



Influence of the thickness of p-GaN ohmic contact layer on the performance of AlGaN-based deep-ultraviolet light-emitting diodes

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ABSTRACT

276 nm AlGaN-based deep-ultraviolet light-emitting diodes (DUV-LEDs) with varying p-GaN thicknesses were investigated. The simulation results demonstrate that DUV-LEDs with an ultra-thin 4 nm p-GaN layer exhibit a 96.9% increase in full-angle total radiant intensity compared to those with a 350 nm p-GaN layer. Meanwhile, the total radiant intensity of the DUV-LEDs with 4 nm p-GaN were all elevated during the degree of polarization (DOP) transition from 1 to -1. The experimental results demonstrate that the maximum external quantum efficiency (EQE) and wall-plug efficiency (WPE) values of 5.3% and 4.0%, respectively, at 4 A/cm² for the DUV-LEDs with a 4 nm p-GaN layer. These figures represent remarkable improvements of 60.6% and 42.8% when compared to DUV-LEDs featuring a 350 nm p-GaN layer. Nevertheless, it's worth noting that the adoption of an ultra-thin p-GaN ohmic contact layer introduced some surface irregularities, potentially affecting the ohmic contact of the p-type layer and resulting in a slight voltage increase, thus tempering the WPE improvement. The light extraction efficiency (LEE) values of 10.0%, 7.4%, 6.7% and 6.3% were extracted for the four samples after fitting the experimental EQE curves by the ABC model.

1. Introduction

In recent years, the imperative of developing AlGaN-based deep-ultraviolet light-emitting diodes (DUV LEDs) has reached a consensus due to its characteristics of low-energy consumption, adjustable wavelength, compact size and non-toxic [1–3]. Moreover, the gradual phase-out of mercury-based lighting sources is mandated, making AlGaN-based DUV-LEDs the most promising alternative [4]. Meanwhile, DUV-LEDs, with a wavelength of 200–280 nm, was reported to be effective in killing the virus during the COVID-19 epidemic [3]. Consequently, AlGaN-based DUV-LEDs have garnered substantial interest for applications spanning water treatment, air purification, virus mitigation and gas sensing [5,6]. Despite their potential, currently reported external quantum efficiency (EQE) of DUV-LEDs is substantially lower than that of InGaN-based blue LEDs (80%) [7]. The modest EQE and wall-plug efficiency (WPE) have been major obstacles preventing the

widespread adoption of DUV-LEDs across various domains. Enhancing the luminous efficiency of DUV-LEDs stands as an urgent and pivotal objective [8]. Typically, the EQE is co-defined by the internal quantum efficiency (IQE) and the light extraction efficiency (LEE) [9]. It has commonly been assumed that the IQE of DUV-LEDs exceeds 60% by reducing the threading dislocation density (TDD), adopting a suitable electron-blocking layer (EBL), adjusting the structure of the active region and improving the Mg doping [10,11]. Nevertheless, the EQE and WPE of major commercially available DUV-LEDs are below 10% and 5%, respectively [12,13]. Another critical factor limiting the EQE and WPE improvement of DUV-LEDs is the poor LEE [14].

The critical factors limiting the LEE include TM-polarized dominated light emission in Al-rich AlGaN QWs [15], total internal reflection (TIR) at the interface of two different refractive index layers [16], and high absorptivity of DUV light by p-GaN [17]. The TM-polarized dominated emission makes most of the light perpendicular to the [0001] direction

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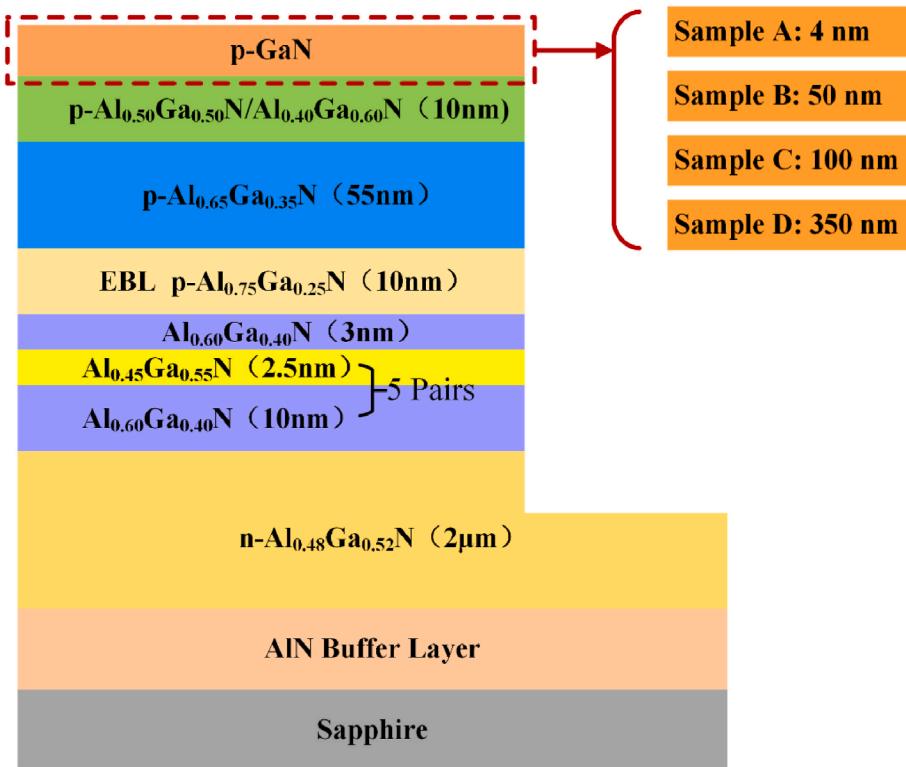


