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Analysis of InGaN-delta-InN quantum wells for light-emitting diodes

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The design of InGaN-delta-InN quantum wells (QWs) leads to significant redshift for nitride active region with large electron-hole wave function overlap ($\Gamma_{\text{e-hh}}$) and spontaneous emission rate. The analysis was carried out by using self-consistent six-band $k\cdot p$ band formalism. The design of active region consisting of 30 Å In$_{0.25}$Ga$_{0.75}$N QW with InN delta-layer leads to large $\Gamma_{\text{e-hh}}$ of $>50\%$ with emission wavelength in the yellow and red spectral regimes, which is applicable for nitride-based light-emitting diodes. © 2010 American Institute of Physics. [doi:10.1063/1.3493188]

High-efficiency InGaN quantum wells (QWs) light-emitting diodes (LEDs) play an important role in solid-state lighting and display applications. Due to the polarization fields in InGaN QW, the electron and hole wave functions are confined in opposite directions leading to reduction of the electron-hole wave function overlap ($\Gamma_{\text{e-hh}}$). The detrimental effect from charge separation becomes more severe, as the emission wavelength of the InGaN QWs is extended into green and red spectral regimes. Several approaches have been proposed to address the charge separation in InGaN QWs as its emission wavelength extends to longer spectral regimes. The optical properties of InGaN-delta-InN QW increases as its emission wavelength extends into green and red spectral regimes. Several approaches have been proposed to address the charge separation in InGaN QWs as its emission wavelength extends to longer spectral regimes. The optical properties of InGaN-delta-InN QW increases as its emission wavelength extends into green and red spectral regimes.

In this work, we present a nitride-based active region with high $\Gamma_{\text{e-hh}}$ by employing InGaN-delta-InN QW. The insertion of ultrathin layer (3–6 Å) of narrow-band gap InN alloy ($E_g=0.69$ eV) in InGaN QW leads to significant enhancement of $\Gamma_{\text{e-hh}}$. In contrast to the existing approaches to enhance the overlap, the optimized $\Gamma_{\text{e-hh}}$ for the InGaN-delta-InN QW increases as its emission wavelength extends to longer spectral regimes. The optical properties of InGaN-delta-InN QW are compared to those of the conventional InGaN QW for LEDs.

The calculation of the band structures and wave functions for InGaN-based QWs with GaN barriers is based on a self-consistent six-band $k\cdot p$ formalism. The details of the numerical model were presented in Ref. 19, and all the computation parameters were obtained from Refs. 24 and 25. In this calculation, all possible transitions between the confined states of the conduction bands and valence bands are taken into account.

To illustrate the challenging issue to redshift the emission wavelength in InGaN QWs, Fig. 1 plots the $\Gamma_{\text{e-hh}}$ (left) and peak emission wavelength (right) as a function of the indium (In) content for InGaN QW with QW thickness $(d_{\text{QW}})$ of $d_{\text{QW}}=2$ nm and $d_{\text{QW}}=3$ nm. As the In-content increases from 5% to 45%, the $\Gamma_{\text{e-hh}}$ decreases from 60% (47%) to 27.8% (6.8%) while the emission wavelength increases from 537 nm (377 nm) to 640 nm (871 nm) for the InGaN QW with $d_{\text{QW}}=2$ nm ($d_{\text{QW}}=3$ nm). Similarly, when the $d_{\text{QW}}$ increases, the emission wavelength extends longer while the $\Gamma_{\text{e-hh}}$ decreases significantly. Thus, it is important to employ QW designs with enhanced $\Gamma_{\text{e-hh}}$, as the emission wavelength is redshifted.

FIG. 1. (Color online) Electron-hole wave function overlap ($\Gamma_{\text{e-hh}}$) (left) and peak emission wavelength (right) vs indium content with InGaN QW thickness ($d_{\text{QW}}$) of $d_{\text{QW}}=2$ nm and $d_{\text{QW}}=3$ nm.

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ally very distinct from the three-layer staggered InGaN QW, where the latter overlap \( \Gamma_{c,h} \) decreases as the emission wavelength extends to the longer spectral regime.

Recently, Che et al. have proposed the use of asymmetric \( \text{GaInN/InN SQW-like} \) structure with InN monolayer thickness, which leads to increase in \( \Gamma_{c,h} \) from the introduction of ultrathin InN layer resulting in strong localization of electron and hole wave functions in the InN/InGaN interface. In contrast to the asymmetric QWs, our approach allows on the insertion of InN delta-layer in the center of InGaN QW, which leads to strong localization of electron and hole wave functions toward the center for the QW.

Figure 3(a) shows the interband transition wavelength versus the thickness (d Å) of the InN layer for 30 Å \( \text{In}_{0.25}\text{Ga}_{0.75}\text{N}/d \) Å InN QW structure. The interband transition wavelength increases as the thickness of the InN layer increases. Figure 3(b) shows the overlap (\( \Gamma_{c,h} \)) versus the thickness (d Å) of the InN layer for 30 Å \( \text{In}_{0.25}\text{Ga}_{0.75}\text{N}/d \) Å InN QW structure. When the InN layer thickness is \( \approx 6 \) Å (as delta layer), the \( \Gamma_{c,h} \) increases as InN layer thickness increases due to the shift of the electron and hole wave functions toward the center of the InGaN QW. Note that the design of InGaN QW with delta-InN layer (<6 Å) allows one to redshift the emission wavelength significantly accompanied by enhancement in the \( \Gamma_{c,h} \). Thus, the role of the InN layer in the InGaN-delta-InN QW structure is very different from that in the InN single quantum well (SQW) [Fig. 3(b)]. When the InN layer thickness is >6 Å, the \( \Gamma_{c,h} \) reduces as InN layer thickness increases, which indicates that the InN layer behaves as SQW.

