Optimizing light extraction efficiency in inclined sidewall type ultraviolet light-emitting diodes with nanopatterned sapphire substrates and photonic crystals

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Research Article

Keywords: Substrate patterning, inclined sidewall, light extraction efficiency, numerical simulation

Posted Date: October 29th, 2023

DOI: https://doi.org/10.21203/rs.3.rs-3491123/v1

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Additional Declarations: No competing interests reported.
Abstract

Herein, we focus on the performance optimization of inclined sidewall (IS) type ultraviolet (UV) light-emitting diodes (LEDs) with either nanopatterned sapphire substrates (NPSSs) or photonic crystals (PCs). The simulation results demonstrate the introduction of substrate patterning plays a crucial role in unlocking the potential of IS type UV LEDs by reducing the generation of high mode resonance within the device. The use of NPSSs design performs exceptionally well in extracting transverse-magnetic (TM) polarized light due to its superior alignment with the inclination design. As a result, the total light extraction efficiencies (LEEs) are significantly improved, increasing from 36.0–57.3%.

1. Introduction

In recent years, there has been a notable trend to phase out conventional mercury lamps in favor of promising alternatives, e.g., ultraviolet (UV) light-emitting diodes (LEDs). The shift is driven by the unbeatable advantages of UV LEDs, including lower power consumption, and their more environmentally-friendly nature compared to mercury lamps (Muramoto et al. 2014). Beyond energy conservation and environmental protection, UV LEDs have also revolutionized various fields with new applications, such as sterilization, intelligent sensing, and promoting plant growth (Kneissl et al. 2019). Notably, the internal quantum efficiencies (IQEs) of UV LEDs have been reported to reach an impressive value of 93% (Sun et al. 2019). However, external quantum efficiencies (EQEs), which are the product of IQEs and light extraction efficiencies (LEEs), an essential indicator evaluating output performance of UV LEDs, have largely remained below 10% (Zheng et al. 2021; Inoue et al. 2017; Wang et al. 2018). The primary bottlenecks for achieving high-efficient and high-power UV LEDs stems from unfavorable LEEs. One particular challenge lies in the refractive index mismatch between the nitride layer and air in UV LEDs with flat substrates, leading to severe total internal reflection (TIR). To mitigate this issue, researchers have explored the use of nano-patterned sapphire substrates (NPSSs) and other optical design concepts to weaken TIR and enhance LEEs (Zhou et al. 2022; Zhmakin 2011). While these methods have shown some success, they have not fully addressed the following two critical challenges.

The first challenge involves the strong parasitic absorption of UV photons in thick p-GaN and electrode materials, which cannot be neglected (Hirayama et al. 2014). Moreover, an increase in the Al component in Al\(_x\)Ga\(_{1-x}\)N (aluminum gallium nitride) layer leads to a higher proportion of transverse-magnetic (TM) (E\(_\parallel\)c) polarized light due to changes in the valence band configuration of Al\(_x\)Ga\(_{1-x}\)N (Xu et al. 2019). However, TM polarized light propagates along the plane whose normal direction parallel to c, hindering light extraction and causing light absorption. Extensive efforts were made through experiments and theoretical simulations to address these two issues. To overcome the parasitic absorption challenge, researchers proposed highly efficient UV LED designs featuring a transparent p-AlGaN contact layer and a high-reflective p-type electrode, resulting in an enhanced LEE and EQE (Maeda and Hirayama 2013). Additionally, the challenge of higher Al component in the active layer and the resulting dominance of TM polarized light has been tackled through innovative chip designs with reasonably sloped sidewalls (Lee et al. 2016; Kim et al. 2015; Luo et al. 2022). For example, researchers have experimented with various
sidewall angles UV micro-LEDs, demonstrating significant improvement in EQEs for LEDs with inclined sidewalls compared to those with perpendicular counterparts (Tian et al. 2021). Others have investigated front and sidewall emission of micro-scale LEDs by designing inclined sidewalls coated with an omni-directional reflector (ODR), leading to substantial increase in total LEE and decreases in sidewall LEEs (Hu et al. 2022). While UV LEDs have seen substantial progress and adoption in recent years, their full potential in terms of EQEs and LEEs is yet to be unlocked.

Inspired by the concept of inclined sidewall type designs in UV LEDs, we present the advanced optical structures that combines inclined sidewall with substrate patterning. Such an optical structure fully exploits the immense potential of inclined sidewall and substrate patterning. The optical performance of this type of UV LEDs is assessed by numerical simulations. The simulation results reveal a significant improvement in light extraction efficiency, attributed to the mitigation of high-order resonance mode generation within the device. Specifically, the enhancement in light extraction efficiency increases from 36.0–57.3%. To gain deeper insights into the light-extraction mechanism, we examine the spatial electric field distribution inside the device. Notably, such a UV LED with a sidewall angle of 40° demonstrates excellent capabilities in extracting TM polarized light. By combining inclined sidewall angles and substrate patterning, our approach opens up exciting possibilities for advancing UV LEDs’ performance and expands their applications in various fields.

