Dominant Transverse-Electric Polarized Emission from 298 nm MBE-Grown AlN-Delta-GaN Quantum Well Ultraviolet Light-Emitting Diodes

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ABSTRACT

III-nitride based ultraviolet (UV) light emitting diodes (LEDs) are of considerable interest in replacing gas lasers and mercury lamps for numerous applications. Specifically, AlGaN quantum well (QW) based LEDs have been developed extensively but the external quantum efficiencies of which remain less than 10% for wavelengths <300 nm due to high dislocation density, difficult p-type doping and most importantly, the physics and band structure from the three degeneration valence subbands. One solution to address this issue at deep UV wavelengths is by the use of the AlGaN-delta-GaN QW where the insertion of the delta-GaN layer can ensure the dominant conduction band (C) - heavy-hole (HH) transition, leading to large transverse-electric (TE) optical output.

Here, we proposed and investigated the physics and polarization-dependent optical characterizations of AlN-delta-GaN QW UV LED at ~300 nm. The LED structure is grown by Molecular Beam Epitaxy (MBE) where the delta-GaN layer is ~3-4 monolayer (QW-like) sandwiched by 2.5-nm AlN sub-QW layers. The physics analysis shows that the use of AlN-delta-GaN QW ensures a larger separation between the top HH subband and lower-energy bands, and strongly localizes the electron and HH wave functions toward the QW center and hence resulting in ~30-time enhancement in TE-polarized spontaneous emission rate, compared to that of a conventional $Al_{0.35}Ga_{0.65}N$ QW. The polarization-dependent electroluminescence measurements confirm our theoretical analysis; a dominant TE-polarized emission was obtained at 298 nm with a minimum transverse-magnetic (TM) polarized emission, indicating the feasibility of high-efficiency TE-polarized UV emitters based on our proposed QW structure.

Keywords: AlN Delta GaN Quantum Well, Ultraviolet, Light Emitting Diodes, Transverse Electric-Polarized

1. INTRODUCTION

III-nitride Ultraviolet (UV) light emitting diodes (LEDs) and laser diodes (LDs) are in strong demand for a wide variety of applications. Specifically, UV LEDs and lasers with emission wavelengths (λ) in the range of 250-350 nm are suitable for water or air purification, sterilization and bio-chemistry[1-4]. Conventionally, AlGaN alloy is intensively considered as a candidate material in such wavelength regime due to its wide direct transition energy range up to 6.2 eV (210 nm)[1-11]. Nevertheless, the AlGaN-based mid- and deep-UV LEDs suffer from low external quantum efficiency (η_{EQE})[6-9] due to the combination of high dislocation density in AlN and AlGaN layers[10-11], low conductivity in p- and n-carrier injection layers[12-13] and physics limits such as severe valence band mixing effect[14-16] in AlGaN quantum well (QW) structures.

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Previous study revealed that spontaneous emission rate and gain characteristics of conventional AlGaN QW are strongly influenced by the crystal-field split-off hole (CH) and heavy hole (HH)/light hole (LH) band-edge energy crossover[14]. Specifically, the three degenerate valence subbands in AlGaN QW are mixed together near the crossover point which results in the deficient conduction band (C) to HH subband transition (C-HH). In addition, the large separation between the electron and hole wavefunctions in such AlGaN QW structure will cause the small wavefunction overlap. As a result, both transverse-electric (TE)-polarized and transverse magnetic (TM)-polarized spontaneous emission rates are low at $\lambda \sim 250\text{-}300$ nm. To address this issue, one possible solution is to use delta QW design[17-18]. Previous studies have demonstrated the insertion of a delta-GaN layer into high Al-content AlGaN QW[17] and AlInN QW[18] structures could largely separate HH/LH and CH subbands and localize the electron and hole wavefunctions toward center of the QW, which consequently results in large TE-polarized spontaneous emission. Nevertheless, the epitaxy challenges of growing high quality AlGaN/AlInN layer on AlN template make it difficult to pursue such QW structure at $\lambda \sim 250\text{-}300$ nm. Alternatively, the use of AlN sub-QW layer instead of previous AlGaN/AlInN sub-QW enables a much straightforward epitaxy growth. Recently, several studies have experimentally demonstrated the use of AlN/GaN superlattices[19] and AlN/GaN quantum dots (QDs)[20-23] for mid- and deep-UV emission. However, the research on physics and polarization properties of AlN-delta-GaN QW is still at the early stage which limits the further development of such QW design at mid- and deep-UV regime.

