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Kyoto University
Carrier Transport and Optical Properties of InGaN SQW With Embedded AlGaN δ-Layer

Jongwoon Park, Akio Kaneta, Mitsuru Funato, and Yoichi Kawakami

Abstract—We investigate the carrier transport and optical properties of a thick InGaN single quantum well (SQW) where an AlGaN δ-layer is embedded. By way of simulation, it is found that the carrier density distribution in the active region is more uniform in such a QW structure, compared to a double QW (DQW) configuration showing a discontinuity in the hole quasi-Fermi level due to the large effective mass of the holes along with the strong piezoelectric field. Through the photoluminescence (PL) measurements, we have shown that the PL peak energy varies depending sensitively on the δ-layer thickness, providing an extra degree of freedom in the wavelength-tuning control. In particular, such a QW structure is highly desired for long-wavelength emission as the wavelength tuning can be achieved with lower indium composition. The embedded δ-layer also increases the wave function overlap between holes and electrons, thereby shortening the PL lifetime. The results of PL measurements are shown to be consistent with the self-consistent numerical results. A possible application of the proposed QW structure is to the design of long-wavelength light-emitting diodes and laser diodes.

Index Terms—AlGaN, carrier transport, delta layer, InGaN, photoluminescence, piezoelectric charge, wave function.

I. INTRODUCTION

THE wide bandgap III–nitride semiconductor materials are of great importance for many semiconductor device applications in lighting [1], [2], full-color display, optical storage, medical applications [3], etc. Despite the tremendous efforts in the growth, the poor crystal quality due to high dislocation densities and the strong piezoelectric field effects induced by large lattice mismatch are still the main limiting factors for their applications [4], especially to InGaN-based long-wavelength (green and red) light-emitting devices that are highly demanded for full-color displays. For long-wavelength tuning, one has to inevitably increase the quantum-well (QW) thickness and/or the indium content. With thick QWs, however, we are faced with a situation where the strong piezoelectric field reduces dramatically the oscillator strength [5], resulting in a decrease of the internal quantum efficiency; whereas several defects such as V-defects, stacking faults, and dislocations [6] are parasitic in QWs with high indium content, causing high nonradiative recombination. Consequently, the threshold current density of laser diodes increases as the emission wavelength increases. Nakamura et al. [7] found that an InGaN-based QW structure with two QWs gave rise to the lowest threshold current for near 400-nm lasers. They also found [8] that for lasers with longer emission wavelength (>435 nm), a structure with only one QW [i.e., single QW (SQW)] showed the lowest threshold current density. The generation of lasing oscillation was not even feasible beyond 475 nm [9] due mainly to the deterioration of the crystal quality. Those defect centers appearing in light-emitting diodes (LEDs) also bring on high sensitivity of device performances to the temperature [10]. With increasing temperature, the decrease in output power for LED with a higher In composition in the multiple QW (MQWs) was higher than that of LED with a lower In content in the MQWs. To make matters worse, the carrier distribution over the QWs is highly nonuniform [11], [12] due to large valence-band offset and low mobility of the holes, which is also crucial for laser performance.

To overcome such pitfalls, we propose a novel QW structure based on a thick InGaN SQW in which an AlGaN δ-layer is embedded. We first investigate the carrier transport property of the QW structure by solving Poisson’s equation and the drift-diffusion equation iteratively. We then analyze the optical [photoluminescence (PL)] properties of the QW structure by time-resolved PL (TRPL) spectroscopy. The effects of varying the In mole fraction of the QWs and the AlGaN δ-layer thickness are also investigated. For a systematic study, we have further solved the effective-mass Schrödinger equation. A numerical investigation of the band structure and material gain offers a clear understanding with regard to the optical behaviors of the QW structures. In the model, the strain effects of those wurzite semiconductor materials are considered and the piezoelectric sheet charge density is incorporated in Poisson’s equation so that the phenomena such as the tilt of the energy band, the spatial separation of electrons and holes, and the charge screening by the injected carriers are all captured. The composition distribution in the QWs is assumed to be homogeneous for simplicity.

