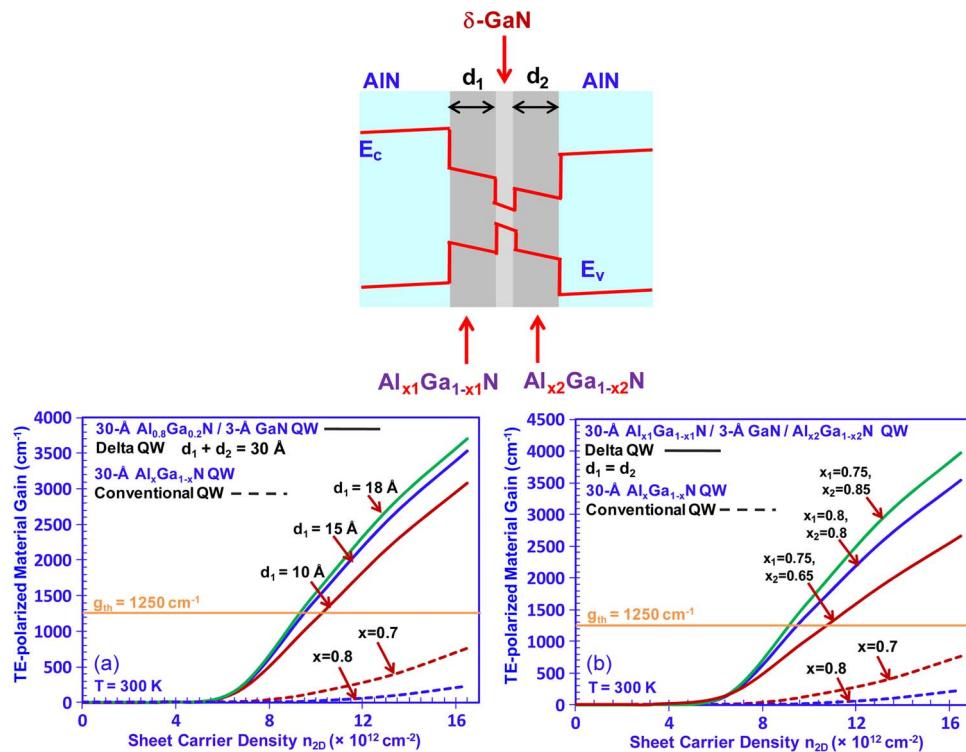


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Jing Zhang, Student Member, IEEE
 Nelson Tansu, Senior Member, IEEE



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Jing Zhang, *Student Member, IEEE*, and Nelson Tansu, *Senior Member, IEEE*

Center for Photonics and Nanoelectronics, Department of Electrical and Computer Engineering,
Lehigh University, Bethlehem, PA 18015 USA

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Abstract: The gain characteristics of AlGaN-delta-GaN quantum wells (QWs) with varying delta-GaN positions and AlGaN QW compositions are analyzed. The use of optimized AlGaN-delta-GaN QWs resulted in ~7-times increase in material gain over that of conventional AlGaN QWs for gain media emitting at ~240 nm. By employing asymmetric AlGaN-delta-GaN QWs, the optimized optical gain can be achievable for AlGaN-delta-GaN QW structure with realistic design applicable for mid- and deep-ultraviolet (UV) lasers. The threshold properties and differential gains are also studied for optimized AlGaN-delta-GaN QWs UV lasers.

Index Terms: III-Nitride, AlGaN-delta-GaN quantum wells (QWs), deep UV (UV) lasers, optical gain, laser diodes.

1. Introduction

The field of III-Nitride semiconductors has applications covering lasers and light-emitting diodes (LEDs) [1]–[16], power electronics [17], thermoelectric [18], [19], photovoltaics [20], and terahertz photonics [21]. Significant advances had been achieved in visible LEDs, especially in addressing the internal quantum efficiency [1]–[4], material epitaxy [5]–[10], extraction efficiency [11], [12], and efficiency droop [13]–[16]. In contrast to the progress in visible emitters [1]–[16], the realization of electrically injected mid- ($\lambda \sim 250$ – 320 nm) and deep-ultraviolet (UV) ($\lambda \sim 220$ – 250 nm) AlGaN quantum wells (QWs) lasers has been limited to $\lambda \sim 320$ – 360 nm [22]–[39], while only optically pumped deep-UV lasers had been realized for shorter emission wavelength [31]. The challenges in realizing the electrically injected mid- and deep-UV AlGaN QWs lasers are attributed to the difficult growths of high Al-content AlGaN and p-AlN and the lack understanding on the physics of high Al-content AlGaN QWs. The optical properties for low [40]–[42] and high Al-content [43], [44] AlGaN QWs lasers have been reported, while the studies are relatively lacking on gain properties of high Al-content AlGaN QWs.

