\ \mathbf{H}_{cv}^{\dagger} & \mathbf{H}_{vv} \end{pmatrix}. \qquad (1)$$

$\mathbf{H}_{cv}$ indicates the direct interaction between the conduction band minimum (CBM) and the valence band maximum (VBM). $\mathbf{H}_{cc}$ and $\mathbf{H}_{vv}$ indicate the conduction band and the valence band without the interaction between CBM and VBM, respectively. The interactions among the other bands were treated as the second order perturbation. $\mathbf{H}_{cv}$ is given by,

$$\mathbf{H}_{cv} = \begin{pmatrix} Q & 0 & R & 0 & Q^* & 0 \\ 0 & Q & 0 & R & 0 & Q^* \end{pmatrix}, \qquad (2)$$

where

$$Q = \frac{1}{\sqrt{2}}\frac{\hbar}{m_0}\langle S|p_x|X\rangle(k_x + ik_y),$$

$$R = \frac{\hbar}{m_0}\langle S|p_z|Z\rangle k_z.$$

Note that $\mathbf{H}_{cv}$ includes $\langle S|p_i|i\rangle (i = x, y, z)$, which is related to the dipole matrix element. Owing to the large energy-gap of GaN and AlN, the 8×8 Hamiltonian can be splitted into the 2×2 Hamiltonian $\mathbf{H}'_{cc}$ for the conduction band and the 6×6 Hamiltonian $\mathbf{H}'_{vv}$ for the valence bands by renomalizing the matrix elements, treating $\mathbf{H}_{cv}$ as the second order perturbation. Then, the parameters in $\mathbf{H}'_{cc}$ and $\mathbf{H}'_{vv}$ were determined independently, by reproducing the band structres near the band edge. The valence bands are shown in Fig. 1. Table 1 indicates the effective masses of the conduction band and the valence bands. $||$ and $\perp$ mean the directions parallel and perpendicular to

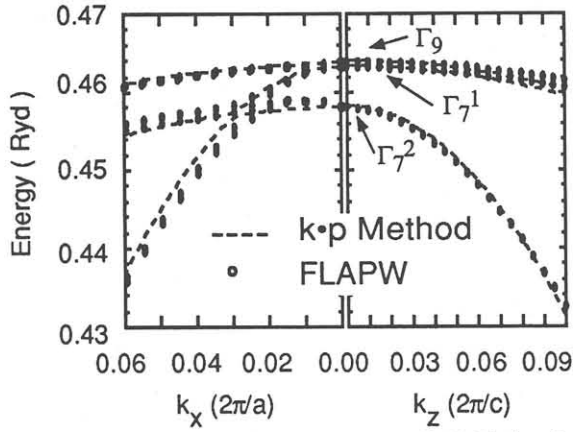

Fig. 1. Valence band structures of GaN by $\mathbf{k}\cdot\mathbf{p}$ method and FLAPW.

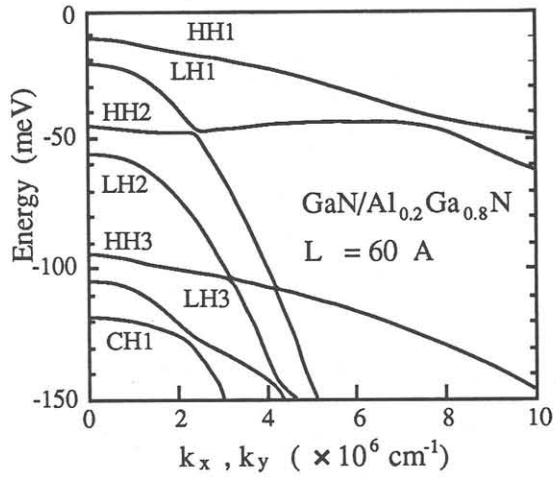

Fig. 2. Subband structures in k_x-k_y plane.

the c-axis, respectively. There are three bands, labeled Γ_9, Γ_7^1, and Γ_7^2 at the Γ point. The eigenstates are given by,

$$|\Gamma_9 \pm \frac{3}{2}\rangle = |X \pm iY, \pm\frac{1}{2}\rangle$$

$$|\Gamma_7^1 \pm \frac{1}{2}\rangle \sim |X \pm iY, \mp\frac{1}{2}\rangle$$

$$|\Gamma_7^2 \pm \frac{1}{2}\rangle \sim |Z, \pm\frac{1}{2}\rangle,$$

when $\Delta_{so} \sim 0$. According to the calculated parameters, Δ_{so} is such a small value of 16 meV that above approximatison is reasonable. Therefore, in the k_z direction, the conduction band is strongly coupled with the only Γ_7^2 state through $k_z p_z$ perturbation and it causes the only Γ_7^2 hole mass to be light. On the other hand, in the k_x direction, the conduction band is strongly coupled with the Γ_9 and Γ_7^1, but the only one of states, which is a linear combination between them ($|\Gamma_9 \pm \frac{3}{2}\rangle + |\Gamma_7^1 \mp \frac{1}{2}\rangle \sim |X\rangle$), is coupled. Then, only one mixed band at the finite wavenumber has small effective hole mass.

