Optical gain in GaN quantum wells with many-body effects

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Band-gap renormalization and Coulomb enhancement due to many-body effects have been studied for wurtzite quantum well structures. Considering the coupling between the chemical potential and the band-gap renormalization, we calculated the band-gap redshifts of a few valence subbands self-consistently in a GaN/ GaAlN quantum well structure using a nonparabolic band approach. We find that the renormalization not only produces redshift but also increases the quasi-Fermi-level separation relative to the effective band-gap. This causes an increase in optical gain for a given carrier density of about 40% compared with the free carrier model due to carrier redistribution by the band-gap renormalization similar to the enhancement by elastic stain. On the other hand, considering the angular dependence of the dipole matrix element, we have obtained an explicit expression for the Coulomb enhancement factor in wurtzite quantum well structures for the first time. Our results show that the band-gap renormalization is the dominant contribution to the optical gain enhancement rather than the "Coulomb/excitonic enhancement" in these structures. [S0163-1829(99)03847-3]

I. INTRODUCTION

Semiconductor lasers based on the wide, direct band-gap group-III nitrides have substantial application potential in light emitters ranging from blue-green to ultraviolet.¹⁻³ Since the first report of a pulsed operation in an In_xGa_{1-x}N quantum well (QW) laser diode (LD) in 1996, there has been much progress at the laboratory level. Now the continuouswave operating lifetime³ of blue-emitting $In_rGa_{1-r}N$ lasers is over 3000 h, though the material quality is still very poor compared with the material used in GaAs-based optoelectronic devices. A clear understanding of the optical processes in nitride materials is an important part of the effort to develop these devices. The transparency carrier density in nitride laser devices⁴ is around 10^{19} cm⁻³ and the exciton binding energy in bulk GaN is of order 30 meV. Both of these are significantly greater than in GaAs-based devices so the Coulomb interaction between carriers must have a significant effect on the optical properties.

There have been many papers published on many-body effects, for example, Refs. 5-9. We have studied the effects of band-gap renormalization and the angular dependence of dipole matrix element on the optical gain in wurtzite QW structures. The angular dependence has usually been ignored in earlier work, for example, Refs. 10-12, and our study suggests that this neglect may overestimate the Coulomb enhancement of the optical gain. We have also developed a much simpler approach for calculation of the optical gain including many-body effects. Our results suggest that bandgap renormalization by many-body effects may be the dominant contribution to the increase of the optical gain due to many-body effects in GaN-based QW structures.

The optical gain with many-body effects in semiconductors can be written as¹³

$$g = \frac{K}{2\hbar\varepsilon V} \sum_{\mathbf{k}} \frac{|\boldsymbol{\mu}_{\mathbf{k}}|^2}{1 - \mathbf{q}(\mathbf{k})} \frac{n_{e\mathbf{k}} + n_{h\mathbf{k}} - 1}{\gamma_{\mathbf{k}} + i(\omega_{\mathbf{k}} - \omega)}, \qquad (1)$$

where the Coulomb enhancement factor is given by

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$$\mathbf{q}(\mathbf{k}) = \frac{-i}{\hbar \mu_{\mathbf{k}}} \sum_{\mathbf{k}' \neq \mathbf{k}} V_{s,|\mathbf{k}'-\mathbf{k}|} \frac{\mu_{\mathbf{k}'}(n_{e\mathbf{k}'}+n_{h\mathbf{k}'}-1)}{\gamma_{\mathbf{k}'}+i(\omega_{\mathbf{k}'}-\omega)}$$
(2)

and where $1/\gamma_k$ is the scattering time of the carriers, μ_k is the dipole matrix element which is roughly proportional to the transition matrix element, $V_{s,q} = V_{s,|\mathbf{k}'-\mathbf{k}|}$ is the Fourier transform of the screened Coulomb potential, and $\hbar \omega_{\mathbf{k}}$ is the transition energy of the electron and hole, which is defined as

$$\hbar \omega_{\mathbf{k}} = \epsilon_{e\mathbf{k}} + \epsilon_{h\mathbf{k}} + \epsilon_{g0} + \Delta \epsilon_g. \tag{3}$$

