Analysis of TM mode light extraction efficiency enhancement for deep ultraviolet AlGaN quantum wells light-emitting diodes with III-nitride micro-domes

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Abstract: Analysis of transverse magnetic (TM) mode light extraction efficiency enhancement for AlGaN quantum wells (QWs) based deep ultraviolet (UV) light-emitting diodes (LEDs) with III-nitride micro-hemisphere and micro-dome structures on the p-type layer are studied and compared to that of the conventional deep-UV LEDs with flat surface. The transverse electric (TE) and TM components of the spontaneous emission of AlGaN QWs with AlN barriers were calculated by using a self-consistent 6-band \( k \cdot p \) method, which shows the TM component overtakes the TE component and becomes the dominant contribution of the spontaneous emission when the Al-content of the AlGaN QWs is larger than 0.66. The TM mode light extraction efficiency of the deep-UV LEDs emitting at 250 nm with AlGaN micro-domes as compared to the conventional LEDs with flat surface is calculated based on three dimensional finite difference time domain (3D-FDTD) method. The effects of the III-nitride micro-dome diameter and height as well as the p-type layer thickness on the light extraction efficiency were comprehensively studied. The results indicate optimized light extraction efficiency enhancement (>7.3 times) of the dominant TM polarized spontaneous emission for deep-UV LEDs with III-nitride micro-domes.

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References and links
Introduction

Ultraviolet (UV) light-emitting diodes (LEDs) based on wide band gap AlGaN quantum wells (QWs) with AlN barriers have a wide range of applications in water/air purification, white light illumination, spectrometry and medical phototherapy [1–4]. Different from the InGaN QWs based LEDs [5–10], it is still challenging to pursue high performance deep-UV LEDs with high internal quantum efficiency due to the challenges to grow high Al-content AlGaN QWs active region and the challenges to grow high material quality, efficient conducting and transparent p-type layer. The low external quantum efficiency of the deep-UV III-nitride
LEDs is also significantly attributed by the low light extraction efficiency, due to 1) total internal reflection from the high refractive index of the nitride semiconductors (n~2.4) in contrast to that of the free space (n = 1), and more importantly, 2) domination of the transverse magnetic (TM) component of the spontaneous emission from the high Al-content AlGaN QWs active region, where TM polarization is polarized along the direction normal to the surface, leading to extremely low light extraction efficiency. Recent approaches for enhancing the light extraction efficiency of III-nitride LEDs mainly focus on the visible InGaN QWs based LEDs by using surface roughening [11,12], photonic crystals [13], SiO2/polystyrene colloidal microspheres [14–17], and graded refractive index materials [18]. Potential issues such as non-uniformity, high cost, limited efficiency enhancement, material degradation and reliability are still required to be addressed in these approaches. Very few studies focus on the light extraction efficiency for deep-UV III-nitride LEDs.

The concept of III-nitride micro-dome structures have been used to enhance the light extraction efficiency of thin-film-flip-chip (TFFC) InGaN QWs LEDs, in which the TE polarization component dominates the total spontaneous emission [19]. Experimental realization of GaN micro-domes have been implemented in InGaN QWs based LEDs, which leads to significant enhancement of light extraction efficiency [20,21]. In this paper, we performed numerical calculations and analyses of dominant TM mode light extraction efficiency enhancement for AlGaN/AlN QWs based deep-UV LEDs emitting at 250nm by forming the III-nitride micro-domes on the p-type layer. Studies show that significant light extraction efficiency enhancement is achievable by optimizing micro-dome size and height, as compared to the conventional LEDs with flat surface.