Therefore, the physics and optical properties of 298 nm AlN-delta-GaN QW UV LEDs are investigated in this study by utilizing both band structure calculations and electroluminescence (EL) measurements. To be more specific, the 6-band $\boldsymbol{k \cdot p}$ model[17-18, 24-28] was employed to calculate the band structures and spontaneous emission properties of the AlN-delta-GaN QW structure with 11 Å delta-GaN thickness. All the parameters in this study are from Ref. 24. From our analysis, the insertion of the thin delta-GaN layer into the AlN sub-QW could strongly separate the HH and CH subbands, which ensures the sufficient C-HH transition. Meanwhile, the electron-hole wavefunction overlap is significantly improved by the use of AlN-delta-GaN QW, which leads to 30 times enhancement in TE-polarized spontaneous emission rate as compared to that of the conventional AlGaN QW at 298 nm. Furthermore, the polarization properties of the proposed structure were also examined experimentally in this study by using polarization-dependent EL measurements on a 298 nm molecular beam epitaxy (MBE)-grown AlN-delta-GaN QW UV LED. The measurements results show great consistency with our theoretical prediction, indicating the dominant TE-polarized emission from proposed AlN-delta-GaN QW structure at mid-UV regime.

2. CONCEPT AND PHYSICS OF ALN-DELTA-GAN QUANTUM WELL

The band energy lineups and wavefunctions of both AlN-delta-GaN QW and conventional $Al_{0.35}Ga_{0.65}N$ QW were calculated and plotted in Figure 1. For AlN-delta-GaN QW, a 11-Å delta-GaN layer is inserted at the center of 20-Å AlN sub-QW region and sandwiched by AlN barriers. The simulated QW structure is similar to the MBE-grown AlN-delta-GaN QW-like LED structure. As discussed earlier, the design of the AlN-delta-GaN QW structure in this study originates from the high Al-content AlGaN-delta-GaN QW structure[17] and hence maintains the benefits of the delta QW design such as improved electron-hole wavefunction overlap and large HH and CH subbands energy separation. Furthermore, the use of the AlN sub-QW as a replacement for AlGaN sub-QW enables a more straightforward process for epitaxy growth. Figure 1 (a) shows the band structures and wavefunctions of ground state conduction band (C1) and valence subband (HH1) at zone center for the proposed AlN-delta-GaN QW structure. Note that the use of delta-GaN layer was utilized as a local minimum to confine the electron and hole wavefunctions, which results in large wavefunction overlap (r_{e_hh} = 74.83%). In contrast, band structures and wavefunctions for conventional $Al_{0.35}Ga_{0.65}N$ QW are also plotted in figure 1 (b). Due to the large internal polarization field and the absence of a local minimum in the conventional QW structure, large separation between electron and hole wavefunctions are realized for conventional $Al_{0.35}Ga_{0.65}N$ QW, which leads to a very small wavefunction overlap (r_{e_hh} = 13.94%). Therefore, the proposed AlN-delta-GaN QW structure could significantly improve the ground state electron and hole (HH1) wavefunction overlap, and large TE-polarized emission can be expected by using such QW design.

The band-edge valence band structures for AlN-delta-GaN QW and conventional $Al_{0.35}Ga_{0.65}N$ QW with carrier density of 5×10^{18} cm^{-3} are also compared in this study to further investigate the physics of such QW design and the results were plotted in figures 2 (a) and 2(b), respectively. For AlN-delta-GaN QW structure, the use of the delta-GaN layer ensures that HH1 subband occupies the highest valence subband while no CH subband exists at the four highest energy levels. Note that both C-HH and C-LH transition contribute to the TE-polarized emission, which indicates the dominant TE-polarized spontaneous emission rate can be achieved for the proposed AlN-delta-GaN QW. As for conventional $Al_{0.35}Ga_{0.65}N$ QW, since Al-content in this study is lower than the valence subband crossover point (57.2%)[14], HH1 is expected to locate at the highest energy level, which is verified in figure 2 (b). In addition, the energy separation between first and second HH/LH subbands in AlN-delta-GaN QW is larger than that in conventional $Al_{0.35}Ga_{0.65}N$ QW, which indicates more sufficient carrier population into HH1 subband for proposed AlN-delta-GaN QW and consequently large TE-polarized spontaneous emission rate.