Here, $\Delta \epsilon_g$ is the band-gap renormalization or self-energy due to the Coulomb interaction which can be written

$$\Delta \epsilon_g = \Delta \epsilon_{CH} + \Delta \epsilon_{SX}, \qquad (4)$$

where

$$\Delta \epsilon_{CH} = \sum_{q \neq 0} V_q [1/\varepsilon(q,\omega) - 1], \qquad (5a)$$

$$\Delta \epsilon_{SX} \cong -\sum_{\mathbf{k}'} V_{s,q} (n_{e\mathbf{k}'} + n_{h\mathbf{k}'}) \big|_{\mathbf{k}=0}.$$
 (5b)

 $\Delta \epsilon_{CH}$ is called Coulomb hole energy or the Debye shift and $\Delta \epsilon_{SX}$ is the screened-exchange shift, which in general is dependent on k. It is an acceptable approximation to use the value at $\mathbf{k} = 0.^{13}$

In Eq. (5a) $\varepsilon(q,\omega)$ is the dielectric function and the screened Coulomb potential:13

$$V_{s,q} = V_q / \varepsilon(q, \omega). \tag{6}$$

According to the single plasma-pole approximation:¹³

$$1/\varepsilon(q,\omega) = 1 + \omega_{\rm pl}^2 / [(\omega + i\gamma)^2 - \omega_q^2], \tag{7}$$

 $\omega_q^2 = \omega_{\rm pl}^2 (1 + q/\lambda) + (\hbar q^2/2m_r)^2$ for where twoа dimensional system. Here λ is the inverse static screening



FIG. 1. The valence-band structures in a 5-nm GaN/Al_{0.2}Ga_{0.8}N QW, (a) without band-gap renormalization and (b) with band-gap renormalization at carrier density of 1.5×10^{19} cm⁻³.

length and $1/\gamma$ is the scattering time of the system. It is common to use the static plasma-pole approximation which sets $\omega + i\gamma = 0$.⁷⁻¹³

In the following sections we consider first the band-gap renormalization and then the effect of Coulomb enhancement on the optical gain.

II. BAND-GAP RENORMALIZATION

Due to the Coulomb interaction between electrons and holes, the band gap is reduced, and this narrowing can be calculated by Eq. (4). In nitride lasers the transparency carrier density is very high, around 10^{19} cm⁻³, and the reduction of the band gap is reported experimentally to be as high as 150-200 meV in nitride devices.¹⁴ We have calculated the band structure for a single 5 nm GaN/Al_{0.2}Ga_{0.8}N quantum well by $\mathbf{k} \cdot \mathbf{p}$ theory using the basis function method,^{15,16} and the resulting valence bands are given in Fig. 1(a) without renormalization. The position of the quasi-Fermi-level is shown for 7.5×10^{12} cm⁻² (1.5×10^{19} cm⁻³) carriers in the well. When several valence bands are populated with carriers it is necessary to adopt a self-consistent iterative approach to determine the quasi-Fermi-levels and the renormalization energies because the renormalization of each band depends upon its respective carrier density, and the hole Fermi-level position at a given carrier density depends in turn upon the separation of the bands.^{17,18} In a GaN quantum well, the separations of the first few valence subbands are usually similar to the thermal energy $(k_B T)$ at room temperature so it is important that this iterative procedure is adopted.

The renormalized band structure, shown in Fig. 1(b) with the corresponding hole Fermi energy, has been calculated by this self-consistent, iterative approach for a carrier density of 7.5×10^{12} cm⁻² in the well using a nonparabolic band ap-



FIG. 2. TE gain spectra in a 5-nm $GaN/Al_{0.2}Ga_{0.8}$ QW at various carrier density (a) without band-gap renormalization and (b) with band-gap renormalization.

proach. Comparison with the free carrier model without renormalization indicates that the Fermi-level separation $(E_{Fe}-E_{Fh})$ relative to the effective band gap is increased when the self-consistent renormalization is considered. In the usual calculation the conduction and valence bands and their respective quasi-Fermi-levels move rigidly under renormalization, and the difference between the quasi-Fermi-level separation and the effective band-gap is unchanged. When the self-consistent iterative scheme is used in this case, the differences in carrier populations in each valence subband are such that the bands renormalize at different rates, resulting in a redistribution of the fixed total number of carriers amongst the bands and a shift in hole quasi-Fermi-level relative to the uppermost band.