2. 3-D FDTD method for calculation of light extraction efficiency

In this work, we propose to enhance the light extraction efficiency of TM polarized spontaneous emission of AlGaN/AlN QWs based deep-UV LEDs emitting at 250nm by using micro-dome structures on the p-type layer. In this study, the LED light extraction efficiency was numerically calculated by using a three-dimensional finite difference time domain (3D-FDTD) method [22]. Note that in the current studies, the feature size of III-nitride micro-domes is in the range of submicron to micron, which is comparable to the emission wavelength from the AlGaN QWs active region. The traditional calculation of light extraction efficiency based on ray tracing is not as accurate. The 3D-FDTD method solves the differential forms of Maxwell’s equations with specific boundary conditions in complex geometries and obtains rigorous and accurate solutions for the electromagnetic wave propagation. The calculation takes into account the frequency dependence of the refractive index and absorption loss of the III-nitride compounds [23]. The light extraction efficiency is defined as the ratio of total extracted light power to the total power generated in AlGaN QWs. In this simulation, the extracted power from LEDs can be obtained by integrating the Poynting vectors over far field projection surface, and the total power emitted from AlGaN/AlN QWs based deep-UV LEDs were calculated by integrating the Poynting vectors surrounding the near field of dipole source.

As shown in Fig. 1, a single dipole source with defined polarization is placed in the AlGaN QWs active region. The lateral dimension of the computational domain is set as 10μm. The boundary condition of the simulation area is perfectly matched layer (PML) boundaries which absorb electromagnetic energy incident upon them. The near field detection plane is set as λ/n away from the top surface of p-type emission surface, where λ is the peak emission wavelength in vacuum from the QWs and n represents the refractive index of the media. The mesh step is set as less than λ/10n, and the average grid points are estimated around 500000 in the computational domain, which generates reasonable accuracy in light extraction efficiency calculation. The light extraction efficiency calculations were performed for both conventional AlGaN QWs deep-UV LEDs with flat surface and the deep-UV LEDs with III-nitride micro-domes on top of the device. Studies show that the light extraction efficiency of a single dipole source has strong dependence on the position of the single dipole source relative to the micro-dome structures. In this study, we took into account the position dependence of the light...
extraction efficiency of the dipole sources and obtained the average value of the light extraction efficiency of the deep-UV AlGaN QWs LEDs with III-nitride micro-domes.

Fig. 1. 2D Schematics of deep-UV AlGaN QWs LEDs with (a) flat surface; and (b) p-type micro-domes on top of the LEDs for enhancing light extraction efficiency.

As compared to the approach based on surface roughening in current LEDs, the use of micro-domes for enhancing the light extraction efficiency provides the advantages of 1) better uniformity; 2) surface morphology controllability; and 3) tunability of the micro-domes shape and size for QWs emitting at different wavelength. Note that the concept of the micro-domes is applicable to LEDs with backside mirror or thin-film-flip-chip (TFFC) LEDs. Our recent studies on light extraction efficiency for TFFC InGaN QWs LEDs by using GaN micro-domes have indicated significant enhancement of light extraction efficiency [19].

3. Results and analysis

3.1 Transverse electric (TE) and transverse magnetic (TM) components in AlGaN QWs LEDs

In AlGaN QWs deep-UV LEDs, the heavy hole (HH), light hole (LH) and crystal-field split-off hole (CH) energy bands in the valence band cross over between HH/LH and CH bands resulting in dominant TM-polarized spontaneous emission and gain for high Al-content AlGaN QWs [24]. For low Al-content Al_{x}Ga_{1-x}N QWs (x<0.66), the dominant transition is between the conduction and HH/LH bands, that is TE polarized spontaneous emission component. For high Al-content Al_{x}Ga_{1-x}N QWs (x>0.66), the dominant transition is between the conduction band and CH band, which is TM polarized spontaneous emission component [24]. In contrast to the dominant TM-polarized emission from the conventional high Al-content AlGaN QWs, the use of new type of active region such as AlGaN-delta-GaN QWs is expected to result in strong TE-dominated polarized spontaneous emission and optical gain [25,26]. Figure 2 plots the spontaneous emission spectra (R_{sp}) for 3-nm Al_{x}Ga_{1-x}N QWs with AlN barriers with x = 0.58, 0.62, 0.66 and 0.7, respectively. The calculations of the band structure and wave functions for AlGaN QWs were carried out by using a self-consistent 6-band k·p method for wurtzite semiconductors, taking into account the valence band mixing, strain effect, polarization fields, and carrier screening effect [27–29]. The band parameters for the III-nitride alloys utilized in our calculations were obtained from [30,31]. The spontaneous emission spectra were calculated at carrier density n = 1x10^{19} cm^{-3}. From Fig. 2, for the AlGaN QWs with x<0.66 (λ>250nm), the spontaneous emission is dominant with the TE polarized component. As the Al-content increases, the TM polarized component becomes the domination of the total spontaneous emission spectra R_{sp}, in agreement with the finding in [24]. Therefore, in AlGaN QWs based deep-UV LEDs, it is important to design device structures to enhance the light extraction efficiency for the TM polarized spontaneous emission component.
Fig. 2. Spontaneous emission spectra (TE and TM modes) for Al\textsubscript{x}Ga\textsubscript{1-x}N QWs LEDs with x = 0.58, 0.62, 0.66, and 0.7. TM spontaneous emission component becomes dominant when x > 0.66.