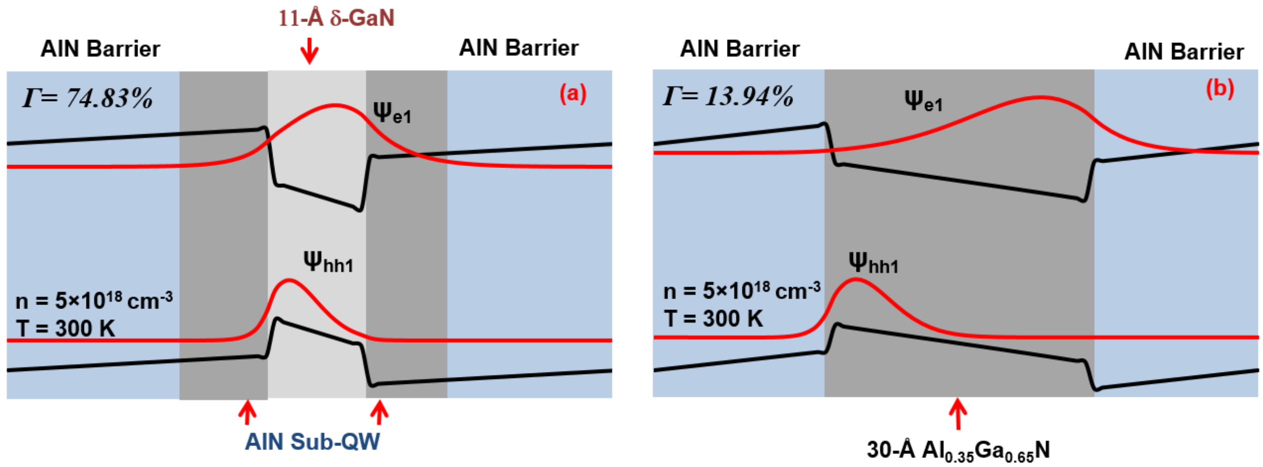

Figure 1. Energy band lineups with ground state electron wavefunction (ψ_{e1}) and heavy hole wavefunction (ψ_{hh1}) at room temperature for (a) AlN-delta-GaN QW (b) conventional $Al_{0.35}Ga_{0.65}N$ QW. The carrier density is 5×10^{18} cm^{-3}.

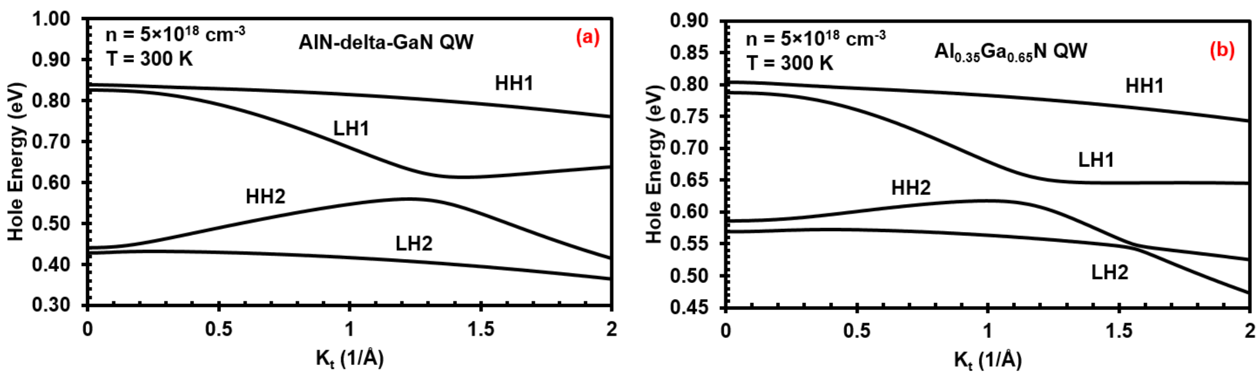

Figure 2. Valence band structure for (a) AlN-delta-GaN QW and (b) conventional $Al_{0.35}Ga_{0.65}N$ QW at room temperature with carrier density of 5×10^{18} cm^{-3}.