This paper is organized as follows. In Section II, the numerical model for the simulation of III–nitride semiconductors is briefly described. Simulation and measurement results, e.g., the carrier transport, PL intensity, and PL decay dynamics, are presented and analyzed in Section III. Finally, a conclusion is drawn in Section IV.

II. MODEL AND IMPLEMENTATION

Built-in interface charge due to spontaneous and piezoelectric polarizations in the GaN material system is incorporated in Poisson’s equation written as [13]

$$\nabla \cdot (\varepsilon \nabla \psi) = -\mathbf{q} (n + N_D - N_A) - \rho_{\text{pi}}$$

(1)
where the variable $\psi$ represents the electrostatic potential, $n$ and $p$ the electron and hole densities, respectively, $N_D$ and $N_A$ the donor and acceptor impurity concentrations, respectively, and $\rho_{pol}$ the polarization charge density given as

$$\rho_{pol} = -\frac{\partial}{\partial x} \left[ e_33 \varepsilon_\perp (x) + 2e_31 \varepsilon_\parallel (x) + P_{sp}(x) \right] \quad (2)$$

where

$$\varepsilon_{\parallel}(x) = \frac{a_{sub} - a(x)}{a(x)} \quad \text{and} \quad \varepsilon_{\perp}(x) = -2\varepsilon_\parallel(x) \frac{C_{13}}{C_{33}} \quad (3)$$

defined as the strain components parallel and perpendicular to the QW plane, respectively. $e_{ij}$ are the coefficients of the piezoelectric tensor and $P_{sp}(x)$ is the spontaneous polarization.

All the parameter values are adopted from [13]. Equation (1) is solved by Newton–Raphson iteration on a finite difference approximation [14], [15]. The piezoelectric field generates the sheet charge density at the interface between a QW and a barrier. By increasing the injection current, however, the piezoelectric field is cancelled out by the free-carrier-induced field [16]. Such a charge screening effect is naturally captured in the model.

The carrier transport in the active region can be described by the following drift-diffusion equation for electrons and holes [15]

$$\frac{\partial n}{\partial t} = \frac{q}{q} \nabla \cdot (\psi \mu_n \nabla \phi_n) + \frac{G - R}{q} \quad (4a)$$

$$\frac{\partial p}{\partial t} = \frac{q}{q} \nabla \cdot (\psi \mu_p \nabla \phi_p) + \frac{G - R}{q} \quad (4b)$$

$$n = n_i \exp \left\{ \left( \psi + \theta - \phi_n \right) / \sqrt{\gamma} \right\} \quad (4c)$$

$$p = p_i \exp \left\{ \left( \phi_p - \left( \psi + \theta - \phi_p \right) / \sqrt{\gamma} \right\} \quad (4d)$$

where the variable $\mu_n$ denotes the electron mobility, $\mu_p$ the hole mobility, and $\phi_n$ and $\phi_p$ the quasi-Fermi potentials for electrons and holes, respectively. All the other parameters are the same as defined in [15] where a detailed implementation is also introduced. To facilitate the numerical calculation, the differential equation (4) is discretized with the box integral discretization scheme [15]. The band-offset ratio ($\Delta E_c/\Delta E_v$) of InGaN–GaN and AlGaN–GaN is assumed to be 0.7/0.3 [17] and 0.67/0.33 [11], [18], respectively. The bandgap energy and the material parameter values such as the refractive index and the electron and hole mobilities used in our simulation are the same as presented in [18]. The effective masses of electrons and holes are adopted from [11].