Fig. 1. The schematic diagrams of the DUV-LED with four different p-GaN thickness ohmic contact layers.

and is emitted from the sidewall, severely weakening the light out of the sapphire side for the flip chip [18]. This anisotropic emission is mainly related to the valence band (VB) of AlGaN with high Al content (>0.25) [19]. Several strategies have been reported to be effective in deceasing TM-polarized dominated emission to improve LEE, such as: employing the staggered QWs and the ultra-thin strained QWs [20,21], optimizing the light emission angle of the side wall of the mesa and employing nano-patterned sapphire substrate (NPSS) [22,23]. Meanwhile, substrate surface roughening is the most common technique for destroying interface TIR to improve LEE [24]. Pernot et al. [25] achieved a 1.5 times improvement in the LEE of the 270 nm DUV-LED by fabricating a moth-eye structure on the backside of a sapphire substrate. Liang et al. [26] prepared nano lens arrays (NLAs) by nanolithography and wet etching techniques, resulting in a 24.7% increase in the optical power of DUV-LED. More importantly, p-GaN is adopted as the ohmic contact layer in DUV-LEDs to reduce the Mg activation energy and achieve an excellent ohmic contact. However, the strong absorption of DUV light by p-GaN becomes the thorniest problem that hinders the LEE improvement of DUV-LEDs [27]. To solve this problem, Takano et al. [28] adopted transparent AlGaN: Mg contact layers and Rh high-reflectance electrodes instead of conventional p-GaN and Ni/Au electrodes to substantially improve the LEE, achieving a maximum EQE of more than 20% at a wavelength of 275 nm. However, this approach causes a significant increase in forward voltage, which is not conducive to improving DUV-LEDs electrical properties. In addition, many research groups have proposed other metal electrodes (such as Al, Au, Mg, and Pd) with high UV reflectance to help enhance LEE [29,30]. To avoid affecting the device's electrical properties, Zhang et al. [31] proposed a laterally over-etched p-GaN layer at the top of truncated cones. This scenario can suppress the absorption of DUV by p-GaN without sacrificing the forward voltage. Thinning p-GaN solutions have come into view further to balance the increasing LEE and the growing operating voltage as well as to simplify the process. Zhang et al. [32] used 7.7 nm ultra-thin p-GaN as an ohmic contact layer to achieve a high DUV transparent p-type layer and adopted Ag-nanodots/Al reflective

electrodes to achieve an enhanced LEE. Although thinning p-GaN has been demonstrated to be effective in improving LEE, the effect of ultra-thin p-GaN on other properties of DUV-LED also deserves further exploration.

In this paper, we synthetically investigate the effects of different p-GaN thicknesses on the LEE, light output power (LOP), surface morphology and I-V characteristics of AlGaN-based DUV-LEDs with 276 nm wavelength. The full-angle radiant intensity of the 4 nm p-GaN structure is enhanced by 96.9% compared to that of the 350 nm p-GaN. However, the surface of ultra-thin p-GaN is more discontinuous and inhomogeneous than thicker p-GaN, which directly deteriorates the p-type layer ohmic contact of DUV-LED. Consequently, the voltage of the sample with 4 nm p-GaN is significantly increased, which is detrimental to the improvement of WPE. The experimental EQE curves were well fitted by the ABC model, and the LEE extracted were 10%, 7.4%, 6.7% and 6.3% for the four structures. In addition, the thinned p-GaN brings a significant increase in light transmission, and high resolution X-ray diffraction (HRXRD) confirms the difference in p-GaN thickness in the structure.