The TE mode optical gain was calculated according to Eq. (1),¹³ including only band-gap renormalization [setting $\mathbf{q}(\mathbf{k})=0$], and the results are shown in Fig. 2. With the results based on the free carrier model being given in Fig. 2(a) for comparison, the results in Fig. 2(b) show the optical gain spectra for various carrier densities in the presence of the band-gap renormalization. The difference in the energy scales of the gain spectra in Figs. 2(a) and 2(b) are due to renormalization. At an injected carrier density of 7.5 $\times 10^{12}$ cm⁻² we obtained a reduction of 140 meV for the effective band gap of the GaN/Al_xGa_{1-x}N well, which is consistent with reported experimental data in Ref. 14.

In a simple model, rigid renormalization of the band gap does not change the magnitude of the gain for a fixed carrier density. Comparison of the two sets of gain spectra shows that the optical gain at a given carrier density is increased significantly when the renormalized band structure is considered. The threshold current of a Fabry-Perot laser is determined by value of gain at the peak of the spectrum, and this is increased by about 40% at a given carrier density. This behavior can be understood by reference to the Bernard-Durraforg condition for transparency, which indicates that the gain is controlled primarily by the difference between the separation of quasi-Fermi-levels ($E_{Fe}-E_{Fh}$) and the photon energy. The minimum photon energy is defined by the effective band gap so the gain is controlled by the difference between $E_{Fe}-E_{Fh}$ and the effective band gap. For a carrier density of 7.5×10^{12} cm⁻², band-gap renormalization produces a 10 meV increase in $E_{Fe}-E_{Fh}$ relative to the effective gap, which, as noted above, increases the peak gain by about 40% compared with the free carrier model. This behavior arises because the redistribution of holes between the valence bands favor the uppermost band, which is also responsible for the TE mode gain. The process is similar to the enhancement of optical gain by elastic strain.

The results in Fig. 2(b) show that as the carrier density increases the effect of renormalization is for the energy of the gain peak initially to increase due to band filling, then to decrease as the rate of band-gap narrowing dominates over the effects of band filling. This behavior offers a means to test our calculations, but at the present time there is no data available for $GaN/Al_xGa_{1-x}N$ QW structures. We may expect similar behavior in other nitride-based systems, such as in $In_xGa_{1-x}N$ QW structures, and there are some experimental data published¹⁹ which shows a similar trend to that predicated here.

The increase in the calculated gain in Fig. 2(b) arises solely from the changes in carrier distribution between valence bands as the results of different rates of band-gap renormalization. It does not include any effect due to the "Coulomb/excitonic enhancement" represented by the term $\mathbf{q}(\mathbf{k})$ in Eq. (1), which describes the increase in polarization of a paired electron and hole. While the overall effect of many-body interactions is, in principle, due to band-gap narrowing and Coulomb enhancement, we argue in the next section that the Coulomb enhancement is not significant for the wurtzite materials being considered here.

III. OPTICAL GAIN IN QUANTUM WELL STRUCTURES

In this section, we discuss the Coulomb enhancement of the optical gain in GaN quantum well structures in detail, considering the spin-orbit interaction and the angular dependence of dipole matrix element. According to the many-body theory, the Coulomb interaction produces an extra enhancement factor as in Eq. (2), and the optical gain is proportional to $1/[1-\mathbf{q}(\mathbf{k})]$ in the Padé approximation. The Coulomb enhancement factor linearly depends on the dipole matrix element $\mu_{\mathbf{k}}$, not only the magnitude of absolute value but also the relative phase angles of the wave functions of the paired electron and hole. As described below, we have considered the angular dependence for the heavy-hole (hh), light-hole (lh), and the crystal-field split-off hole (cs) in wurtzite material, and we find that the enhancement is reduced compared with the results when only the absolute value of the matrix element $|\mu_k|$ is used. The angular dependence of μ_k has often been ignored, and only the absolute value of $\mu_{\mathbf{k}}$ has been used in the literature.⁷⁻¹³ We show that this may overestimate the Coulomb enhancement, which has often predicted an increase in optical gain^{10-12,20,21} of 50% or more. We derive below an explicit expression for the Coulomb enhancement factor in wurtzite QW structures.