For the calculation of the band structure and material gain of the QW structure, we have also solved the effective mass Schrödinger equation [19]–[21] expressed as for the valence band

$$\sum_{j=1}^{6} (H_{ij} + \delta_{ij}E^v(z)) \phi_{m}^j(z) = E_{m}^v \phi_{m}^j(z), \quad i = 1, 2, \ldots, 6 \quad (5)$$

with the $6 \times 6$ effective-mass Hamiltonian defined as

$$H_{6 \times 6} = \begin{bmatrix} H_U & 0 \\ 0 & H_L \end{bmatrix} \quad (6)$$

where $H_U$ and $H_L$ are 3 $\times$ 3 matrices with the relation of $H_U = (H_L)^*$, and

$$H_U = \begin{bmatrix} F & K_t & -iH_t \\ K_t & G & \Delta + iH_t \\ iH_t & \Delta + iH_t & \lambda \end{bmatrix} \quad (7)$$

$$F = \Delta_1 + \Delta_2 + \lambda + \theta$$

$$G = \Delta_1 - \Delta_2 + \lambda + \theta, \quad \Delta = \sqrt{\Delta_3}$$

$$\lambda = \frac{\hbar^2}{2m_0} \left( A_1 k_z^2 + A_2 k_t^2 \right) + D_1 \varepsilon_{zz} + D_2 (\varepsilon_{xx} + \varepsilon_{yy})$$

$$\theta = \frac{\hbar^2}{2m_0} \left( A_3 k_z^2 + A_4 k_t^2 \right) + D_3 \varepsilon_{zz} + D_4 (\varepsilon_{xx} + \varepsilon_{yy})$$

$$K_t = \frac{\hbar^2}{2m_0} A_5 k_t^2, \quad H_t = \frac{\hbar^2}{2m_0} A_6 k_z k_t \quad (8)$$

for the conduction band

$$\left[ \frac{n^2}{2} \left( \frac{k_z^2}{m_e^*} + \frac{k_t^2}{m_h^*} \right) + E^c(z) \right] \varphi_n(z) = E_{m}^c \varphi_n(z). \quad (9)$$

The valence ($E^v(z)$) and conduction ($E^c(z)$) band edge profiles appearing in (5) and (9) are obtained after solving Poisson’s equation (1) and conventional drift-diffusion equation (4). Therefore, the effect of free-carrier screening is also considered in the calculation of quantum energy levels. To calculate the energy levels of the valence ($E^v_{m}$) and conduction ($E^c_{m}$) bands and the associated wave functions of $\varphi_m(z)$ and $\varphi_n(z)$, (5) and (9) are spatially discretized with a standard central differencing scheme and solved with the inverse power method [22]. All the parameter values and more detailed descriptions are available in [19]–[21].

The optical gain is calculated by [20], [21]

$$g(\hbar\nu) = g_{sp}(\hbar\nu) \left[ 1 - \exp \left( \frac{\hbar\nu - \Delta F}{kT} \right) \right] \quad (10a)$$

$$g_{sp}(\hbar\nu) = \frac{q^2 \pi}{n_\tau \varepsilon_0 m_e^* m_h^*} \sum_{\sigma=\pm} \sum_{i=1}^{L} \int \frac{k_d dk_t}{2\pi} \left( M_{\sigma} \gamma_{m}(k_t) \right)^2 \times f_{\sigma m}(k_t) \left[ 1 - f_{\sigma m}^v'(k_t) \right] \frac{\hbar \gamma}{\pi} \times \frac{[E^v_{\sigma m}(k_t) - \hbar\nu]^2 + (\hbar \gamma)^2}{(\hbar \gamma)^2} \quad (10b)$$
with the TE-polarized matrix element express as

$$
|M_x^{nm}(k_L)|^2 = \left|\frac{\langle S|x|X\rangle^2}{4} \left\{ \langle \varphi_n^{(1)}|\varphi_m^{(1)} \rangle^2 + \langle \varphi_n^{(2)}|\varphi_m^{(2)} \rangle^2 \right\} \right|^2,
$$

for $\sigma = U$ \hspace{1cm} (11a)

$$
|M_x^{nm}(k_L)|^2 = \left|\frac{\langle S|x|X\rangle^2}{4} \left\{ \langle \varphi_n^{(4)}|\varphi_m^{(4)} \rangle^2 + \langle \varphi_n^{(5)}|\varphi_m^{(5)} \rangle^2 \right\} \right|^2,
$$

for $\sigma = L$. \hspace{1cm} (11b)

All the variables appearing in (10) and (11) are the same as defined in [20] and [21].