When the heterojunction is perpendicular to the $c-$axis, k_z becomes an operator in $\mathbf{H}'_{cc}$ and $\mathbf{H}'_{vv}$. The subband structures are evaluated by solving the matrix differncial eigenvalue problems. We will discuss it in detail elsewhere. Figure 2 shows the valence subband structures of $GaN/Al_{0.2}Ga_{0.8}N$ quantum well. The parameters in the calculation are shown in the Table 1. The band-offsets and the other parameters in ternary layer are determined by the virtual crystal approximation. The band off-set ΔE_v between GaN and AlN was 0.82 eV by the first-principles calculation. This value is merely derived from the energy difference of the Γ_9s between GaN and AlN . The quantum well length is 60 $\AA$. Here we labeled the subbands as HH_i (Γ_9:heavy hole), LH_i (Γ_7^1:light hole) and CH_i (Γ_7^2:crystal field splitting), whose naming corresponds to the case in k_x-k_y plane. Note here that the subband energy dispersions have similar characteristics of bulk ones. As a result, there are strong mixings but the nonparabolicity of the dispersion are weak. Then, the effective hole masses in k_x-k_y plane are approximately given by $m_{\rm HH} \sim 1.6$ and $m_{\rm LH} \sim 0.15$, respectively. These are the same as the bulk masses. Generally, this property would be observed for the other Group-III nitrides materials since the spin-orbit coupling in a N atom is not dominant. As for the CH subbands, the CH_1 is weakly coupled with LH_2. Thus, $m_{\rm CH}$ is still heavy. This weak coupling modifies the only HH_2 subband compared with HH_1 and HH_3 at $k \sim 6 \times 10^6 cm^{-1}$ due to the same space parity of the HH_1 and HH_3 envelope functions.

3. Optical Gain

In order to calculate the optical gain, the momentum matrix element should be evaluated. From eq. 1, it is derived analytically as,

$$P^2 = \hbar^2\left(\frac{1}{m_e^*} - \frac{1}{m_0}\right)\frac{(E_g + \Delta_{cr} + \Delta_{so})E_g + \frac{2\Delta_{cr}\Delta_{so}}{3}}{2(E_g + \frac{2}{3}\Delta_{so})}, \quad (3)$$

where Δ_{cr} is the crystal field splitting energy. On the other hand, P can be evaluated from the first-principles calculation, by fitting the energy dispersion near the band edge from the 8 × 8 Hamiltonian to the first-principles calculation result. For GaN, both values are 1.08 Ryd$\hbar^2/2m_0$ from eq. (3) and 0.96 Ryd$\hbar^2/2m_0$ from first-principles calculation. Thus, eq. (3) is the very reliable expression of the momentum matrix element.

The optical gain in terms of the interband transition between the conduction subbands and the valence subbands of GaN/AlGaN quantum well has been calculated, using the above momentum matrix elements. Figure 3 shows the maximum gain as a function of the carrier density in the wells, comparing with the similar structures of the $GaAs/Al_{0.4}Ga_{0.6}As$ and

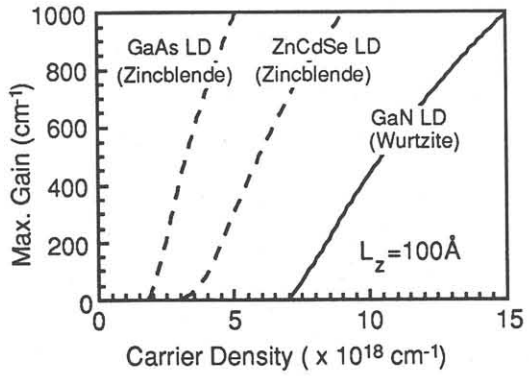

Fig. 3. Maximum gain as a function of carrier density.

$Zn_{0.8}Cd_{0.2}Se/ZnS_{0.06}Se_{0.94}$ quantum wells. The well length is 100 Å. It becomes evident that the treshold density of GaN/AlGaN quantum well lasers needs twice or more than that of the conventional ones, if their cavity losses and the optical confinments are not so different among them. This is mainly caused by the large hole effective masses and the small spin-orbit spiltting energy of the GaN/AlGaN quantum well.

In conclusions, we have studied on the optical gain of wurtzite GaN/AlGaN quantum wells, from the first-principles calculation by way of the $\mathbf{k}\cdot\mathbf{p}$ method. According to the calculated parameters, the wurtzite GaN/AlGaN quantum well structure has the large hole effective masses and the small spin-orbit spiltting energy. It cause the higher carrier density to obtaine the enough optical gain. To overcome this problem, the excitonic effect, propsed by the author[5], might be useful. Since the wide-gap materials have large exciton binding energies, excitonic effect can realize large optical gain with small carrier density, by adding a localized state in the energy-gap. We will discuss the strain effect for the optical gain as well.

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Table I. The effective masses of electron (a) and hole (b) for AlN and GaN. All values are in units of a free electron mass m_0.

(a)

	m_c^*	$m_c^{\parallel}$	$m_c^{\perp}$
AlN	0.27	0.33	0.25
GaN	0.18	0.20	0.18

(b)

	$m^{\parallel}_{\Gamma_9}$	$m^{\parallel}_{\Gamma_7^1}$	$m^{\parallel}_{\Gamma_7^2}$	$m^{\perp}_{\Gamma_9}$	$m^{\perp}_{\Gamma_7^1}$	$m^{\perp}_{\Gamma_7^2}$
AlN	3.68	3.68	0.25	6.33	0.25	3.68
GaN	1.10	1.10	0.15	1.65	0.15	1.10

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