2. Structures and parameters

The detailed structure schematics of the DUV-LED with four different p-GaN thickness ohmic contact layers are shown in Fig. 1. Epitaxial structures of DUV-LEDs were grown by metal-organic chemical vapor deposition (MOCVD). The device structure consists of the following: an AlN buffer layer, an n-AlGaN layer (Si: $5 \times 10^{18} \text{ cm}^{-3}$), the luminescent layer consisting of a 5-periodic quantum wells (QWs) and quantum barriers (QBs, Si: $3 \times 10^{18} \text{ cm}^{-3}$), the last barrier layer, the electron blocking layer (EBL, Mg: $1 \times 10^{18} \text{ cm}^{-3}$), the p-AlGaN hole-injection layer (Mg: $3 \times 10^{18} \text{ cm}^{-3}$), and the transition layer with gradient Al component (the Al mole fraction linearly decreased from 0.50 to 0.40), and the topmost layer is the p-GaN ohmic contact layer. We designed p-GaN ohmic contact layers with different thicknesses of 4 nm, 50 nm, 100 nm and 350 nm corresponding to Sample A, Sample B, Sample C and

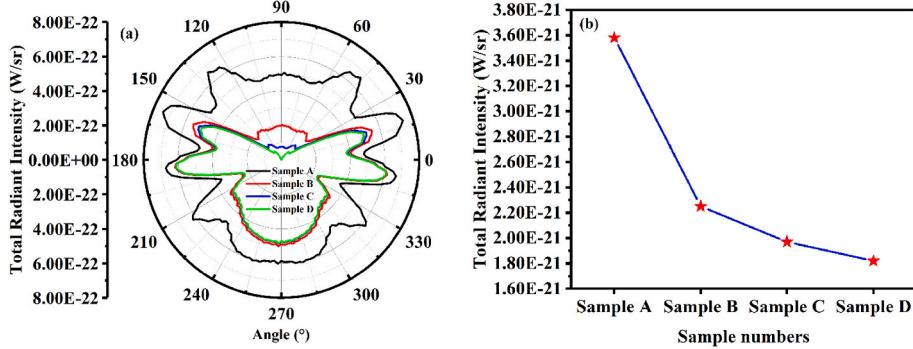


Fig. 2. (a) Simulated angular emission patterns and (b) trend of total radiant intensity for Samples A, B, C and D.

Sample D, respectively. Subsequently, epitaxial wafers of DUV-LEDs were prepared as $500 \times 500 \mu\text{m}^2$ flip-chips. The room-temperature (RT) light output power (LOP) and EL emission spectrum were measured by adopting a calibrated integrating sphere and spectrometer (Everfine). The surface morphology was surveyed by atomic force microscopy (AFM) (Bruker Dimension Edge). High-resolution X-ray diffraction (HRXRD) measurement was performed using Jordan Valley QC3 instrument. The optical transmission spectra measurement was performed using Persee TU-1901 ultraviolet and visible spectrophotometer. In this study, the in-depth physical mechanisms of the DUV-LED structure are investigated by the SILVACO TCAD simulation program. This program calculates full-angle total radiant intensity by solving physical equations such as the Schrödinger equation. In this work, the absorption coefficients and refractive indices of GaN and AlGaN for 275 ± 5 nm deep ultraviolet light can be referred to other literatures [7]. Therefore, the simulated radiant intensity can be applied to represent the LEE. Other parameters for the group III-nitride semiconductor can be found in our previous work [33,34].

3. Results and discussion

To reveal the in-depth mechanism of the LEE enhancement of DUV-LEDs by ultra-thin p-GaN, the angular emission pattern profiles were calculated for DUV-LEDs with different p-GaN thicknesses, as shown in Fig. 2(a). Reich et al. [35] calculated the relationship between the degree of polarization (DOP) and the Al component in the AlGaN quantum well grown on bulk AlN using the $\mathbf{k}\cdot\mathbf{p}$ theoretical model. The TM-polarized emission modes are more than 90% in our designed structure since the Al components of quantum wells and barriers are 45% and 60%, respectively, so set the light emission angle $\theta = 80^\circ$ in our simulation. In Fig. 2(b), we can notice that the total radiant intensity of all angles gradually increases as the p-GaN thickness decreases, with an increase of 96.9% for Sample A compared to Sample D. This proves that adopting an ultra-thin p-GaN ohmic contact layer in DUV-LEDs can effectively increase the light extraction at full angles. In addition, the total radiant intensity decreases exponentially when increasing from 4 nm to 50 nm, decreasing by 58.8%. At the same time, the total radiant intensity increase from 100 nm to 350 nm can be found to decline gradually, decreasing by only 8.3%. This is in basic agreement with the