Figure 3 plots both TE-polarized (solid and dash dot line) and TM-polarized (dash line) spontaneous emission spectra for AlN-delta-GaN QW (black) and conventional $Al_{0.35}Ga_{0.65}N$ QW (red) at carrier density of 5×10^{18} cm^{-3}. The spontaneous emission rate calculations in this study are based on the Fermi's Golden rule with considering all the transitions between the conduction bands and valence subbands. More simulation method details can be found in Ref. 26. For the proposed AlN-delta-GaN QW, large TE-polarized spontaneous emission rate is achieved at peak emission wavelength λ_{peak} = 298 nm with minimum TM-polarized output, which was attributed to the dominant C-HH transition. As discussed earlier, the insertion of delta-GaN layer for the proposed structure could not only improve the electron-hole wavefunction overlap, but also ensure that the ground state HH subband occupies the highest energy level, which indicates the dominant transition is C-HH transition from such QW structure and therefore dominant TE-polarized emission. As for the conventional $Al_{0.35}Ga_{0.65}N$ QW, the TE-polarized spontaneous emission rate is larger than TM-polarized emission due to the absence of CH subband at the four highest valence energy subbands. Note that up to 30 times improvement in TE-polarized spontaneous emission rate can be realized by the use of AlN-delta-GaN QW as compared to that of the conventional $Al_{0.35}Ga_{0.65}N$ QW due to the improved wavefunction overlap and large energy separation between first and second HH/LH subbands. Figure 3 inset shows the spontaneous emission radiative recombination rate per volume (R_{sp}) as a function of carrier density up to 1×10^{19} cm^{-3} for both AlN-delta-GaN QW and conventional $Al_{0.35}Ga_{0.65}N$ QW. Significantly larger TE-polarized R_{sp} is realized for entire carrier density range by the use of AlN-delta-GaN QW, which demonstrates such QW structure is promising for mid- and deep-UV LEDs.

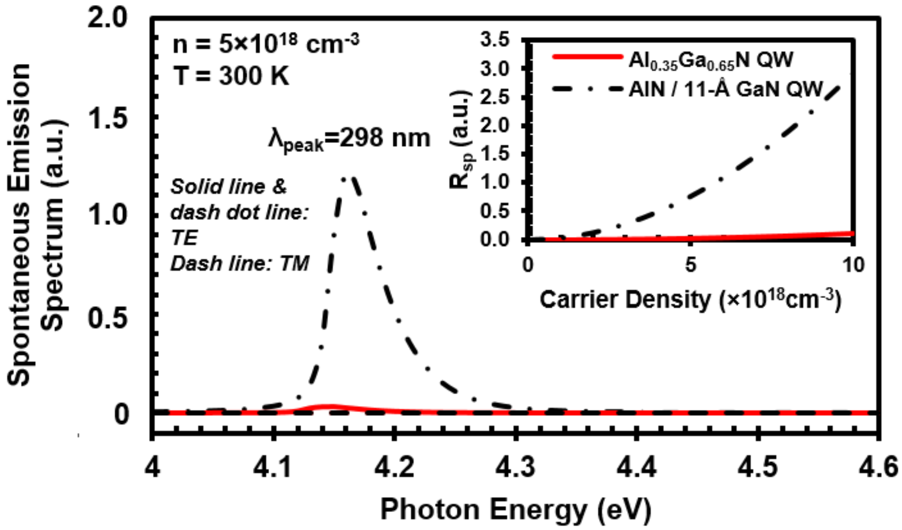

Figure 3. TE-polarized (solid line and dash dot line) and TM-polarized (dash line) spontaneous emission spectra of AlN-delta-GaN QW (black) and conventional $Al_{0.35}Ga_{0.65}N$ QW at n = 5×10^{18} cm^{-3}. Inset: R_{sp} as a function of carrier density up to n = 1×10^{19} cm^{-3} for both AlN-delta-GaN QW and conventional $Al_{0.35}Ga_{0.65}N$ QW.