2. Modeling and simulation methods

In this study, we employed the finite element method to obtain spatial-resolved electromagnetic distributions, by solving Maxwell’s equations coupled with the frequency domain response (Li et al. 2022). Perfectly matched layers (PMLs) with a fixed thickness of 300 nm to absorb electromagnetic wave of top and bottom boundaries were employed. The simulation structures were simplified by setting the lateral size to 15 µm, and using perfect electric conductors (PECs) at the boundaries. Additionally, the finite sapphire thickness of 2 µm was used to replace the approximate millimeter-scale substrate thickness. To simulate the light emission process, an individual dipole source positioned at the center of the multi-quantum well (MQWs) region, representing the complex electron-hole pair recombination process and generating electromagnetic waves. The light emitted by dipole propagated predominantly in the plane perpendicular to the polarization direction. This dipole source had an emission wavelength of 280 nm, and the optical constants of related materials were obtained from references (Polyanskiy 2023). To evaluate the change in LEE, detectors at two specific sites, i.e., site 1 was around the dipole source, and site 2 was positioned in the air region. By calculating the Poynting vector of these regions, the ratio of the total power extracted from site 2 and that from site 1 can be obtained, which serves as a representative measure for the LEE.

3. Results and discussions

For flip-chip UV LEDs with a p-GaN layer, the well-designed thickness of the p-GaN layer plays a crucial role in improving light extraction efficiency since that the optical cavity is able to influence angle-
dependent reflectivity through the adjustments in the direction of reflection light (Zhang et al. 2019). This effect can be confirmed through numerical simulations using a simplified model, as depicted in the insert of Fig. 1(a). The simulations involved UV light incidence at various angle $\alpha$ with a fixed wavelength of 280 nm. The lateral boundary conditions were set as periodic boundaries, while the top and bottom boundary conditions utilized PMLs.

Firstly, we investigated the angle-integrated reflectivity (Ref.) of a p-AlGaN/dielectric/metal structure by varying relevant parameters, i.e., electrode materials and the thickness of the p-AlGaN, using numerical simulation simulations, as shown in Fig. 1(a). To illustrate the positive influence of adopting Al electrode materials, we compared two cases: one with Ni and Ag electrodes without a dielectric layer (i.e., dielectric layer thickness $t_d = 0$ nm, metal thickness $t_m = 300$ nm), and the other one with an Al electrode. The values of Ref. for the Ni and Ag cases were relatively low, reaching 38.8% and 36.4%, when the thickness of p-AlGaN was 140 nm. However, the Al electrode case exhibited considerable enhancement in reflectivity. In addition, an oscillation behavior induced by the optical cavity was observed in the p-AlGaN thickness range from 50 to 150 nm, though the fluctuating range was less obvious compared to the counterpart with p-GaN, which is attributed to the strong absorption of the p-GaN layer (Mondal et al. 2021). The maximum reflectivity of 90.0% is obtained when the p-AlGaN thickness was 140 nm. This indicates that the combination of a high-reflection Al electrode and an ultraviolet transparent p-AlGaN film can increase reflectivity by 53.6%. It is worth noting that the combined action of a high-reflectivity electrode and a p-AlGaN UV-transparent layer is crucial for enhancing reflectivity. This p-AlGaN/dielectric/metal structure can also be effectively utilized to design sidewall omni-direction reflection structures (ODRs) (Zheng et al. 2020; Kim et al. 2008).