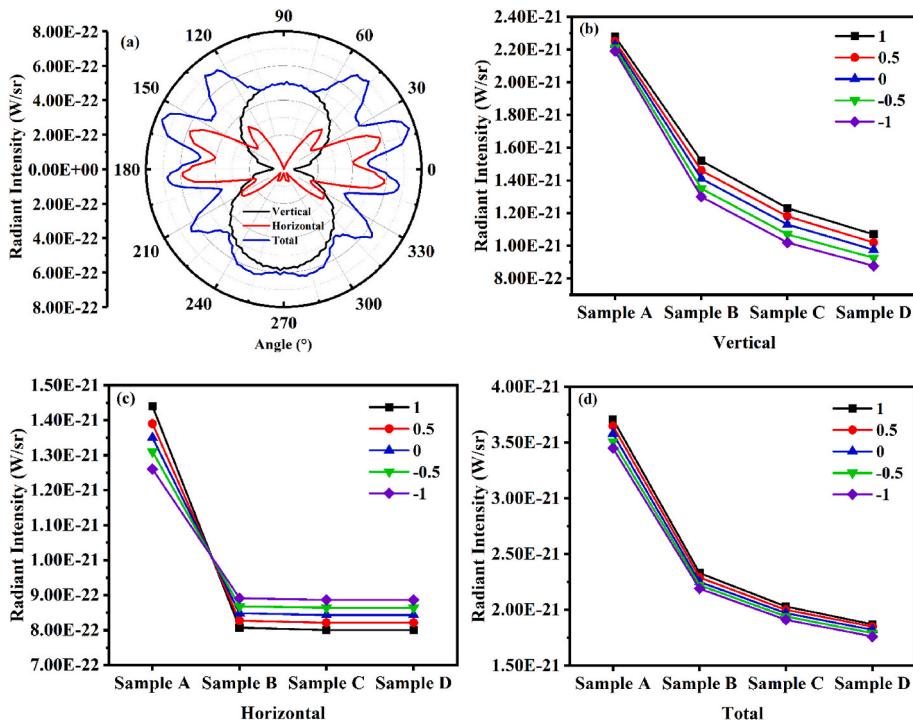


Fig. 3. (a) Simulated angular emission patterns for vertical, horizontal and total radiation intensity (Sample A for example). Radiant intensity with different DOP in (b) vertical, (c) horizontal and (d) total for Sample A, B, C and D.