In our model based on the conventional bulk carrier transport equations [15], the effect of quantum carrier capture [23] is neglected. Therefore, the carrier density in the lowest bound states calculated by it could be a little overestimated. Even so, we have used the bulk carrier transport model combined with the effective mass Schrödinger equation, since the effect of the delta-layer on the overall carrier transport, especially in the presence of piezoelectric charges, is our main concern in this work. As mentioned, this model is indeed capable of capturing the piezoelectric field effect and the screening effect as well, which are key issues in GaN-based semiconductor devices.

### III. RESULTS AND DISCUSSION

InGa−GaN SQW samples were grown on (0001) sapphire substrates by metal–organic vapor phase epitaxy (MOVPE). In the QW structure shown in Fig. 1, a 1-nm-thick AlGaN δ-layer is embedded in the center of a 5-nm-thick InGaN QW (i.e., 2 nm In$_{0.16}$Ga$_{0.84}$N − 1 nm Al$_{0.05}$Ga$_{0.95}$N − 2 nm In$_{0.16}$Ga$_{0.84}$N). The indium composition and overall well thickness are measured to be 16% and 4 nm (±2 nm − In$_{0.10}$Ga$_{0.87}$N + 2 nm − In$_{0.16}$Ga$_{0.84}$N), respectively, by the x-ray rocking curve analysis. The AlGaN δ-layer was grown at the same growth temperature as the InGaN QW layer. Low (740 °C) and high (1320 °C) temperature deposited GaN buffer layers were used to enhance the quality of uppergrown barriers and QWs. The samples have an undoped SQW that is sandwiched between 6.2-nm-thick GaN barriers. In the PL measurement, they were excited with 1.5 ps pulses from a frequency-doubled Ti:sapphire laser. The laser wavelength is 400 nm and the repetition rate is 80 MHz. All measurements were carried out at 13 K.

#### A. Carrier Transport Property

The carrier transport to the QWs plays an important role in the spontaneous emission efficiency and thus laser performance. Ignoring the piezoelectric charges in the simulation [11], the hole
distribution over three In$_{0.25}$Ga$_{0.75}$N — In$_{0.02}$Ga$_{0.98}$N QWs for 461-nm lasers is very uniform. In the presence of piezoelectric charges, however, we have found that the holes have difficulty in entering the QWs due to their large effective mass. Consequently, the hole distribution is highly inhomogeneous with lower concentration in the $n$-side QW (the right-hand side of the diagram) as evident in Fig. 2, showing the energy band profile and carrier distribution in the active region consisting of two 2-nm-thick In$_{0.16}$Ga$_{0.84}$N QWs separated by a 7-nm-thick Al$_{0.05}$Ga$_{0.95}$N barrier. We can clearly see the discontinuity in the hole quasi-Fermi level ($F_h$) in both QWs, implying a difficulty in the hole transport. Due to the large conduction band offset, the electron distribution is also nonuniform with lower concentration in the $p$-side QW (the left-hand side of the diagram). The partial charge screening effect by the injected carriers is thus observed in the $n$-side QW. Such an inhomogeneous carrier distribution could be one of the main reasons that the lowest threshold current density is achieved when the number of QWs is only one (i.e., SQW) for the lasing wavelengths longer than 435 nm [8], [12]. If one has to use a thin SQW for the reason, however, the temperature and the current overflow in the active region would be issues for high current injection [12], since the carriers are overcrowded in the active region and the confinement factor of the SQW is very low, which is in proportion to the active layer thickness.