3.2 Source position dependence analysis of light extraction efficiency for deep-UV AlGaN QW LEDs with III-nitride micro-domes (micro-hemispheres)

To study the effects of the III-nitride micro-dome (micro-hemisphere) size and p-type layer thickness on the light extraction efficiency of the TM polarized spontaneous emission component in AlGaN QWs deep-UV LEDs, Fig. 3 shows the light extraction efficiency enhancement of the AlGaN QWs LEDs ($\lambda_{\text{peak}} = 250$ nm, full width half maximum (FWHM) = 10 nm) with different source positions along the micro-dome diameter. Figure 3(a) shows the schematics of two parameters: micro-dome diameter ($D$) and p-type layer thickness ($P_{\text{type}}$), which were used for the extraction efficiency calculation. Figure 3(b) plots the light extraction efficiency of the TM dipole source ($\lambda = 250$ nm) located along the diameter of the micro-dome with various diameters ($D = 100$ nm up to 500 nm). The top p-type layer thickness is set as 300 nm. Studies show that the light extraction efficiency strongly depends on the position of the TM dipole source along the diameter of the micro-domes with $D > 300$ nm: the extraction efficiency reaches maximum for the dipole source locating around the center region under the micro-domes, and decreases along the radius of the micro-domes. For $D < 300$ nm, the light extraction efficiency of the TM polarized $R_e$ is relatively constant for the dipoles locating along the diameter of the micro-domes. Note that the case for $D = 0$ represents the conventional AlGaN QWs LEDs with flat surface.

The light extraction efficiency of the TM dipole sources located along the diameter of the micro-domes with various p-type layer thicknesses was also investigated. Figure 4 shows the light extraction efficiency as a function of TM dipole source position along the micro-dome diameter. The p-type layer thickness ranges between $P_{\text{type}} = 300$ nm to $P_{\text{type}} = 700$ nm. The diameter of micro-dome is set as $D = 500$ nm. Note that the light extraction efficiency of the conventional AlGaN QWs deep-UV LEDs with flat surface was calculated for comparison, in which the p-type layer thickness is 300 nm. The studies show that the light extraction efficiency has a strong position dependence of the TM dipole source along the diameter of the micro-domes, when the p-type layer thickness is thinner than 400 nm. The light extraction efficiency shows less position dependence for p-type layer thickness $P_{\text{type}} > 400$ nm.
Fig. 3. (a) Schematic of AlGaN QWs LEDs with p-type micro-hemispheres, where $D$ represents the diameter of the micro-hemisphere and $P_{\text{type}}$ represents the thickness of the p-type layer; and (b) TM mode light extraction efficiency as a function of the TM dipole source position relative to the micro-hemispheres with $D = 0$ (flat surface), $D = 100\text{nm}$, $D = 200\text{nm}$, $D = 300\text{nm}$, $D = 400\text{nm}$, and $D = 500\text{nm}$.