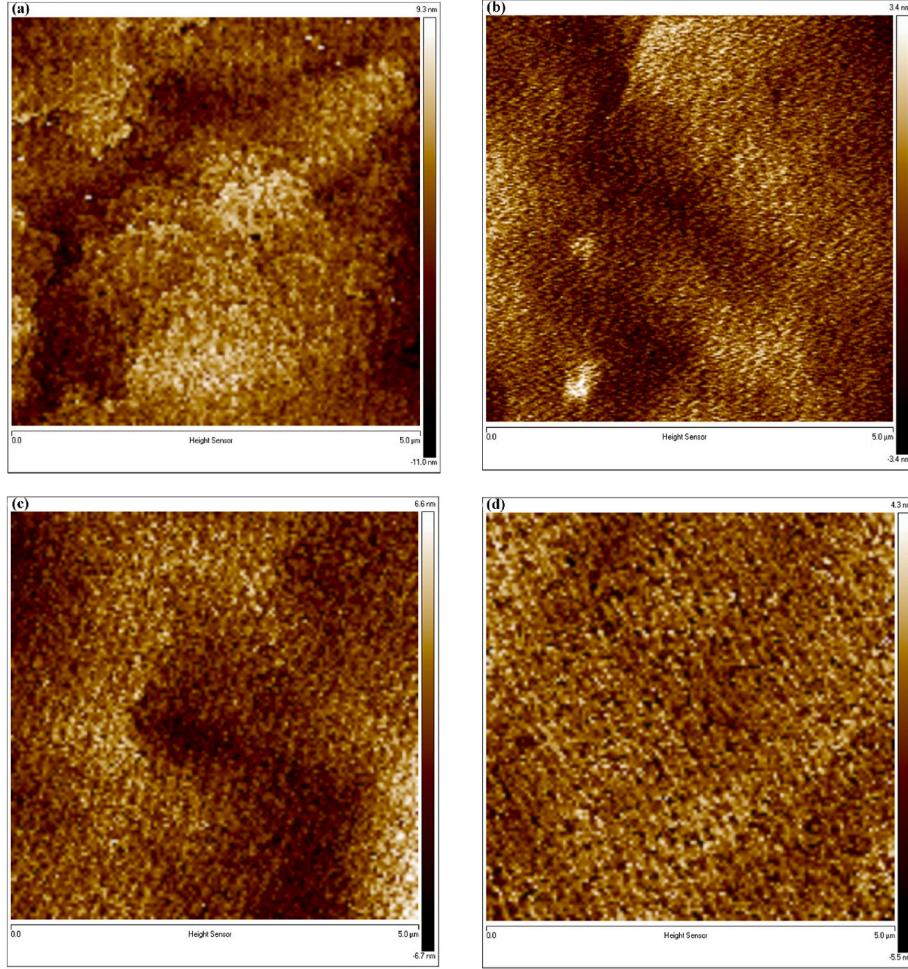


Fig. 4. The $5 \mu\text{m} \times 5 \mu\text{m}$ atomic force microscopy (AFM) images of the surface (p-GaN) of Sample A, B, C and D.

results reported by Zheng et al. [36] that the total LEE variation is minimal when the p-GaN is increased to a certain thickness. It is mainly due to the fact that the p-GaN side entirely absorbs the light incident on the thick p-GaN.

As we designed or shorter wavelength DUV-LEDs in QWs with Al component ≥ 0.45 , it is highly imperative to consider the effect of TE-polarized and TM-polarized light emission on LEE. It has been demonstrated that TM-polarized emission gradually replaces TE-polarized emission as the Al component increases in the QWs, which has a detrimental effect on the light extraction of conventional DUV-LED structures and flip-chips [16]. Accordingly, investigating the relationship between optical polarization emission characteristics and p-GaN thickness can provide new ideas for device design. In general, the TE-polarized and TM-polarized emission modes can be varied in the simulation by changing the light emission angle θ , which is the angle between the light emission path and the c-axis (only the TE-polarized is at $\theta = 0^\circ$ and only the TM-polarized is at $\theta = 90^\circ$) [36,37]. Based on the variation of θ , the electric field intensities I_{\perp} and I_{\parallel} can be calculated by the following equations:

$$I_{\parallel} = I_{TE_y} \sin^2 \theta + I_{TM} \cos^2 \theta,$$

$$I_{\perp} = I_{TE_x},$$

where I_{TM} is the intensity of TM-polarized emission, I_{TE_x} and I_{TE_y} represent the intensities of TE-polarized emission along x and y directions, respectively. The DOP can be calculated as follows:

$$DOP = (TE_{total} - TM_{total}) / (TE_{total} + TM_{total}),$$

where TE_{total} and TM_{total} are integrated optical intensities and calculated as follows:

$$TE_{total} = I_{TE_y} \cos^2 \theta + I_{TE_x},$$

$$TM_{total} = I_{TM} \sin^2 \theta.$$

With different θ from 0° to 90° , we can calculate the different DOP as 1, 0.5, 0, -0.5 , -1 , referring to only TE-polarized, TE-polarized dominant, unpolarized, TM-polarized dominant, and only TM-polarized, respectively. Thus, depending on the variation of DOP from 1 to -1 , we calculated the variation with different p-GaN thicknesses in vertical, horizontal and total radiant intensity, as shown in Fig. 3(a)-(d). In Fig. 3(c), it can be found that the trend of the horizontal radiant intensity of the Sample A during the variation of DOP from 1 to -1 is different from the other three samples, which is that the horizontal radiation intensity of Sample A is decreasing from 1 to -1 . The main reason is that the horizontal radiant intensity includes the components of TM-polarized and TE-polarized emissions. With 4 nm p-GaN, the TE-polarized component in the horizontal direction determines the radiation intensity of the DUV-LED in the horizontal direction because the light absorption is greatly reduced. In addition, the variation magnitude of the horizontal radiant intensity is significantly decreased as the p-GaN thickness increases from 50 nm to 350 nm. This indicates that as the thickness increases, the p-GaN absorption of the DUV light enhances and reaches saturation, so the TM-polarized component determines the horizontal radiation intensity variation. The radiant intensity of the TM-polarized is independent of the p-GaN thickness, so the variation tends