Figure 1(b) provided a detailed illustration of the angle-integrated reflectivity (Ref.) of the sidewall ODR structure (i.e., the thickness of the dielectric layer $t_d \neq 0$) as a function of the thickness of the dielectric layer. The reflectivity curves for different dielectric materials, such as MgF$_2$ ($n_m = 1.39$ at wavelength of 280 nm) ODR (red line), SiO$_2$ ($n_s = 1.49$ at wavelength of 280 nm) one (blue line), and HfO$_2$ ($n_h = 2.05$ at wavelength of 280 nm) one (black line), displayed similar periodic oscillation behaviors due to the effect of the optical cavity. It was observed that during the variation of $t_d$, the ODR structure with MgF$_2$/Al acted as an excellent antireflection design, indicating that a smaller refractive index of the dielectric layer increases the angle-integrated reflectivity of the sidewall ODR structure (Oh et al. 2017). To elucidate the underlying reasons for the positive role of MgF$_2$ in enhancing reflectivity, angle dependent reflectivity and spatial electric field distribution were investigated, as shown in Fig. 1(c)-(d). Figure 1(c) demonstrates angle dependent reflectivity (Ref.$\alpha$) curves for the cases with/without MgF$_2$ layer. It is evident that the Ref.$\alpha$ curve of case with MgF$_2$ layer exhibits nearly omnidirectional enhancement compared to the other case, as shown in Fig. 1(c). The normalized distributions of electric-field intensities for 0° and 40° cases for p-AlGaN/MgF$_2$/Al and p-AlGaN/Al structures are depicted in Fig. 1(d). The significant impedance differences at the interface can lead to serious internal reflection phenomena (Son et al. 2012). In the 40° case, the parasitic absorption in the Al electrode was prevented due to the existence of total internal reflection at the p-AlGaN/MgF$_2$ interface.
Figure 2(a) illustrates the schematic diagram of the simulated device with a NPSS or/and PC structure. The thicknesses of the sapphire substrate, AlN buffer layer, n-AlGaN electron transport layer, MQWs (multiple quantum wells), p-AlGaN hole transport layer, Al metal layer were set to 2 µm, 3 µm, 2.2 µm, 58 nm, 140 nm, 300 nm, respectively. The typical parameters of NPSSs or PCs were fixed at 1.5 µm (Period $p$) and 1.1 µm (height $h$), respectively. Notably, the UV LED featured an inclined sidewall with a 250 nm-thick MgF$_2$ dielectric interlayer and an Al metal cladding layer. Figure 2(b) displays the radiation pattern emitted by a single electric dipole. The left side of Fig. 2(b) clearly shows that: 1) The direction of the dipole moment is along the y-axis parallel to the direction of film growth. 2) Emission along the x-axis is much stronger than that along the y-axis, indicating anisotropic emission (Kim et al. 2015). 3) Most of the emitted light travels along the x-axis. In contrast, the main propagation direction of TE (transverse-electric) polarized light is perpendicular to TM polarized light on the right side of Fig. 2(b). For UV LEDs featuring an inclined sidewall structure, adopting a rational sidewall angle can significantly improve LEEs (Tian et al. 2021). Therefore, the results in Fig. 2(c)-(d) provide further insights into the influence of the sidewall angle $\theta$, ranging from 25° to 85°, on LEEs in UV LEDs with an inclined sidewall coated with an ODR structure. Figure 2(c) shows the effect of various structure designs, i.e., inclined sidewall (IS), composite design of inclined sidewall and NPSSs (IS & NPSS), and composite design of inclined sidewall and PCs (IS & PC) on TM polarized light extraction in detail. It is evident that LEEs for all three cases display similar trends as the sidewall angle $\theta$ changes. Specifically, LEEs increase to a maximum for a sidewall angle $\theta$ of up to 40°, and then decrease as the sidewall angle $\theta$ increases from 40° to 85°. Furthermore, at a sidewall angle $\theta$ of 40°, the UV LED with IS exhibits the lowest LEE value of 40.8% among the three structure designs. Notably, the latter two cases show significant LEEs enhancement compared to UV LEDs with an IS structure, indicating that the addition of NPSSs or PCs can tap into the greater potential of the inclined sidewall ODR structure. Similarly, Fig. 2(d) demonstrates the light extraction of TE polarized light for the IS, IS & NPSS, and IS & PC structure designs at different sidewall angles. Compared to the IS type structure, the IS & NPSS type and IS & PC type structure designs exhibit higher LEEs for all sidewall angles $\theta$, suggesting that the LEEs enhancement for the latter two structure designs can be attributed to the existence of a roughened interface. Figure 2(e) summarizes the LEEs at a sidewall angle $\theta$ of 40° for the IS, IS & NPSS, and IS & PC structure designs. The IS & NPSS structure design demonstrates the highest LEE value. On the other hand, TE polarized light is more sensitive to the IS & PC structure among the three typical structures. It is observed that the IS & NPSS type and the IS & PC structure can improve total LEEs by 21.3% and 18.3%, respectively, compared to the IS structure. The ratio of TM polarized and TE polarized light follows the reference (Mondal et al. 2021), and further discussion on this aspect will be presented in the later section. Notably, Fig. 2(f) depicts the LEEs response with polarization angles of the dipole moment. The information contained in Fig. 2(f) suggests that: 1) The LEE of UV LED with the IS & NPSS structure is the least sensitive to the orientation of the dipole moment among the three structure cases. 2) Typical orientations of the dipole moment, i.e., TE and TM polarized light cases, align with the results shown in Fig. 2(c)-(e). 3) The LEE values from this figure provide valuable reference for MQWs.
A deeper understanding of the light-extraction mechanism of UV LEDs with IS, IS & PC, IS & NPSS structures at a sidewall angle $\theta$ of 40° is revealed through the spatial electric field distribution in Fig. 3. In the case of TM polarized light, the radiation patterns of the IS and IS & PC structures were basically similar. However, the incorporation of NPSSs at the sapphire/AlN interface disrupted these patterns, preventing the generation of numerous hot spots in the AlN region. These hot-spots are a result of high-orders mode resonance (Yang et al. 2019). As depicted in Fig. 3(a) and Fig. 3(c), the IS and IS & PC structures showed clear hot spots in regions such as AlN and AlGaN, indicating that light was trapped in these regions. This observation further underscores the superior LEEs value of the IS & NPSS structure compared to the IS & PC structure at a sidewall angle $\theta$ of 40°. In contrast, as shown in Fig. 3(f), although NPSSs help in reducing the formation of hot-spots in the AlN region to extract a higher proportion of light, the extracted light propagates laterally in the sapphire region, which is not conducive to further extraction into the air region. Conversely, the presence of PCs in the IS & PC structure alters the radiation pattern of TE polarized light compared to the IS case, as shown in Fig. 3(b) and 3(d), allowing a higher ratio of light to leak into the air region. This improvement in light extraction in the air region can be attributed to the reduction in high-mode resonance generation within the device (Qian et al. 2023).