Fig. 4. TM mode light extraction efficiency as a function of the TM dipole source position relative to the micro-domes with p-type layer thickness of $P_{\text{type}} = 300\text{nm}$, $P_{\text{type}} = 350\text{nm}$, $P_{\text{type}} = 400\text{nm}$, and $P_{\text{type}} = 700\text{nm}$. The micro-hemisphere diameter is set as $D = 500\text{nm}$.
3.3 Effect of micro-dome (micro-hemisphere) size and p-type layer thickness on light extraction efficiency for deep-UV AlGaN QW LEDs

The total light extraction efficiency of the TM polarized spontaneous emission component of the deep-UV AlGaN QWs LEDs (λ = 250nm) considering source position dependence for different diameter of micro-hemispheres were calculated. Figure 5(a) plots the ratio of the light extraction efficiency enhancement of the AlGaN QWs LEDs (λ_{peak} = 250nm, FWFM = 10nm) with III-nitride micro-hemispheres as a function of the micro-hemisphere diameter (D). The top p-type layer thickness is constant of 300nm. Note that the extraction efficiency enhancement for D = 0 represents the case for the conventional LEDs with flat surface, which is normalized to 1. As the micro-hemisphere diameter D increases, the light extraction efficiency enhancement ratio increases. The enhancement ratio increases significantly from 1 (D = 0) to 5.7 (D = 200nm). As the micro-hemisphere diameter D increases from D = 200nm to D = 600nm, the enhancement ratio increases slightly. Considering of the limited p-type layer thickness in real devices, it is favorable to form relatively small diameter of the micro-hemispheres (D<200nm) to eliminate potential effect on the AlGaN QWs active region.

![Graph](image)

Fig. 5. (a) Light extraction efficiency enhancement of the TM polarized spontaneous emission component for AlGaN QWs LEDs with AlGaN micro-hemispheres emitting at 250nm as a function of the micro-hemisphere diameter, and (b) Light extraction efficiency of the TM polarized spontaneous emission component for AlGaN QWs LEDs with AlGaN micro-hemispheres emitting at 250nm as a function of the p-AlGaN layer thickness. The micro-hemisphere diameter is 500nm. The light extraction efficiency of conventional deep UV LEDs with flat surface is plotted as a comparison.
The dependence of the light extraction efficiency of the TM polarized spontaneous emission component for the deep-UV AlGaN QWs LEDs ($\lambda_{\text{peak}} = 250\text{nm}$) with various p-type layer thicknesses was studied and the results are shown in Fig. 5(b). The light extraction efficiency of the TM polarized component for the conventional LEDs with p-type thickness of 300nm is plotted as reference. The light extraction efficiencies of the TM polarized component for the LEDs with III-nitride micro-hemispheres (D = 500nm) were calculated for various p-type layer thickness from 300nm up to 700nm. Large enhancement of the light extraction efficiency was observed for different p-type layer thickness. The enhancement factor ranges between 5.8 and 6.2 times for the deep-UV LEDs with III-nitride micro-hemispheres (D = 500nm) as compared to that of the conventional LEDs with flat surface, which indicates there is no strong dependence of the light extraction efficiency of the TM polarized spontaneous emission component on the p-type layer thickness. The LEDs with p-type layer thickness of 300nm shows the largest enhancement of 6.2 times. Considering of the growth challenges of high quality p-type layer in deep-UV AlGaN QWs LEDs [32,33], relative thin p-type layer thickness ranges between 200 and 300nm is preferable for the epitaxy of the LED device.

3.4 Effect of micro-dome size and shape (micro-hemiellipsoid) on light extraction efficiency for deep-UV AlGaN QWs LEDs

The light extraction efficiency from deep-UV AlGaN QWs LED with micro-domes was studied by tuning the micro-dome height h ($h \neq D/2$). The results show that optimized micro-dome structure for the maximum light extraction efficiency is not necessary occurred from the micro-domes with $h = D/2$ (micro-hemisphere). The geometric structure of the general micro-dome structure on p-type layer is shown in Fig. 6(a), where D represents the diameter of the micro-domes and h represents the height of the micro-domes ($h \neq D/2$).