Our recent work [43] revealed the valence subbands crossover in high Al-content AlGaN QW leads to strong conduction (C)-crystal-field split-off hole (CH) transition, which results in large transverse-magnetic (TM)-polarized optical gain for $\lambda \sim 220$ – 230 nm. Recent experimental works have confirmed the dominant TM-polarized emission for shorter wavelength with higher Al-content

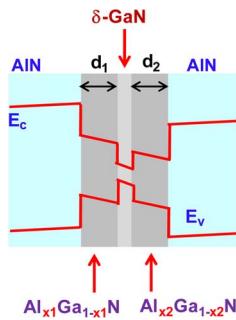


Fig. 1. Schematic energy band lineup of $\text{Al}_{x1}\text{Ga}_{1-x1}\text{N}/\text{delta-GaN}/\text{Al}_{x2}\text{Ga}_{1-x2}\text{N}$ QW with AlN barriers.

AlGaN QWs LEDs [45], [46], in agreement with our prediction [43]. The subsequent paper has studied about the temperature and barrier effect on the polarization properties of AlGaN QW [47]. Recent theoretical work [48] has confirmed the crossover of the valence subbands for AlGaN alloys on $\text{Al}_{0.85}\text{Ga}_{0.15}\text{N}$ substrate, in agreement with our finding [43]. The subsequent theoretical work [49] has discussed the strain effect by using various AlGaN substrates on the crossover in AlGaN. Garrett and coworkers have experimentally confirmed our prediction of the CH/HH crossover for AlGaN QWs from the transverse-electric (TE) ($\lambda \sim 253$ nm) to TM ($\lambda \sim 237$ nm) photoluminescence polarization switching [50].

In order to address the issue of low optical gain at $\lambda \sim 250$ – 300 nm, we recently proposed the AlGaN-delta-GaN QW structure [51] by inserting an ultrathin GaN layer into high Al-content (x) $\text{Al}_x\text{Ga}_{1-x}\text{N}$ -delta-GaN QW active region. The use of AlGaN-delta-GaN QWs resulted in strong valence subband mixing, which led to large TE-polarized gain at $\lambda \sim 240$ – 300 nm attributed to the dominant C–HH transition. Recent experimental work [52] has reported the polarization properties of the deep-UV emission from AlN/GaN short-period superlattices, which revealed that stronger TE-polarized emission from the use of a very thin GaN in AlN active region similar to our prediction [51]. Note that the use of InGaN-delta-InN QW had been used for achieving improved overlap design in visible LEDs [53], [54].

In this paper, we present a comprehensive study on the optical gain and threshold characteristics of AlGaN-delta-GaN QWs with various delta-GaN positions and AlGaN QW compositions for mid- and deep-UV lasers. The band structure and wave function calculations are based on the six-band $\mathbf{k} \cdot \mathbf{p}$ formalism for wurtzite semiconductors taking into account the valence band mixing, strain effect, polarization fields, and carrier screening effects [55]–[59], with the III-Nitride band parameters and band offsets ratio ($\Delta E_c/\Delta E_v = 70/30$) obtained from references [59]–[61]. The spontaneous and piezoelectric polarizations follow the treatments in [62] and [63], respectively.

2. Concept and Band Structure for AlGaN-Delta-GaN QWs

Fig. 1 shows the schematic of the AlGaN-delta-GaN QW. Our previous work [51] revealed that the use of symmetric high Al-content AlGaN-delta-GaN QWs led to large TE-polarized gain at $\lambda \sim 240$ – 300 nm. In this paper, we present a comprehensive study of the asymmetric AlGaN-delta-GaN QWs. The asymmetric QWs can be introduced by engineering the thicknesses of the AlGaN layers (d_1, d_2) and/or the Al contents of the AlGaN layers (x_1, x_2) surrounding the delta-GaN layer.