Figure 4(a) shows the spontaneous emission spectra for conventional 30 Å \( \text{In}_{0.25}\text{Ga}_{0.75}\text{N} \) QW, 30 Å \( \text{In}_{0.25}\text{Ga}_{0.75}\text{N}/3 \) Å InN QW, 30 Å \( \text{In}_{0.25}\text{Ga}_{0.75}\text{N}/4 \) Å InN QW and 30 Å \( \text{In}_{0.25}\text{Ga}_{0.75}\text{N}/6 \) Å InN QW with carrier density \( n=5\times10^{18} \text{ cm}^{-3} \) at \( T=300 \text{ K} \). From the Figure 4(b), it is observed that the emission wavelengths are 6 Å, 3 Å, and 2 Å for the conventional 30 Å \( \text{In}_{0.25}\text{Ga}_{0.75}\text{N} \) QW, 30 Å \( \text{In}_{0.25}\text{Ga}_{0.75}\text{N}/3 \) Å InN QW, and 30 Å \( \text{In}_{0.25}\text{Ga}_{0.75}\text{N}/6 \) Å InN QW, respectively. The observed emission wavelengths are in agreement with the theoretical calculations.
significant redshift as compared to that of the conventional InGaN QW. The 30 Å In$_{0.25}$Ga$_{0.75}$N/3 Å InN QW shows a redshift from 492 nm (conventional InGaN QW) to 590 nm with ~3.4 times higher of the peak spontaneous emission spectra (1.34 × 10$^{24}$ s$^{-1}$ cm$^{-3}$ eV$^{-1}$) than that of the conventional one (3.9 × 10$^{26}$ s$^{-1}$ cm$^{-3}$ eV$^{-1}$) at n = 10$^{18}$ cm$^{-3}$. The In$_{0.25}$Ga$_{0.75}$N QW with 6 Å InN delta-layer shows a redshift from 492 nm (conventional InGaN QW) to 747 nm with ~7 times higher of the peak spontaneous emission spectra (2.73 × 10$^{27}$ s$^{-1}$ cm$^{-3}$ eV$^{-1}$) than that of the conventional one at n = 10$^{18}$ cm$^{-3}$.

Figure 4(b) illustrates the spontaneous emission radiative recombination rate per unit volume (R$_{sp}$) for conventional 30 Å In$_{0.25}$Ga$_{0.75}$N QW, 30 Å In$_{0.25}$Ga$_{0.75}$N/3 Å InN QW, 30 Å In$_{0.25}$Ga$_{0.75}$N/4 Å InN QW, and 30 Å In$_{0.25}$Ga$_{0.75}$N/6 Å InN QW as a function of carrier density. For the 30 Å In$_{0.25}$Ga$_{0.75}$N/3 Å InN QW structure, the R$_{sp}$ is enhanced by 4–4.6 times at each carrier density as compared to that for conventional 30 Å In$_{0.25}$Ga$_{0.75}$N QW. The enhancement of the R$_{sp}$ for the 30 Å In$_{0.25}$Ga$_{0.75}$N/4 Å (6 Å) InN QW ranges between 5.2–8.3 (6.4–12) times.

Note that high quality InN alloy have been reported for material grown by metal organic chemical vapor deposition (MOCVD) (Refs. 27–33) and molecular beam epitaxy (MBE). The growths of InN material by MBE have resulted in high electron mobility in the order of 2370 cm$^2$/V s. The use of pulsed MOCVD has also resulted in high optical quality InN alloy.26,35 Recent experimental studies by MBE have also indicated the capabilities to grow InN with monolayer precision.26,37

The key idea from this work is to illustrate the advantage arises from the insertion of narrow-band gap delta-layer in InGaN QW, which enables the extension of emission wavelength while resulting in QW with large matrix element and large radiative recombination rate. Experimental studies are required to clarify on the optimized design for realistic InGaN-delta-InN QW LEDs, which require the need to take into account the large lattice mismatch and phase separation issues in InN/InGaN heterostructure, as well as current injection efficiency in nitride LEDs.38

Our analysis assumes that the InN delta-layer inserted in InGaN QW as uniform ultra-thin layer, thus the active region is treated as two-dimensional QW structure. However, the InN nonuniformity or clustering may lead to quantum-dot like characteristics, which will require further investigation. However, it is important to point out that the challenges in the high precision control in the epitaxy of very thin InN layer may present potential advantage, in particular for realizing broadband white emission from the potential thickness variation or InN clustering from the InN delta-layer.

In summary, the design of delta-InN layer inserted in the InGaN QW results in the ability to extend its emission wavelength into yellow and red spectral regime, with significantly enhanced matrix element and spontaneous emission rate. The design of 30 Å InGaN QW with 3 Å (6 Å) InN delta-layer shows redshift in the emission wavelength by ~100 nm (~250 nm) with enhancement of the spontaneous emission rate of ~4–4.6 times (~6.4–12 times) as compared to that of the conventional InGaN QW. The InGaN-delta-InN QW has potential for achieving high-efficiency nitride LEDs and lasers emitting in the yellow and red spectral regime.

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