In wurtzite material, such as the nitrides, the band-edge wave functions of the valence bands can be written explicitly as^{22}

$$\begin{split} \mathrm{hh} \rangle &= -\left(\alpha^{*}/\sqrt{2}\right) |(X+iY)\uparrow\rangle + \left(\alpha/\sqrt{2}\right) |(X-iY)\downarrow\rangle, \\ |\mathrm{lh}\rangle &= \left(\beta/\sqrt{2}\right) |(X-iY)\uparrow\rangle - \left(\beta^{*}/\sqrt{2}\right) |(X+iY)\downarrow\rangle, \\ |\mathrm{cs}\rangle &= \beta^{*} |Z\uparrow\rangle + \beta |Z\downarrow\rangle, \end{split}$$
(8)

where

$$\alpha = e^{i3(\pi/4 + \phi/2)} / \sqrt{2}, \quad \beta = e^{i(\pi/4 + \phi/2)} / \sqrt{2},$$
$$\phi = \arctan(k_y / k_y).$$

These bands are doubly degenerate under the so-called "cubic approximation."²²

The band-edge wave functions of electron in the *s*-like conduction band can be described as $\langle S \uparrow |$ or $\langle S \downarrow |$ including the spin momentum. The dipole matrix elements in a QW structure can be represented as (writing explicit results for only the spin-up orientation $\langle S \uparrow |$ here, for more details see Refs. 22 and 23 and pp. 192–199 in Ref. 13): For the TE mode,

$$\mu_{\mathrm{TE}}(k,\phi) = \langle \Psi_{\mathbf{k}}^{e} | ex | \Psi_{\mathbf{k}}^{h} \rangle = [I_{\mathrm{hh}}(k) e^{-i3\phi/2} + I_{\mathrm{lh}}(k) e^{i\phi/2}] \\ \times \langle S \uparrow | ex | X \uparrow \rangle / 2$$
(9)

and for the TM mode,

$$\mu_{\rm TM} = \langle \Psi_{\mathbf{k}}^{e} | ez | \Psi_{\mathbf{k}}^{h} \rangle = I_{\rm cs}(k) e^{i\phi/2} \langle S \uparrow | ez | Z \uparrow \rangle /2.$$
(10)

 $I_{\rm hh}$, $I_{\rm lh}$, and $I_{\rm cs}$ represent the envelope function overlap integrals for the quantum confined heavy holes, light holes, and crystal-field split-off holes with the electrons in conduction band, respectively, with the wave functions calculated by $\mathbf{k} \cdot \mathbf{p}$ theory using the basis function method.

In a QW structure, the Coulomb enhancement factor in Eq. (2) can be explicitly written to include the angular dependence:

$$\mathbf{q}(k,\phi) = \frac{-ie^2}{8\pi^2 \varepsilon \hbar \,\mu(k,\phi)} \int dk' \,k' \frac{f_{ek'} + f_{hk'} - 1}{\gamma_{k'} + i(\omega_{k'} - \omega)} \\ \times \int_0^{2\pi} d\phi' \frac{\mu(k',\phi')}{q\varepsilon(q,0)}, \tag{11}$$

where $q = |\mathbf{k} - \mathbf{k}'| = \sqrt{k^2 + k'^2 - 2k k' \cos \theta}$ and $\theta = (\phi - \phi')$. Substituting Eqs. (9) and (10) into Eq. (11), we can obtain

the enhancement factor for the TE mode:

$$q_{\rm TE}(k,\phi) = \frac{I_{\rm hh}(k) \, q_1(k,\phi) + I_{\rm lh}(k) q_2(k,\phi) e^{i2\phi}}{I_{\rm hh}(k) + I_{\rm lh}(k) e^{i2\phi}}, \quad (12)$$