For the AlGaN-delta-GaN QWs, the energy levels of the HH and light hole (LH) subbands are higher than those of the CH subband, which leads to the dominant C–HH transition. The difference in the effective masses of the electrons and holes leads to different spreading of the wave functions for electrons and holes in III-Nitride-based QWs. In the case of identical effective masses for both electrons and holes, the optimized overlap will occur with the delta position at the center of the QWs. However, the effective masses for holes are larger than those of electrons in nitride-based QWs; thus, the optimization of the overlap can be achieved by using engineering of the delta layer

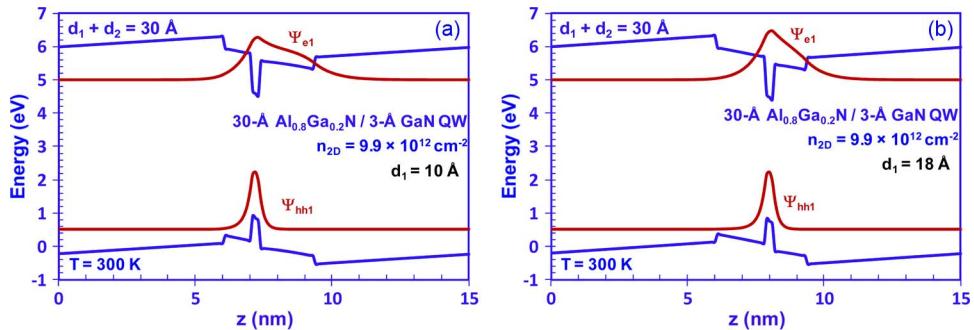


Fig. 2. Energy lineups with electron wavefunction EC1 and hole wave function HH1 for the 30-Å Al_{0.8}Ga_{0.2}N/3-Å GaN QW with (a) d₁ = 10 Å, and (b) d₁ = 18 Å.

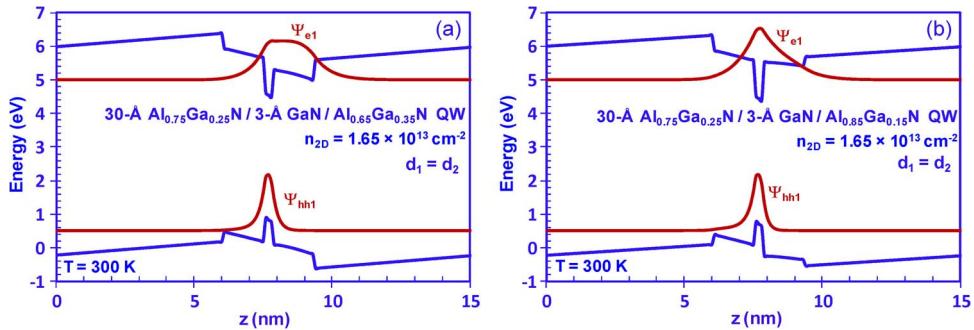


Fig. 3. Energy lineups with electron and hole wavefunctions for (a) the 30-Å Al_{0.75}Ga_{0.25}N/3-Å GaN/Al_{0.65}Ga_{0.35}N QW, and (b) the 30-Å Al_{0.75}Ga_{0.25}N/3-Å GaN/Al_{0.85}Ga_{0.15}N QW.

position (d₁, d₂) [Fig. 2(a) and (b)] or different compositions of AlGaN QW sublayers (x₁, x₂) [see Fig. 3(a) and (b)].

Fig. 2(a) and (b) shows the energy lineups with electron wavefunction EC1 and hole wave function HH1 for the 30-Å Al_{0.8}Ga_{0.2}N/3-Å GaN QW with different d₁ thicknesses (d₁ + d₂ = 30 Å) at the sheet carrier density (n_{2D}) of 9.9 × 10¹² cm⁻² (T = 300 K). For the 30-Å Al_{0.8}Ga_{0.2}N/3-Å GaN QW structure with d₁ = 10 Å in Fig. 2(a), the electron–hole wavefunction overlap (Γ_{e_hh}) is obtained as ~63.51%. By engineering the delta QW structure with d₁ = 18 Å, as shown in Fig. 2(b), the electron and hole wavefunctions are strongly localized toward the center of the QW active region, attributing to the engineered spreading of the wavefunctions, which leads to the enhanced $\Gamma_{e_hh} \sim 73.92\%$.