3. MBE-GROWN ALN-DELTA-GAN QUANTUM WELL

To experimentally confirm the polarization properties of proposed QW structure, an AlN-delta-GaN QW UV LED is investigated in this study, which is grown on AlN/sapphire substrate by plasma-assisted MBE. Figure 4 shows the schematic of the MBE-grown AlN-delta-GaN QW-like LED heterostructure. The active region contains 8-period AlN/GaN QW-like heterostructure which is sandwiched by Mg:$Al_{0.5}Ga_{0.5}N$ and Si:$Al_{0.77}Ga_{0.23}N$ carrier injection layers. From cross-sectional transmission electron microscopy (TEM) image (figure 4), the thickness of the delta-GaN QW layer is precisely controlled as 3-4 monolayers (MLs) while the thickness of the AlN layer is engineered as 2.5 nm. More growth and device fabrication details can be found in Ref.20-23 .

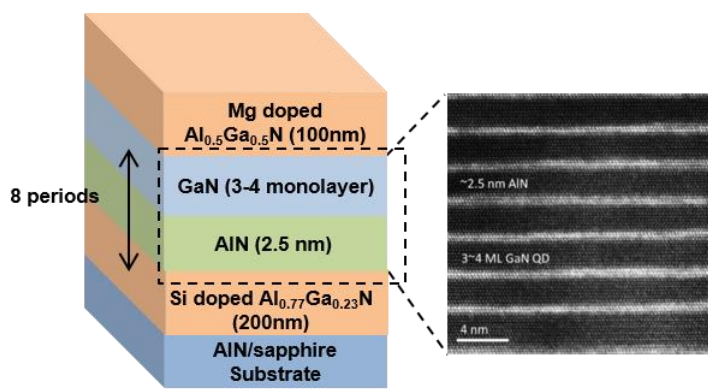

Figure 4. Schematic of MBE-grown AlN-delta-GaN QW UV-LED structure and cross-sectional TEM image of the active region. The thickness of the delta-GaN sub-QW region is 3-4 MLs

The emission properties of the MBE-grown AlN-delta-GaN QW LED were examined by EL measurements. The LED devices were electrically pumped by a pulsed current source with 5% duty cycle and 10 kHz frequency. The emission light was collected by an optical fiber which is connected to a spectrometer. Figure 5 (a) shows EL spectra of the MBE-grown AlN-delta-GaN QW LED with different current densities (***j*** = 2 – 23 A/cm^2). The peak emission wavelength is observed at 298 nm corresponding to the AlN-delta-GaN QW active region, which is similar with the simulation results. Figure 5 (b) exhibits the integrated EL intensity as a function of current density, showing the increasing trend as the current density increase.

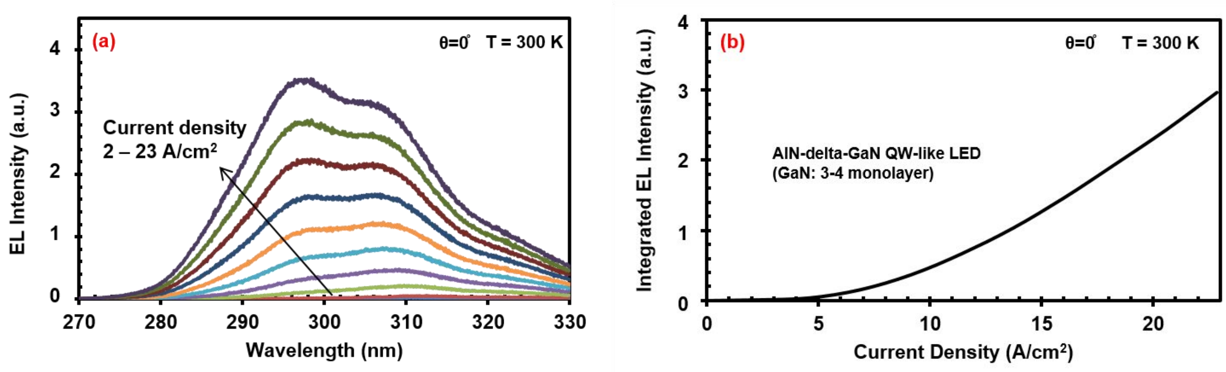

Figure 5. (a) EL spectra from the MBE-grown AlN-delta-GaN QW-like UV-LED with different current density (***j*** = 2 – 23 A/cm^2) (b) Integrated EL intensity of MBE-grown AlN-delta-GaN QW-like UV LED as a function of current injection level at room temperature.