In the proposed QW structure where a 1-nm-thick AlGaN $\delta$-layer is embedded in the center of a 5-nm-thick InGaN SQW, however, the discontinuity in $F_h$ has disappeared as shown in Fig. 3. As a result, highly uniform carrier distribution is observed. Furthermore, the charge screening effect is more pronounced in both QWs. It is apparent that the carrier distribution is getting inhomogeneous with increasing emission wavelength due to increased indium content (i.e., increased band offset). From the simulation results, therefore, it is our natural expectation that the threshold current density may be much lowered for long-wavelength lasers based on such a QW structure, since the internal quantum efficiency of spontaneous emission may increase by virtue of the uniform carrier distribution in the active region. In addition, one may be released from the concerns related to the temperature and the current overflow that could be issues in a SQW structure unavoidably employed for long-wavelength emission under high bias current.

B. Optical Properties: PL Intensity and PL Decay Dynamics

In the proposed QW structure, a coupling between QWs exists in the sense that the $\delta$-layer can be regarded as a very...
thin barrier. Namely, the QW structure is similar to a DQW system with a very thin AlGaN barrier. In order to perceive the optical behaviors of such a QW structure, we have first calculated the in-plane subband dispersion for different δ-layer thicknesses and presented the results in Fig. 4. For a comparative study, we have also calculated the band structures of 2-nm-thick and 4-nm-thick SQWs without a δ-layer. As seen in Fig. 4, the lowest conduction subband (C1) of the 2-nm-thick SQW is split into two subbands in the QW with the δ-layer. The separation increases further with decreasing δ-layer thickness. In the end, when the δ-layer thickness is zero, those separated subbands become the subbands (C1 and C2) of the 4-nm-thick SQW, a phenomenon known as the effect of a well coupling. Similar behavior also appears in the valence band; namely, those four subbands split from the HH1 and LH1 subbands of the 2-nm-thick SQW eventually become the HH1, LH1, HH2, and LH2 subbands of the 4-nm-thick SQW. Therefore, the transition energy of the
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-\layer thickness. We
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In
\(nm\)\)
\(N\ SQW\)
\(In\)
\(N\)-layer embedded in
\(N\)-layer
\(eV,\)
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\(-\layer\)
\(N\ SQW\)
\(In\)
\(N\)-layer
\(eV,\)
\(2n\ m\)
\(N\ SQW\)
\(QW\)
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,
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-\layer thicknesses in the absence of
undoped
4-nm-thick
\(In_{0.16}Ga_{0.84}N\)\ SQW\((-\triangle-),\)
\(In_{0.16}Ga_{0.84}N\)\ (2 nm) –
\(A_{0.05}Ga_{0.95}N\)\ (1 nm)–\(In_{0.16}Ga_{0.84}N\)\ (2 nm)\ QW\((-\square-),\)
and
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Fig. 5. Low-temperature (13 K) continuous-wave PL spectra of nominally
undoped 4-nm-thick
\(In_{0.16}Ga_{0.84}N\)\ SQW\((-\triangle-),\)
\(In_{0.16}Ga_{0.84}N\)\ (2 nm) –
\(A_{0.05}Ga_{0.95}N\)\ (1 nm)–\(In_{0.16}Ga_{0.84}N\)\ (2 nm)\ QW\((-\square-),\)
and
2n
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\(-\layer\)
.

Fig. 6. Material gain spectra for different\(-\layer\) thicknesses in the absence of
piezoelectric charge when the carrier density is equal to \(3 \times 10^{19}\)\ cm\(^{-3}\).