where

$$q_{1}(k,\phi) = \frac{-ie^{2}}{8\pi^{2}\varepsilon\hbar I_{\rm hh}(k)}$$

$$\times \int dk'k' I_{\rm hh}(k') \frac{f_{ek'} + f_{hk'} - 1}{\gamma_{k'} + i(\omega_{k'} - \omega)}$$

$$\times \Psi(k,\phi,k',-\frac{3}{2})$$
(13)

and

$$q_{2}(k,\phi) = \frac{-ie^{2}}{8\pi^{2}\varepsilon\hbar I_{\rm lh}(k)} \\ \times \int dk' \, k' I_{\rm lh}(k') \frac{f_{ek'} + f_{hk'} - 1}{\gamma_{k'} + i(\omega_{k'} - \omega)} \\ \times \Psi(k,\phi,k',\frac{1}{2}).$$
(14)

For the TM mode:

$$q_{\mathrm{TM}}(k,\phi) = q_{3}(k,\phi) = \frac{-ie^{2}}{8\pi^{2}\varepsilon\hbar I_{\mathrm{cs}}(k)}$$

$$\times \int dk'k' I_{\mathrm{cs}}(k') \frac{f_{ek'} + f_{hk'} - 1}{\gamma_{k'} + i(\omega_{k'} - \omega)}$$

$$\times \Psi(k,\phi,k',\frac{1}{2}). \tag{15}$$

Here, $\Psi(k, \phi, k', -3/2)$ and $\Psi(k, \phi, k', 1/2)$ are represented by

$$\Psi(k,\phi,k',m/2) = \int_{-\phi}^{2\pi-\phi} d\theta \frac{e^{im\theta/2}}{q\varepsilon(q,0)}.$$
 (16)

To demonstrate our approach, for the sake of simplicity, we here only discuss the TM mode. For the spin-up states $\langle S \uparrow |$, the Coulomb enhancement factor is

$$q_{\rm TM} = q_r + iq_I \tag{17}$$

for the spin-down states $\langle S \downarrow |$, the dipole matrix element and Coulomb enhancement factor are

$$\mu_{\rm TM}(k,\phi) = I_{\rm cs}(k) e^{-i\phi/2} \langle S \downarrow | ez | Z \downarrow \rangle/2, \qquad (18)$$

$$q_{\rm TM} = -q_r + iq_I, \tag{19}$$

where

$$q_{r} = \frac{-e^{2}}{2\pi^{2}\varepsilon\hbar} \int dk' \times \left(k' \frac{I_{cs}(k')}{I_{cs}(k)} \frac{f_{ek'} + f_{hk'} - 1}{\gamma_{k'} + i(\omega_{k'} - \omega)} \int_{0}^{\cos(\phi/2)} dy \frac{1}{Y\varepsilon(Y,0)} \right),$$
(20)

$$Y = \sqrt{(k+k')^2 - 4k \, k' y^2},$$

$$q_{I} = \frac{-e^{2}}{2\pi^{2}\varepsilon\hbar} \int dk' \\ \times \left(k' \frac{I_{cs}(k')}{I_{cs}(k)} \frac{f_{ek'} + f_{hk'} - 1}{\gamma_{k'} + i(\omega_{k'} - \omega)} \int_{0}^{\sin(\phi/2)} dx \frac{1}{X\varepsilon(X,0)}\right),$$

$$(21)$$

$$X = \sqrt{(k-k')^{2} + 4kk'x^{2}}.$$

We see that the real parts of the enhancement factor for the spin up and spin down are of opposite sign. It therefore appears as if there is an increase in optical gain for one spin orientation (e.g., spin up) and decrease for the other orientation, which should not be so because the spin-orbit interaction does not split the double degeneracy. However, if we consider any particular magnitude of k, the optical enhancement should be integrated over all directions (ϕ), thus

$$g_{\rm TM} \propto \int dk \, (k \cdots) \int_0^{2\pi} d\phi \{ 1/[1 - q_{\rm TM}(k, \phi)] \}$$
$$\cong \int dk (k \cdots) \int_0^{2\pi} d\phi (1 + q_r + iq_I + q_r^2 - q_I^2 + \cdots).$$
(22)

We note that

$$\int_{0}^{2\pi} d\phi(q_r)^{2n+1} = 0 \tag{23}$$

because of the symmetry feature of q_r in ϕ ; therefore only the even terms of q_r contribute to the enhancement, and this removes the difference between the spin-up and spin-down orientations.