4. POLARIZATION-DEPENDENT EL MEASUREMENT RESULTS

To further study the polarization characteristics of the MBE-grown AlN-delta-GaN QW LED, a polarization-dependent EL setup is built in house and shown in figure 6(a), similar with Refs. 28-31. Specifically, the LED device is fixed on a stationary stage and its emission light is filtered by a Glan-Taylor polarizer and collected by a spectrometer. The polarizer and optical fiber are placed on a rotatable holder. The angle θ represents the rotation angle between c-axis and the optical fiber. In addition, $I_{//}$ (electric field in y-z plane) and $I_{\perp}$ (electric field along x-axis) can be resolved by the rotation of the polarizer about light emitting direction. Note that at a particular angle (θ ≠ 90º), $I_{//}$ and $I_{\perp}$ are not sole TM and TE components, but fulfill the following equations[28-30]:

$$I_{//} = I_{TEy}\cos^2\theta + I_{TM}\sin^2\theta \quad (1)$$

$$I_{\perp} = I_{TEx} \quad (2)$$

where I_{TEx} and I_{TEy} are TE-polarized emission intensities along x and y directions, respectively. In addition, I_{TEx} and I_{TEy} have same value for general case because there is no anisotropic emission in the x-y plane. Therefore, the total TE-component and TM-component lights can be expressed as

$$TE_{total} = I_{TEy}\cos^2\theta + I_{TEx} \quad (3)$$

and

$$TM_{total} = I_{TM}\sin^2\theta \quad (4)$$

Specially, at θ = 90º, the measured $I_{//}$ represents the total TM-component emission while $I_{\perp}$ is identified as the total TE-component. Therefore, several research groups usually study the device polarization properties by applying edge-emitted EL measurements[2, 29].

In this study, the polarization properties were studied at θ = 45º with current density of 40 A/cm^2 and plotted in figure 6(b). The results show the $I_{\perp}/I_{//}$ ratio from MBE-grown AlN-delta-GaN QW UV-LED is 1.149 corresponding to TE/TM ratio of 4.05. The polarization-dependent EL measurements verified the dominant TE-polarized emission from MBE-grown AlN-delta-GaN QW LED. Previous theoretical study in section 2 has demonstrated that the dominant TE-polarized emission is originated from the prevailing C-HH transition. The insertion of the delta-GaN sub-QW region could significantly improve the electron-hole wavefunction overlap and largely separate the ground state HH subband with lower energy subbands, which ensures the sufficient carrier population into HH1 subband and dominant C-HH transition. With the TE/TM ratio of 4.05 for AlN-delta-GaN QW LED at θ = 45º, the degree of polarization ***P***, which is defined as ***P*** = (TE-TM)/(TE+TM), is calculated as 0.60. Large positive ***P*** value indicates large TE-polarized emission as compared to TM-component.