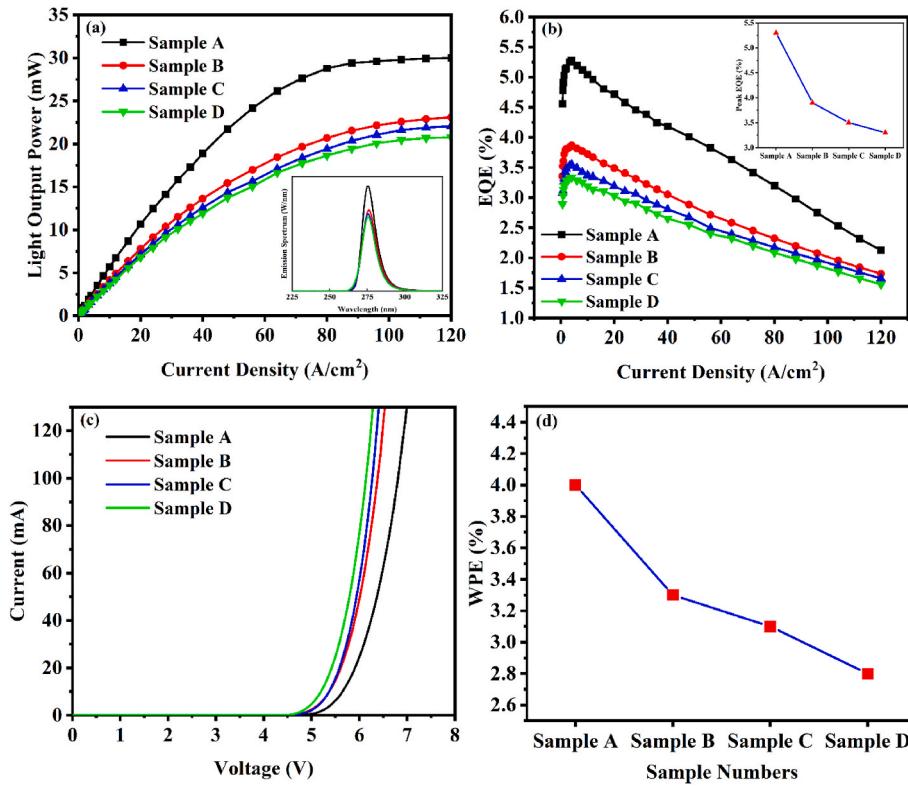


Fig. 5. The experimental results of (a) light output power (LOP) and (b) external quantum efficiency (EQE) as a function of current density; (c) the I-V characteristics of DUV-LEDs with varied p-GaN thickness, (d) the peak WPE trend for Sample A, B, C and D. The inset in (a) shows the EL emission spectra of DUV-LEDs at 100 mA, (b) shows the peak EQE trend.

to be gradual. In Fig. 3(b) and (d), the vertical and total radiant intensity trends are basically the same during the shift of DOP from 1 to -1. Normally, the vertical direction is determined by the TE-polarized fraction. This suggests that the TE-polarized are the main contributor to the LEE in the conventional device structure [38]. More importantly, observing the change of the total radiant intensity with the DOP for the different samples, it can be found that the variety of the total radiant intensity for Sample A, B, C, and D remains identical, i.e., there is a decreasing trend during the DOP from 1 to -1. This result demonstrates that using an ultra-thin 4 nm p-GaN is more beneficial to improve the LEE when the DUV light is in any optical polarization of emission.

Fig. 4(a)-(d) show the AFM images of p-GaN surfaces with different thicknesses. The root mean square (RMS) values of the p-GaN surfaces for Sample A, B, C and D were tested to be 5.71 nm, 3.92 nm, 3.71 nm and 3.16 nm, respectively. These results demonstrate that the use of ultra-thin p-GaN significantly increases the surface roughness. The p-GaN surface uniformity and continuity at 4 nm are the worst in the AFM images. Typically, The Al component in p-AlGaN is less than EBL (75%), which generates compressive stress on p-AlGaN, and the stress and relaxation degree introduced by the lattice mismatch between GaN and p-AlGaN directly affect the growth quality of p-GaN. In addition, the GaN decomposition during the cooling phase of growth thins the p-GaN causing the thickness to be less than the calculated growth thickness [39]. These reasons contribute to the discontinuity and inhomogeneity of Sample A, which may expose the underlying p-AlGaN layer and can directly affect the ohmic contact.

In Fig. 5(a), the LOP continuously decreases as the p-GaN thickness increases. The LOP of Sample A, B, C and D are 28.8 mW, 20.7 mW, 19.4 mW and 18.6 mW, respectively, at a current density of 80 A/cm². The inset of Fig. 5(a) clearly shows that the EL emission wavelengths of the four samples are about 276 nm, and the spectral intensity is greatly enhanced in the 4 nm p-GaN structure compared to the other structures. The function of EQE versus current density is shown in Fig. 5(b). At a