Fig. 3(a) and (b) shows the energy band lineups with electron wavefunction EC1 and hole wave function HH1 for the 30-Å Al_{0.75}Ga_{0.25}N/3-Å GaN/Al_{0.65}Ga_{0.35}N QW and Al_{0.75}Ga_{0.25}N/3-Å GaN/Al_{0.85}Ga_{0.15}N QW with n_{2D} = 1.65 × 10¹³ cm⁻² at T = 300 K, and the thickness d₁ is kept as identical with the thickness d₂. For the 30-Å Al_{0.75}Ga_{0.25}N/3-Å GaN/Al_{0.65}Ga_{0.35}N QW, the design consisting of asymmetric QW with different Al contents (75% and 65%) results in Γ_{e_hh} of ~60.31%. By engineering the Al contents of the AlGaN layers as x₁ = 0.75 and x₂ = 0.85 [see Fig. 3(b)], the electron and hole wavefunctions are pushed toward the center of the QW active region, as the band gap of Al_{0.85}Ga_{0.15}N is larger than that of Al_{0.75}Ga_{0.25}N, which results in the improved $\Gamma_{e_hh} \sim 78.83\%$. Therefore, the matrix element will be enhanced attributing to the improved Γ_{e_hh} , which will contribute to the optical gain by using the optimized asymmetric AlGaN-delta-GaN QW structures.

3. Optical Gain Characteristics of Asymmetric AlGaN-Delta-GaN QWs

Fig. 4(a) shows the TE-polarized optical gain spectra for 30-Å Al_{0.8}Ga_{0.2}N/3-Å GaN QWs with n_{2D} = 1.65 × 10¹³ cm⁻² at T = 300 K with varying d₁ thicknesses. For the asymmetric QW with

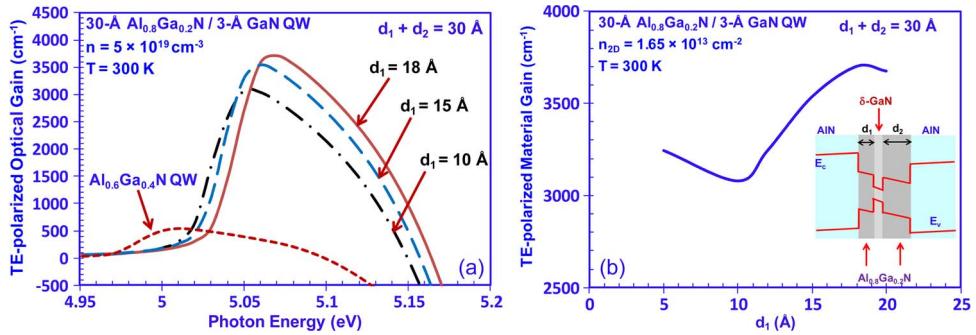


Fig. 4. (a) TE-polarized optical gain spectra for 30-Å Al_{0.8}Ga_{0.2}N/3-Å GaN QW with varying d₁ thicknesses, and (b) TE-polarized material peak gain as a function of the d₁ thickness for the 30-Å Al_{0.8}Ga_{0.2}N/3-Å GaN QW with n_{2D} = 1.65 × 10¹³ cm⁻² at T = 300 K.

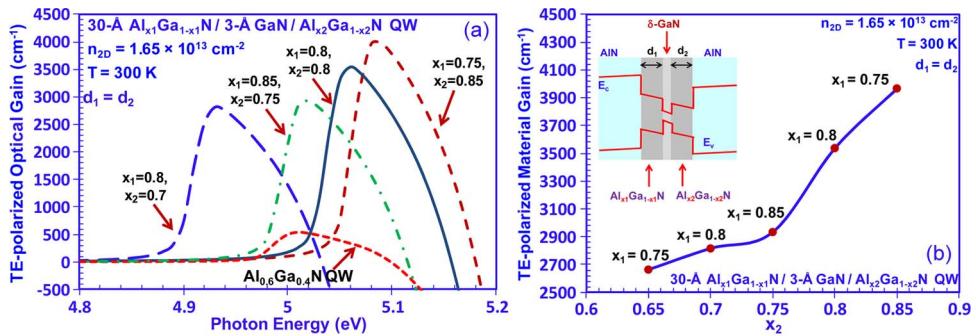


Fig. 5. (a) TE-polarized optical gain spectra for 30-Å Al_{x1}Ga_{1-x1}N/3-Å GaN/Al_{x2}Ga_{1-x2}N QW with varying combinations of the Al contents x₁ and x₂, and (b) TE-polarized material peak gain for the 30-Å Al_{x1}Ga_{1-x1}N/3-Å GaN/Al_{x2}Ga_{1-x2}N QW with n_{2D} = 1.65 × 10¹³ cm⁻² at T = 300 K.