![Fig. 6. (a) Schematic of AlGaN QWs LEDs with p-type micro-domes, where D represents the diameter of the micro-dome and h represents the height of the micro-dome, and (b) Light extraction efficiency enhancement ratio of the TM polarized spontaneous emission component for AlGaN QWs LEDs with micro-domes emitting at 250nm as a function of the micro-dome height h. The yellow squares indicate the cases for micro-hemispheres ($h = D/2$).](image-url)
Taking into account the TM source position dependence, the total light extraction efficiency enhancement ratio was calculated and plotted in Fig. 6(b) for micro-dome diameter sizes $D = 100\text{nm}$, $D = 125\text{nm}$, $D = 200\text{nm}$, $D = 300\text{nm}$ and $D = 500\text{nm}$ with different micro-dome height ranging from $h = 0$ (flat surface) to $h = 250\text{nm}$. The cases for $h>250\text{nm}$ were not calculated due to the limitation of p-type layer thickness ($P_{\text{type}} = 300\text{nm}$). Note that the yellow squares on each curve indicate the light extraction efficiency with micro-hemisphere structure ($h = D/2$). The light extraction efficiency at $h = 0$ represents the case for the conventional LED with flat surface. From Fig. 6(b), the optimized micro-dome structure for the highest light extraction efficiency occurs when $h>D/2$ for the micro-dome structures with $D = 100\text{nm}$, $D = 125\text{nm}$ and $D = 200\text{nm}$. For micro-domes with diameter $D = 300\text{nm}$ and $D = 500\text{nm}$, the light extraction efficiency increases as the increase of micro-dome height (here, the height of the micro-domes are limited by the p-type layer thickness). For deep-UV AlGaN QWs LED with III-nitride micro-domes emitting at 250nm, the light extraction efficiency could be optimized by tuning both the diameter $D$ and the height $h$ of the micro-domes. The optimized enhancement ratio of 2.4, 7.2, 7.3, 6.8 and 6.1 could be achieved at $\lambda_{\text{peak}} = 250\text{nm}$ for the micro-dome diameter of $D = 100\text{nm}$, $D = 125\text{nm}$, $D = 200\text{nm}$, $D = 300\text{nm}$ and $D = 500\text{nm}$, respectively.

3.5 Far field TM polarized emission pattern from deep-UV AlGaN QWs LED with III-nitride micro-domes

Figure 7 plots the far field TM polarized emission pattern (with 90° as the normal to the LED emission surface) for AlGaN QWs deep-UV LEDs with flat surface, with micro-hemispheres ($D = 200\text{nm}$ and $D = 500\text{nm}$, $P_{\text{type}} = 300\text{nm}$) and with micro-domes ($D = 200\text{nm}$, $h = 175\text{nm}$, $P_{\text{type}} = 300\text{nm}$). The far field emission pattern indicates that the LED structure with III-nitride micro-hemispheres has significant enhancement of the TM emission component for a wide range of angles, especially in the directions normal to the LED device surface. By tuning the height of the micro-hemisphere to form the micro-dome structures, the light extraction efficiency could be further enhanced. From Fig. 7, the light extraction efficiency of TM polarized spontaneous emission component is significantly enhanced in a wide range of angles by using the micro-dome structures. The increase in far field radiance of the deep-UV LEDs with III-nitride micro-domes can be attributed to the enhanced scattering of photons and enlargement of the photon escape cone from the micro-domes.

![Fig. 7. Far field emission pattern of the TM polarized spontaneous emission component for deep-UV AlGaN QWs LEDs with (a) flat surface (x3); (b) AlGaN micro-hemispheres ($D = 200\text{nm}$), (c) AlGaN micro-hemispheres ($D = 500\text{nm}$), and (d) AlGaN micro-domes ($D = 200\text{nm}$, $h = 175\text{nm}$). The p-type layer thickness is 300nm.](image-url)
4. Summary

In summary, 3-D FDTD simulations were performed to calculate the light extraction efficiency for both conventional AlGaN QWs deep-UV LEDs with flat surface and the LEDs with III-nitride micro-domes. The studies focus on the enhancement of light extraction efficiency of TM-polarized spontaneous emission component, which is the dominant component in AlGaN QWs deep-UV LEDs. With p-type layer thickness of 300nm and III-nitride micro-dome diameter of 200nm and height of 175nm, the TM polarized light extraction efficiency shows 7.3 times enhancement as compared to that of the conventional LEDs. The far field pattern shows significant enhancement of TM-polarized extraction efficiency for a wide range of polar angles. The design of the LEDs with III-nitride micro-domes has great potential to significantly enhance the total light extraction efficiency of the AlGaN QWs deep-UV LEDs, which will contribute to enhancement of the total external quantum efficiency of the LEDs.

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