We can now obtain the first nonzero approximation for the optical gain:

$$g_{\rm TM} \propto \int dk (k \cdots) \int_0^{2\pi} d\phi \{ 1/[1 - (q_r^2 - q_I^2)] \}$$
 (24)

since the first term of q_I mainly contributes to the imaginary part of the complex optical gain, relating to the index change, and the contributions from higher-order terms are very small. The results are the same for the spin-up and -down orientation, which is as expected since the spin-orbit coupling does not split the double degeneracy. On the basis of Eq. (24), the overall Coulomb enhancement can be approximately described as

$$g \propto 1/(1-\mathbf{q}^2). \tag{25}$$

The above result does not depend on any particular dielectric function and it merely results from the consideration of the angular dependence of the dipole matrix element. The form obtained here [Eq. (25)] contrasts with that which is conventionally used:¹³

$$g \propto 1/(1-\mathbf{q}). \tag{26}$$

Using this form the Coulomb enhancement is overestimated compared with the result obtained here by including the angular dependence of the dipole matrix element. For example,

and

when Eq. (26) gives an enhancement of 50%, our result with the angular dependence consideration in Eq. (25) predicts only about a 10% increase in the optical gain. It is more complicated for the TE mode; however, the results are similar. There were some theoretical calculations^{11,12} which gave a 30-50 % increase in the optical gain in GaN QW structures using the conventional model. We can only obtain an optical gain enhancement of a few percent when the angular dependence is considered as above. Comparing the 40% increase by the band-gap renormalization shown in the previous section, we therefore conclude that the increase in optical gain due to redistribution of holes by renormalization is more important than the increase due to Coulomb/excitonic enhancement of the dipole (or transition) matrix element per *e*-*h* pair. Our treatment for the "Coulomb enhancement factor" can be extended to cubic phase semiconductors, including bulk materials. We also expect a similar treatment can be adopted in the more advanced theory which is introduced by Chow and co-workers.^{24–26} They dealt with the carrier collision effects at the level of quantum kinetic theory in the semiconductor Bloch equations, but the Coulomb enhancement was treated in conventional way as in Eq. (26). It has also been suggested that the band-gap renormalization might be reduced according to this theory. Supposing the band-gap renormalization is halved, we then obtain an optical gain increase of about 20% at a carrier density 1.5×10^{19} cm⁻³. The Coulomb enhancement factor is expected to follow the reduction of the renormalization as they are both controlled by the quasi-Fermi-level separation; see Eqs. (1) and (2). We can see that the increase in gain by the renormalization is still greater than the Coulomb enhancement according to the calculation presented here.

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IV. SUMMARY

We have examined the effects of many-body interactions on the optical gain of the wurtzite QW structures in detail, and the spin-orbit interaction and the angular dependence of dipole (or transition) matrix elements have been considered for the first time to our knowledge. By including the angular dependence of the dipole matrix elements, we were able to obtain an explicit expression for the Coulomb enhancement in wurtzite QW structures. The form which we have derived gives a smaller enhancement of the gain than the expressions commonly used in the literature. We have also considered band-gap renormalization in these structures by a selfconsistent iterative approach and find that there is an increase in the quasi-Fermi-level separation relative to the effective band gap because the different rates of the renormalization result in redistribution of holes between the various valence bands. This strong renormalization process causes a redshift of the gain peak with increasing carrier density and causes a significant increase in peak optical gain. When combined with our analysis of the Coulomb enhancement process, our calculation suggests that the dominant many-body effect on the optical gain of these structures is carrier redistribution due to renormalization rather than "excitonic/Coulomb enhancement" of the dipole (or transition) matrix element.

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