QW with the\(-\layer\) always lies between or is rather bounded by the ones of those
2-nm-thick and 4-nm-thick SQWs.
This numerical result is consistent with the measured one in
Fig. 5, showing the low-temperature luminescence spectra of
4-nm-thick
\(In_{0.16}Ga_{0.84}N\)\ SQW,\ \(In_{0.16}Ga_{0.84}N\)\ (2 nm) –
\(A_{0.05}Ga_{0.95}N\)\ (1 nm)–\(In_{0.16}Ga_{0.84}N\)\ (2 nm)\ QW,\ and
2n
m
-\layer\)
\(-\layer\)
.

It would be more desirable to make a direct comparison at the
same PL peak wavelength. To this end, we have so increased the
In mole fraction of the 2-nm-thick SQW and the QW with
the\(-\layer\) as to emit the light around the green wavelength of
520 nm. In fact, the measured result in Fig. 5 gives us a hint that
the QW structure with the\(-\layer\) requires lower indium composition for long-wavelength tuning. Through the x-ray rocking
curve analysis, the indium content of the QW with the\(-\layer\) grown at 990°C is shown to be about 5% lower than that of the
2-nm-thick SQW at 950°C. Fig. 9(a) shows the PL decay
dynamics measured around the emission peak of 520 nm. Little
change is observed in the PL lifetime of the 2-nm-thick SQW
(almost no change from the one in Fig. 8) due most likely to its
very small thickness. It is likely that an increase in strain-induced
piezoelectric charge does not affect the PL decay
dynamics of a thin SQW much. However, the deterioration of crystal
quality would be much pronounced due to high indium composition,
which is the root cause for high threshold current density of
long-wavelength lasers [7]–[9]. This could also be the limiting
factor for employing a thin SQW structure for long-wavelength emission, besides the aforementioned issues such as the
temperature and the current overflow in the QW region. On
the other hand, the PL lifetime of the QW with the\(-\layer\)
is increased to 254 ns, but still much shorter than that of the
4-nm-thick SQW.
Fig. 7. Energy band diagram and wave function of (a) 5-nm-thick InGa$_{0.5}$N SQW and (b) InGa$_{0.5}$N/40/50/41/0/AlGa$_{0.5}$N/40/50/41/0/InGa$_{0.5}$N sandwiched between 10-nm-thick GaN barriers at zero bias current.

Fig. 8. Logarithmic plot of PL decay dynamics of nominally undoped 2-nm-thick InGa$_{0.5}$N SQW, InGa$_{0.5}$N/40/50/41/0/AlGa$_{0.5}$N/40/50/41/0/InGa$_{0.5}$N QW, and 4-nm-thick InGa$_{0.5}$N SQW.

To investigate the effect of the δ-layer thickness on the emission peak, we have grown more samples emitting photons with the green PL peak energies (i.e., in the green wavelength region) and measured their PL spectra as shown in Fig. 9(b). The PL peak energy of the QWs with 0.5-, 1-, and 2-nm-thick δ-layers is measured to be 2.325 eV(λ = 533.3 nm), 2.366 eV(λ = 523.9 nm), and 2.433 eV(λ = 509.6 nm), respectively.

In agreement with a conclusion drawn earlier in this section, the transition energy (PL peak wavelength) of the QW structure is reduced (increased) with decreasing δ-layer thickness.

IV. CONCLUSION

We have investigated the carrier transport and optical properties of a thick InGaN SQW where an AlGaN δ-layer is embedded. It has been demonstrated by way of simulation that a difficulty in the hole transport is dramatically reduced in the QW structure with the δ-layer, possibly enhancing the internal quantum efficiency of spontaneous emission and thus reducing the threshold current density of long-wavelength lasers based on such a QW structure. The PL peak energy depends sensitively on the δ-layer thickness, which offers an extra degree of freedom in emission wavelength tuning. We have also addressed that
the QW with the δ-layer needs a smaller amount of indium for long-wavelength tuning compared to the half-thick SQW, a feature highly desired for the design of long-wavelength light-emitting devices. Due to the increased wave function overlap by the embedded δ-layer, the QW structure also has shorter PL lifetime compared to the same-thick SQW.

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