d₁ = 18 Å, the TE-polarized optical gain is larger than that of the symmetric QW with d₁ = 15 Å, attributing to the enhanced Γ_{e-hh} from the optimized AlGaN-delta-GaN QW structure. For the asymmetric QW with d₁ = 10 Å, the optical gain is slightly lower due to the weaker confinement of the electron and hole wavefunctions. Note that the peak emission wavelengths (λ_{peak}) for the asymmetric QWs with d₁ = 10 Å and 18 Å are ~246 nm and ~245 nm, respectively, which are very similar with that of the symmetric QW. In comparison with the conventional Al_{0.6}Ga_{0.4}N QW, the optimized asymmetric delta QW (d₁ = 18 Å) shows ~6 times enhancement in the TE-polarized optical gain for mid-UV spectral regime.

Fig. 4(b) shows the TE-polarized material peak gain (g_{peak}^{TE}) as a function of the d₁ thickness for the 30-Å Al_{0.8}Ga_{0.2}N/3-Å GaN QW with n_{2D} = 1.65 × 10¹³ cm⁻² at T = 300 K. With the d₁ thicknesses ranging from 5 Å up to 20 Å, the TE-polarized material gain varies from ~3078 cm⁻¹ (d₁ = 10 Å) up to ~3703 cm⁻¹ (d₁ = 18 Å). Therefore, very large optical gain can be maintained for emission wavelength ~245 nm for the asymmetric AlGaN-delta-GaN QW structures with different delta-GaN positions.

Fig. 5(a) illustrates the TE-polarized gain spectra for 30-Å Al_{x1}Ga_{1-x1}N/3-Å GaN/Al_{x2}Ga_{1-x2}N QW with n_{2D} = 1.65 × 10¹³ cm⁻² at T = 300 K with combinations x₁ and x₂. For the optimized delta QW with Al contents of x₁ = 0.75 and x₂ = 0.85, very large TE-polarized gain (g_{peak}^{TE} ~ 3967 cm⁻¹) can be obtained at λ_{peak} ~ 244 nm, attributed to the improved Γ_{e-hh} from the asymmetric QW. For the asymmetric cases of Al_{0.85}Ga_{0.15}N/3-Å GaN/Al_{0.75}Ga_{0.25}N QW (x₁ = 0.85, x₂ = 0.75) and Al_{0.8}Ga_{0.2}N/3-Å GaN/Al_{0.7}Ga_{0.3}N QW (x₁ = 0.8, x₂ = 0.7), large optical gains can be obtained with λ ~ 244–252 nm, which are ~6–7 times larger than that of the conventional QW emitting at similar wavelengths.

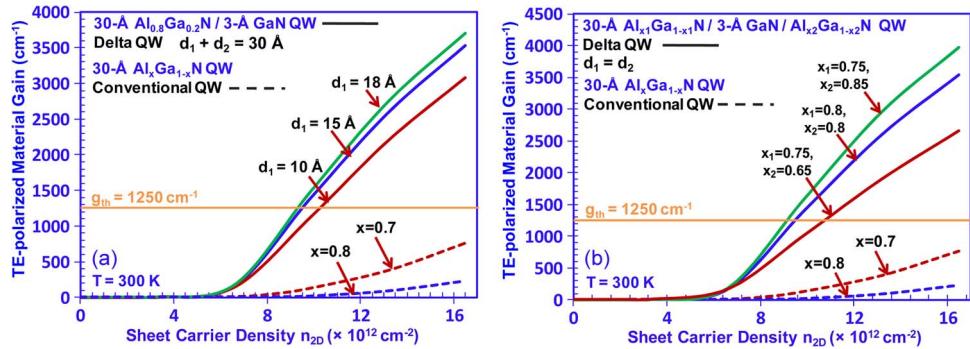


Fig. 6. TE-polarized material gain as a function of sheet carrier density for (a) 30-Å Al_{0.8}Ga_{0.2}N/3-Å GaN QW with varying d₁ thicknesses, and (b) 30-Å Al_xAl_{1-x}N/3-Å GaN/Al_{x2}Al_{1-x2}N QWs, in comparison with conventional 30-Å Al_xAl_{1-x}N QW (x = 0.7, 0.8).