current density of 4 A/cm², the peak EQE for the four samples were 5.3%, 3.9%, 3.5% and 3.3%, respectively. In the inset of Fig. 5(b), it can be found that the trend of the peak EQE variation of the four samples is first steeper and then slower, and is generally consistent with the trend of the total radiant intensity of the simulations mentioned above. This indicates that the change in EQE is caused by LEE. The I-V characteristics of the four samples are shown in Fig. 5(c), and the voltages of Sample A, B, C and D are 6.3 V, 5.9 V, 5.8 V and 5.6 V at 40 mA, respectively. The remarkable increase in voltage of Sample A can be explained in several ways. Firstly, it has been shown that the p-contact resistance increases rapidly as the p-GaN thickness decreases [40]. Moreover, the p-GaN growth process can introduce unintentional aluminium due to diffusion or memory effect of MOCVD, which can reduce the doping efficiency of Mg and result in a lower hole concentration of p-GaN. Secondly, it is known from AFM analysis that there is a risk of exposing the lower AlGaN layer due to the poor continuity of the ultra-thin p-GaN. The poor conductivity of p-AlGaN affects the ohmic contact of the p-type electrode. Finally, the p-GaN contact layer may be too thin to shield the energy band bending caused by band shifts and polarization electric fields, thus increasing the Schottky barrier height [40]. In addition, to verify the feasibility of employing a 4 nm p-GaN ohmic contact layer, we simultaneously fabricated a p-GaN-free structure. The test results were a voltage of 8.5 V at 40 mA and an LOP of 21.4 mW at 80 A/cm². Compared with the 4 nm p-GaN structure, the voltage increases by 34.9% and the LOP decreases by 34.6%. The increase in voltage degrades the WPE drastically and generates more heat. Meanwhile, the absence of p-GaN decreases the Mg doping concentration and is detrimental to forming good ohmic contacts. Therefore, the ultra-thin 4 nm p-GaN is a more suitable thickness for epitaxial growth and improving optoelectronic performance. As can be seen in Fig. 5(d), the peak WPE are 4.0%, 3.3%, 3.1%, and 2.8% for Sample A, B, C, and D, respectively. By comparing Sample A and Sample B at the same current density (4 A/cm²), it can be found that the LOP increases by 37.4%,

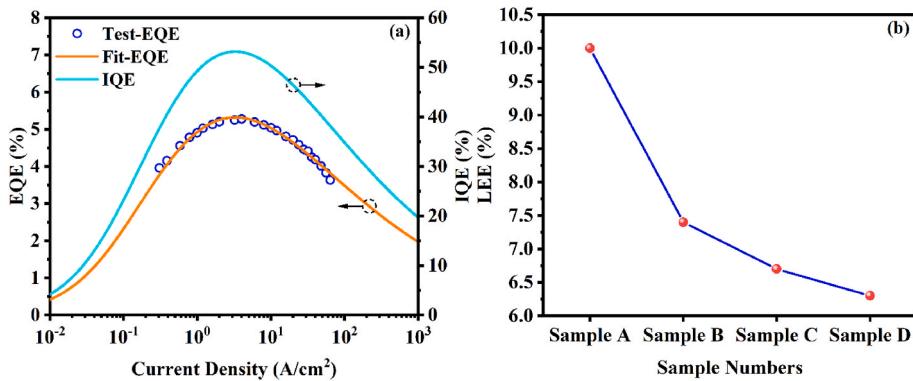


Fig. 6. (a) EQE curve fitting of the DUV-LED with 4 nm thickness p-GaN using the ABC model and the extracted IQE curve, (b) the extracted LEE for Sample A, B, C and D.

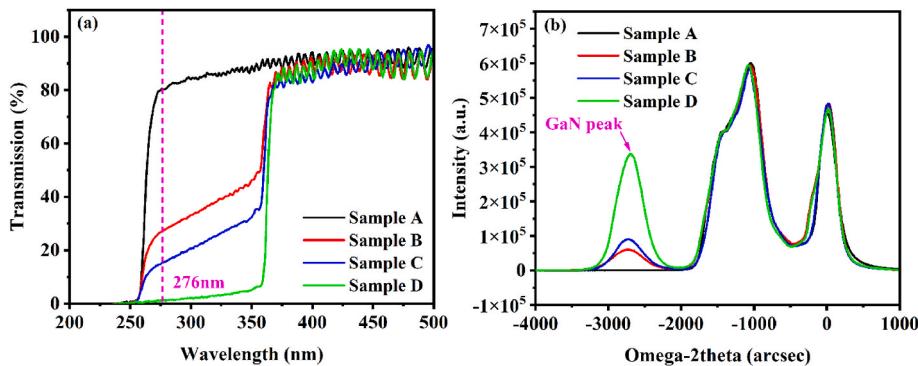


Fig. 7. (a) Optical transmission spectra of DUV-LED structures with different thickness of p-GaN layer and (b) HRXRD ω -2 θ scanning curves of the samples with varied p-GaN thicknesses.

while the WPE increases by 21.2%. This indicates that the increase in voltage hampers the WPE.