Furthermore, Fig. 4 presents angle-dependent transmissivity (Tra.) curves and the corresponding electric field distributions for PC and NPSS substrates at $\beta = 0°$ and 10°. This additional information provides further insights into Fig. 2(e). The results reveal that a significant portion of TM polarized light experiences reflection by inclined ODR structures and redirects towards the vicinity of $\beta = 10°$ (Lee et al. 2016; Zheng et al. 2020). As a consequence, UV LEDs employing the IS & NPSS design outperform these with IS & PC design in terms of extracting TM polarized light. Notably, the simulated results from Fig. 4(b) demonstrate complete agreement with Fig. 4(a).

4. Conclusions

In summary, we introduced two optical designs (i.e., IS & NPSS and IS & PC), and conducted a series of numerical investigations to explore their optical performance in UV LEDs. By analyzing spatial electric field distributions, we elucidated the light-extraction mechanism. The results demonstrate the significant influence of sidewall angle on LEEs. Notably, a sidewall angle of $\theta = 40°$ greatly enhances LEEs of TM polarized light. Furthermore, the IS & NPSS (LEE = 57.3%) and IS & PC (LEE = 54.3%) designs effectively increase the light-extraction potential compared to the IS structure (LEE = 36.0%), mainly by reducing the generation of high mode resonance within the device. Importantly, our findings highlight the crucial role of rational substrate design in extracting light redirected by sidewall ODR structures. We anticipate that this research will garner attention and contribute to the advancement and commercialization of highly efficient AlGaN-based UV-LEDs.

Declarations

Funding. This work was supported by the National Natural Science Foundation of China under Grant 61974149; by the Youth Innovation Promotion Association of the Chinese Academy of Sciences under
Data availability. The data that support the findings of this study are available from the corresponding author upon reasonable request.

Disclosures. The authors declare no conflicts of interest.

References


**Figures**
Figure 1

(a) Angle-integrated reflectivity (Ref.) for p-AlGaN/metal (i.e., Al, Ni and Ag) structures with varying p-AlGaN thickness. (b) Angle-integrated reflectivity (Ref.) for p-AlGaN/dielectric (i.e., MgF$_2$, SiO$_2$ and HfO$_2$)/Al structures with different dielectric layer thickness. (c) Angle dependent reflectivity (Ref.$\alpha$) as a function of the angle of incidence $\alpha$ with/without the MgF$_2$ layer. (d) Typical spatial electric field distributions for p-AlGaN/MgF$_2$/Al and p-AlGaN/Al structures at $\alpha = 0^\circ$ and 45°.
Figure 2

(a) Simulated device with the NPSS or/and PC substrates and an inclined sidewall ODR structure. (b) Emission patterns of TM and TE polarized light in air. (c) Calculated LEEs as a function of the sidewall angle $\theta$ for (c) TM polarized light and (d) TE polarized light. (e) A summary of calculated LEEs for the three related cases with different substrate configurations. (f) Calculated LEEs as a function of the polarization angles of the dipole moment.
Figure 3

Simulated electric field distributions inside the UV LEDs featuring a (a)/(b) flat, (c)/(d) PC, and (e)/(f) NPSS substrates for TM/TE polarized light cases.
Figure 4

(a) Angle-dependent transmissivity (Tra.) as a function of $\beta$. (b) Typical electric field distributions for two exemplary incident angles, $\beta = 0^\circ$ and $10^\circ$. 