Fig. 5(b) shows the TE-polarized material peak gain for the 30-Å Al_xAl_{1-x}N/3-Å GaN/Al_{x2}Al_{1-x2}N QW with $n_{2D} = 1.65 \times 10^{13}$ cm⁻² at T = 300 K. By varying the Al contents of the AlGaN layers surrounding the delta-GaN layer, the TE-polarized material peak gains range from ~ 2700 cm⁻¹ up to ~ 4000 cm⁻¹. Therefore, the optimized asymmetric QW structures with different Al contents can lead to enhanced optical gain. Also, large TE-polarized gain can be maintained by different combinations of the Al contents of the AlGaN QWs, which will provide flexibility in the experimental realizations of the AlGaN-delta-GaN QWs mid- and deep-UV lasers.

4. Threshold Properties and Differential Gains of AlGaN-Delta-GaN QWs

Fig. 6(a) shows the TE-polarized material gain as a function of sheet carrier density for both 30-Å Al_{0.8}Ga_{0.2}N/3-Å GaN QWs with various d₁ thicknesses, and conventional 30-Å Al_xAl_{1-x}N QW (x = 0.7, 0.8) at T = 300 K. The $g_{\text{peak}}^{\text{TE}}$ values of the AlGaN-delta-GaN QW structure (~ 3100 – 3700 cm⁻¹) are found to be significantly larger than that of the conventional high Al-content AlGaN QWs (~ 200 – 800 cm⁻¹) at high $n_{2D} = 1.65 \times 10^{13}$ cm⁻². The optimized asymmetric QW structure with d₁ = 18 Å achieves ~ 1.2 times larger material gain than that of the symmetric QW structure, attributing to its improved matrix element.

To illustrate the effect of different Al contents of the AlGaN QWs, Fig. 6(b) shows the TE-polarized material gain as a function of sheet carrier density for 30-Å Al_xAl_{1-x}N/3-Å GaN/Al_{x2}Al_{1-x2}N QWs and conventional 30-Å Al_xAl_{1-x}N QWs (x = 0.7, 0.8) at T = 300 K. Attributing to the reduced charge separation effect, the optimized asymmetric 30-Å Al_{0.75}Ga_{0.25}N/3-Å GaN/Al_{0.85}Ga_{0.15}N QW achieves ~ 1.4 times larger material gain than that of the symmetric QW. Thus, the TE-polarized lasing is feasible for asymmetric AlGaN-delta-GaN QW lasers with $\lambda \sim 240$ – 250 nm.

To analyze the threshold properties of mid- and deep-UV lasers, AlGaN QW lasers with optical confinement factor (Γ_{opt}) of 0.02 [41] were used in the analysis. Based on the transfer matrix method [64], the Γ_{opt} for the asymmetric and symmetric QWs are calculated as almost identical. Thus, the modal gain comparison for the QWs will be governed by the difference in the material gains. The internal loss (α_i) in typical AlGaN lasers is 14 cm⁻¹ [35]. The laser cavity length is assumed as 500 μm [35], [41] with end-facet reflectivities of 95% and 35%, which corresponds to mirror loss (α_m) of 11 cm⁻¹ and threshold gain (g_{th}) of ~ 1250 cm⁻¹. The threshold sheet carrier density (n_{2D}^{th}) is 9.273×10^{12} cm⁻² for the symmetric 30-Å Al_{0.8}Ga_{0.2}N/3-Å GaN QW. For the optimized structure with d₁ = 18 Å [see Fig. 6(a)], the n_{2D}^{th} is 9.042×10^{12} cm⁻². Similarly, for optimized 30-Å Al_{0.75}Ga_{0.25}N/3-Å GaN/Al_{0.85}Ga_{0.15}N QW, the n_{2D}^{th} is 8.976×10^{12} cm⁻². Thus, the n_{2D}^{th} for both optimized AlGaN-delta-GaN QW structures with different delta-GaN positions and varying Al contents are reduced compared with the symmetric QW.