To investigate the LEE of DUV-LEDs more comprehensively, the tested EQE curves can be fitted by the carrier recombination model (ABC model). The current density equation is as follows:

$$J = qd(An + Bn^2 + Cn^3)$$

where q is the elementary charge, n is the injected carrier concentration, d is the effective active-region thickness, A is the nonradiative recombination rate, B is the radiative recombination rate and C is the Auger recombination rate. IQE and EQE are defined as:

$$IQE = \frac{Bn^2}{An + Bn^2 + Cn^3}$$

$$EQE = LEE \times \frac{Bn^2}{An + Bn^2 + Cn^3}$$

For the DUV-LED, the asymmetry of carrier transport (the hole mass is much larger than the electron) causes electron-hole recombination to occur mostly in the last quantum well close to the p-type layer. Therefore, in the ABC model fitting of this paper, d is set equal to the thickness of the last well. Other more details can be found in other literature [41]. Sample A fitted EQE curve and IQE curve are shown in Fig. 6(a). The parameters extracted from the fit are as follows: $A = 3.5 \times 10^6$, $B = 3.4 \times 10^{-12}$, $C = 6.4 \times 10^{-31}$, $d = 2.5$ nm, $LEE = 10\%$, and $IQE_{max} = 52.8\%$ at a current density of 4 A/cm². From this, we can calculate the LEE of the other three samples as 7.4%, 6.7% and 6.3%, respectively, with a LEE improvement of 58.7% comparing 4 nm and 350 nm. In Fig. 6(b), it is easy to find that the trend of LEE is consistent with the total radiant intensity of the simulation and the peak EQE variation trend of the

experiment.

In Fig. 7(a), we measured the optical transmission spectra of epitaxial wafers with different thicknesses of p-GaN for normal incidence light. At 276 nm, by comparing the 4 nm and 350 nm p-GaN structures, the light transmission rate of the DUV-LED increases from 1.4% to approximately 80%, which greatly reduces light loss. We will find that the optical transmission rate continues to decrease as the p-GaN thickness increases. As shown in Fig. 7(b), the High-resolution X-ray diffraction (HRXRD) ω -2 θ scanning results of four samples. It can be found that the different peaks on the left side correspond to different p-GaN thicknesses. Since the intensity of the GaN peak in Sample A is more than two orders of magnitude lower than the other samples, the peak is barely visible in the curve. In addition, the other curves are basically the same indicating that the structure is the same except for the thickness of p-GaN.

4. Conclusion

In conclusion, we have comprehensively and systematically investigated the effects of different thicknesses of p-GaN ohmic contact layers on the LEE, LOP, surface morphology and I-V characteristics for AlGaN-based DUV-LEDs emitting at 276 nm. The simulation results show that the total radiant intensity is enhanced by 96.9% compared to 4 nm and 350 nm p-GaN. Meanwhile, the total radiant intensity of the DUV-LEDs with 4 nm p-GaN were all elevated during the DOP transition from 1 to -1. As the p-GaN is thinned, the RMS of the four structures significantly increases, which is 5.71 nm, 3.92 nm, 3.71 nm and 3.16 nm, respectively. Sample A has the worst surface continuity and uniformity, which is not conducive to forming ohmic contacts. The experimental results showed that EQE and WPE were improved by 60.6% and 42.8% by comparing 4 nm and 350 nm p-GaN structures, respectively. Thinning p-

GaN deteriorates the ohmic contact of the device and generates higher Joule heating, which can hinder WPE improvement. The experimental EQE curves were well fitted by the ABC model, and the LEE of the four structures were extracted as 10%, 7.4%, 6.7% and 6.3%, respectively, with a LEE improvement of 58.7% comparing 4 nm and 350 nm. Additionally, optical transmission spectra reveal a significant increase in the transmission rate of light as the thickness of p-GaN decreases. The HRXRD ω -2 θ scanning curves confirm that the four structures are nearly identical except for the difference in p-GaN thickness. This work lays the groundwork for optimizing the structure of DUV-LEDs by thinning the p-GaN layer.

CRediT authorship contribution statement

Yiwei Cao: Writing – review & editing, Writing – original draft, Visualization, Software, Investigation. **Quanjiang Lv:** Writing – review & editing, Software, Project administration, Funding acquisition, Data curation, Conceptualization. **Ju Liu:** Software, Investigation. **Tianpeng Yang:** Validation, Resources, Investigation, Conceptualization. **Tingtong Mi:** Validation, Investigation. **Xiaowen Wang:** Validation, Investigation. **Shuti Li:** Funding acquisition, Software. **Junlin Liu:** Writing – review & editing, Supervision, Project administration, Funding acquisition, Data curation, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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