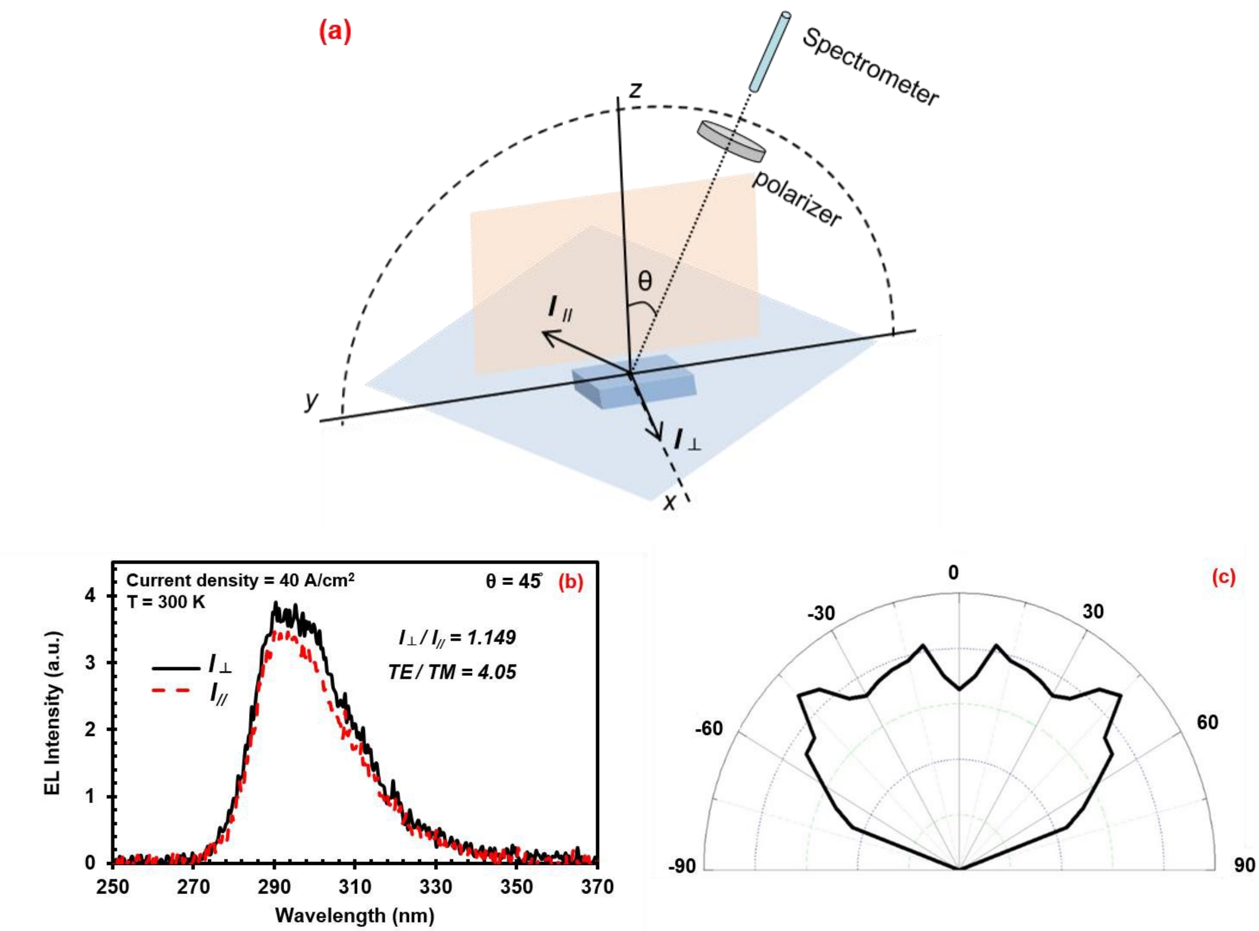

Figure 6. (a) Schematic diagram of the polarization-dependent EL measurements setup, the θ represents the angle between the spectrometer and c-axis; (b) Polarization-dependent EL spectra from the AlN-delta-GaN QW-like LED at θ = 45º with current density of 40 A/cm^2; (c) Light emission pattern of the AlN-delta-GaN QW-like LED with current density of 40 A/cm^2.

The light emission pattern of the MBE-grown AlN-delta-GaN QW LED is also investigated in this study and plotted in figure 6(c). The highest EL intensity is realized at θ = 45º and the rabbit-ear-shape for TM-polarized emission is not obvious in this radiation pattern, which is consistent with the far field pattern of a 320 nm AlGaN QW at ***P*** = 0.6 [32]. Therefore, the light emission pattern of the AlN-delta-GaN QW-like LED again verifies the dominant TE-polarized emission from the proposed structure.

5. SUMMARY

In summary, the polarization characteristics and the underlying physics of 298 nm AlN-delta-GaN QW are investigated in this study. Based on the band structure and wavefunction calculation, the insertion of delta-GaN layer could strongly improve the electron-hole wavefunction overlap and ensure the sufficient carrier population into the ground state HH subband, which results in the dominant C-HH transition. From the 6-band $\boldsymbol{k\cdot p}$ simulation, up to 30-times TE-polarized spontaneous emission rate was achieved by the use of the proposed AlN-delta-GaN QW structure as compared to that of the conventional AlGaN QW. The polarization characteristics of AlN-delta-GaN QW structure were also experimentally investigated in this study by a home-made polarization-dependent EL measurements setup. The measurements on a 298 nm MBE-grown AlN-delta-GaN QW LED with 3-4 ML GaN sub-QW layer confirm the prevailing TE-polarized emission, which indicate the proposed AlN-delta-GaN QW structure is promising for high-efficient mid- and deep-UV LEDs.

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