The spontaneous emission rates and peak modal gains (with $\Gamma_{\text{opt}} = 0.02$ [41]) comparisons for both symmetric and asymmetric AlGaN-Delta-GaN QWs are presented in Figs. 7 and 8, respectively. The comparison studies were performed for AlGaN-Delta-GaN QWs with different delta layer

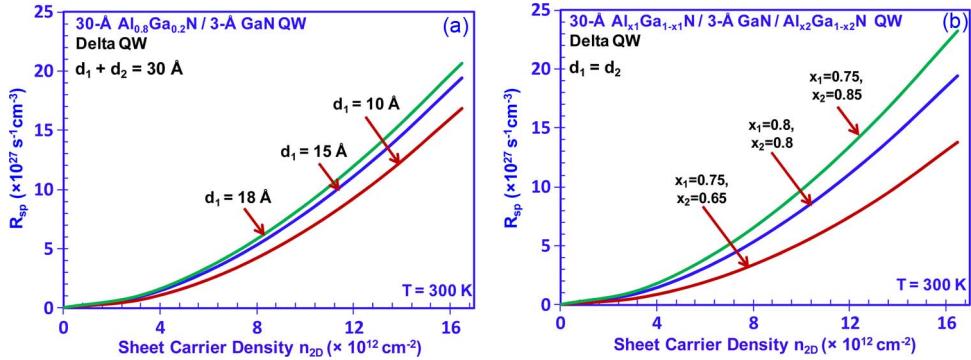


Fig. 7. R_{sp} as a function of sheet carrier density for both symmetric and asymmetric AlGaN-Delta-GaN QWs to illustrate (a) effect of delta positions, and (b) effect of Al contents in AlGaN QWs.

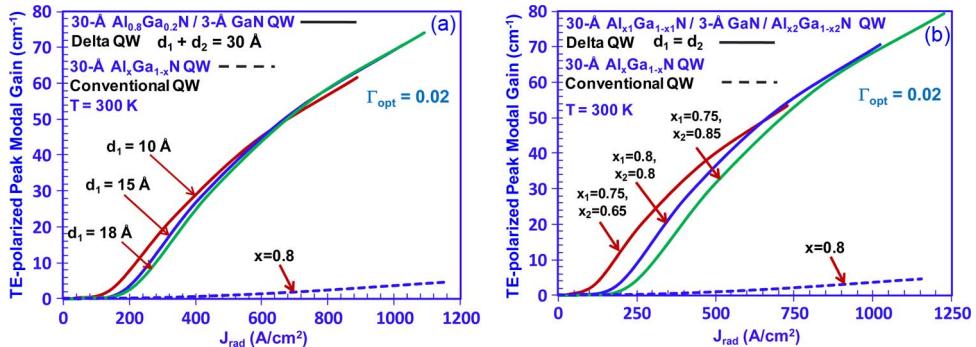


Fig. 8. Modal gains as a function of radiative current density for AlGaN-Delta-GaN QWs and conventional $\text{Al}_{0.8}\text{Ga}_{0.2}\text{N}$ QW with different (a) delta positions, and (b) Al contents in AlGaN QWs.

position (d_1, d_2) [see Figs. 7(a) and 8(a)] and different AlGaN QW sublayer compositions [see Figs. 7(b) and 8(b)]. By comparing the R_{sp} for different delta-layer positions [see Fig. 7(a)], the asymmetric delta QW with $d_1 = 18 \text{ \AA}$ shows higher R_{sp} ($\sim 2.07 \times 10^{28} \text{ s}^{-1} \text{ cm}^{-3}$ with $n_{2D} = 1.65 \times 10^{13} \text{ cm}^{-2}$) than those of the other structures, attributed from the improved overlap ($\Gamma_{e,hh} \sim 73.92\%$). Fig. 7(b) shows that the optimized R_{sp} was obtained from the use of that for $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/3\text{-}\text{\AA}\text{ GaN}/\text{Al}_{0.85}\text{Ga}_{0.15}\text{N}$ QWs attributed to the optimized C-HH overlap of 78.83%. The delta QWs exhibited significantly higher modal gain for any radiative current density (J_{rad}) injection level [see Fig. 8(a) and (b)], in comparison with those the conventional QW. The total recombination current density J_{tot} in the QW active region includes both the radiative and nonradiative current densities ($J_{tot} = J_{rad} + J_{non-rad}$) [58], and $J_{non-rad}$ ($\sim A \cdot n_{th} + C \cdot n_{th}^3$) represents the dominant part of the J_{tot} in AlGaN-based QW [41], [58]. Thus, the reduction in n_{th} is important for suppressing monomolecular ($\sim A \cdot n_{th}$) and Auger ($\sim C \cdot n_{th}^3$) recombination currents at threshold.

The differential gain properties are also analyzed for both symmetric and asymmetric AlGaN-Delta-GaN QWs to illustrate effect of delta positions [see Fig. 9(a)], as well as effect of Al contents [see Fig. 9(b)]. For both cases, the differential gains first increase with higher carrier densities, which can be attributed to the carrier screening effect. After reaching the maximum, the differential gains start to decrease with increasing carrier densities, which is due to the band filling effect. In Fig. 9(a) and (b), the peak differential gains of the optimized asymmetric AlGaN-delta-GaN QW structures are higher than those of the symmetric QW structures, which indicates that the optimized AlGaN-delta-GaN QW structures will be applicable for high-speed modulation lasers.

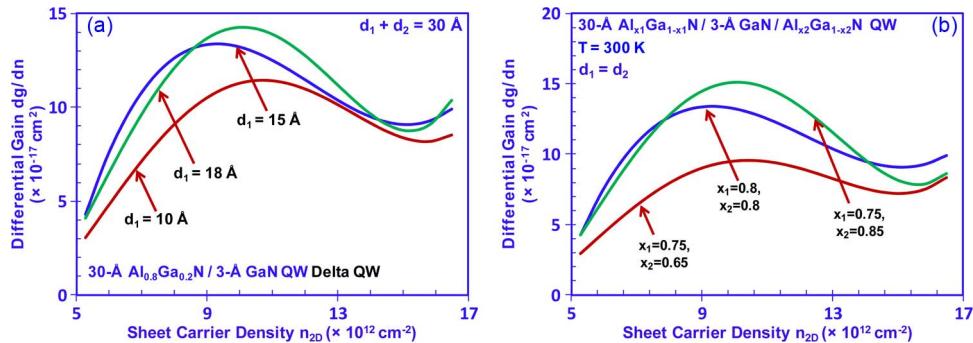


Fig. 9. Differential gain as a function of sheet carrier density for AlGaN-Delta-GaN QWs to illustrate the effect of (a) delta positions, and (b) Al contents of AlGaN QWs

5. Summary

In summary, the comprehensive optimization studies on the gain characteristics of AlGaN-delta-GaN QWs with various delta-GaN positions and AlGaN compositions are analyzed. The optimized asymmetric AlGaN-delta-GaN QWs result in ~ 7 times increase in material gain, in comparison with that of the conventional QWs. Recent works had reported the TE-polarized gain from the following: 1) $\text{Al}_{0.7}\text{Ga}_{0.3}\text{N}/\text{AlN}$ QWs with low Al-content nanocluster “quantum dot” features within the $\text{Al}_{0.7}\text{Ga}_{0.3}\text{N}$ QW layers [65], [66] and 2) thin GaN “quantum dot” structures embedded in AlN barriers [67], which are consistent with the dominant TE-polarized gain from our prediction for high Al-content AlGaN QWs consisting of low band-gap GaN delta layer embedded in the active region [51]. Large material gains can be maintained at $\lambda \sim 240\text{--}250$ nm for the asymmetric AlGaN-delta-GaN QWs [see Fig. 4(b)]. Despite the improved material gain for the asymmetric QWs, the finding shows that large material gain can be obtained for both symmetric and asymmetric AlGaN-delta-GaN QWs [see Fig. 4(b)], which indicates the flexibility and robustness in the experimental implementations of this concept in devices. Thus, by employing asymmetric QW design with optimized delta-GaN layer position and asymmetric AlGaN-composition layers, the optimized optical gain and lower threshold carrier densities are achievable for the AlGaN-delta-GaN QW with realistic design applicable for mid- and deep-UV lasers. Recent works by metalorganic chemical vapor deposition (MOCVD) had reported the growths of AlN/ GaN superlattice structures with thin GaN layers in the order of $\sim 0.9\text{--}2.5$ monolayers [52]. Thus, the growths of the AlGaN-delta-GaN QW is expected to be practical for implementation in deep/mid-UV LEDs or lasers.

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