

Investigation of light extraction efficiency comparison of AlGaIn-based deep- and mid-ultraviolet flip-chip light-emitting diodes with patterned sapphire substrate

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ABSTRACT

Nitride-based ultraviolet (UV) emitters have attracted substantial attentions for various applications due to compact sizes and higher energy efficiencies. Despite the remarkable improvement in external quantum efficiency (η_{EQE}) for near-UV light-emitting diodes (LEDs), typical η_{EQE} for planar mid- and deep-UV LEDs is still low (<10%). One of the primary reasons for such low η_{EQE} is the strong anisotropic emission due to dominant transverse-magnetic (TM)-polarized output in high Al-content AlGaIn quantum wells (QWs) while conventional planar LED structure favors extracting light traveling along c-axis. Here, we investigated the polarization dependence light extraction efficiency ($\eta_{\text{extraction}}$) of AlGaIn-based flip-chip UV LEDs emitting at 230 nm and 280 nm with microdome-shaped patterning on sapphire based on three-dimensional (3D) finite-difference time-domain (FDTD) simulations. Our results show that microdome-shaped patterning on sapphire substrate is predominantly beneficial in enhancing TM-polarized output where up to 6.1-times and 2.4-times enhancement in TM-polarized $\eta_{\text{extraction}}$ can be achieved for 230 nm and 280 nm flip-chip UV LEDs with microdome-shaped patterned sapphire substrates respectively as compared to conventional flip-chip UV LEDs with flat sapphire substrates. In contrast, very minimal transverse-electric (TE)-polarized $\eta_{\text{extraction}}$ enhancement (<1%) can be obtained from both 230 nm and 280 nm flip-chip UV LEDs with microdome-shaped patterned sapphire substrates. In particular, microdomes with diameter ≥ 200 nm for the investigated 280 nm UV LEDs are acting as reflector that severely limit light extraction through sapphire substrate. It is expected that this study will shed light on further optimizations of flip-chip UV LED designs for both deep-UV and mid-UV regimes.

Keywords: microdome-shaped patterning, flip-chip light-emitting diodes, patterned sapphire substrate, polarization-dependent light extraction efficiency, quantum well structure, ultraviolet light-emitting diodes

1. INTRODUCTION

III-nitride-based materials have drawn significant attention as ultraviolet (UV) emitters due to the wide direct band-gap energy of ternary AlGaIn alloy between 3.4 eV for GaN and 6.2 eV for AlN. Accordingly, nitride-based UV emitters are considered as promising candidates in replacing conventional UV light sources for various applications such as sterilization, purification, biological and chemical sensing attributed to their compact sizes, longer lifetime, robustness and absence of harmful materials such as mercury and lead¹⁻⁴. Despite the tremendous progress on near-UV light-emitting diodes (LEDs), the efficiency of AlGaIn-based mid- and deep-UV LEDs is still low where < 10% of external quantum efficiency (η_{EQE}) has been reported for planar structure AlGaIn-based quantum well (QW) UV LEDs with emission wavelength (λ) < 300 nm³. Disregard the growth material quality, this relatively low UV LED performance is assumed to arise from the strong UV light absorption in the p-GaN contact layer and the anisotropic emission from high Al-content AlGaIn QWs¹⁻⁷.

As a result, various approaches have been proposed to improve the light extraction efficiency ($\eta_{\text{extraction}}$) for UV LEDs including flip-chip structures⁸, surface roughing⁹, patterned sapphire substrates¹⁰, transparent p-contact layer¹¹, surface plasmon¹², photonic crystal patterns¹³ and nanorod structures¹⁴. Above all, the combination of patterned sapphire substrate and flip-chip devices are widely adopted InGaIn-based LEDs considering the tradeoff between the complexities in fabrication process and manufacturing cost. In addition, the use of patterned sapphire substrate can also help to minimize dislocation density which reduces the possibility of photons trapping in these defect sites. Previous simulation study on InGaIn/GaN flip-chip LEDs with patterned sapphire substrates¹⁵ has demonstrated ~115% enhancement in $\eta_{\text{extraction}}$ while experimental study on 282 nm AlGaIn-based UV LEDs with patterned sapphire substrates¹⁶ has reported

up to 98% improvement in LED performance as compared to LEDs with flat sapphire surfaces. In spite of these encouraging results, there are very limited works on understanding the polarization-dependent $\eta_{\text{extraction}}$ for flip-chip UV LEDs with patterned sapphire substrates, which is particularly important for AlGaIn-based UV LEDs as emission from QW with $\lambda < 250$ nm is primarily transverse-magnetic (TM) dominant whereas $\lambda > 250$ nm is mostly transverse-electric (TE) dominant^{17,18}.

Therefore, in this work, we examine the effect of microdome-shaped array patterning on sapphire substrate for flip-chip UV LEDs based on three-dimensional (3D) finite-difference time-domain (FDTD) method. In particular, we study the polarization dependence $\eta_{\text{extraction}}$ of 230 nm and 280 nm AlGaIn-based flip-chip UV LEDs with microdome-shaped array on sapphire substrates arranged in hexagonal pattern. Our results show that microdome-shaped patterning is predominantly beneficial in enhancing TM-polarized output where up to 6.1-times and 2.4-times enhancement in TM-polarized $\eta_{\text{extraction}}$ can be achieved for 230 nm and 280 nm AlGaIn-based flip-chip UV LEDs with microdome-shaped patterned sapphire substrates respectively as compared to conventional UV LEDs on flat sapphire substrates. On the contrary, very minimal TE-polarized $\eta_{\text{extraction}}$ enhancement (<1%) can be obtained from both 230 nm and 280 nm flip-chip UV LEDs with microdome-shaped array patterned sapphire substrates. Specifically, microdomes with diameter ≥ 200 nm for the investigated 280 nm UV LEDs are acting as reflector that severely limit the light extraction through the sapphire substrate. Despite more TM-polarized $\eta_{\text{extraction}}$ enhancement than TE-polarized $\eta_{\text{extraction}}$ enhancement can be achieved from the investigated 230 nm and 280 nm UV LEDs with microdome-shaped pattern sapphire substrates, the $\eta_{\text{extraction}}$ for TM-polarization ($\sim 0.1 - 0.7\%$ for 230 nm and $\sim 1.1 - 2\%$ for 280 nm) is still comparatively smaller than TE-polarization ($\sim 10.3 - 13.4\%$ for 230 nm and $\sim 8.2 - 13.1\%$ for 280 nm) since planar structure is generally advantageous for extracting light propagates in vertical direction (parallel to c-axis). It is expected that this study will shed light on further optimizations of flip-chip UV LED with microstructure patterned sapphire substrate for both deep-UV and mid-UV regimes to achieve high-efficiency AlGaIn-based mid- and deep-UV LEDs.

2. 3D FDTD SIMULATION

3D FDTD method¹⁹ is employed to investigate the $\eta_{\text{extraction}}$ for AlGaIn-based multiple quantum well (MQW) flip-chip UV LEDs with microdome-shaped array patterning on sapphire substrates emit at 230 nm and 280 nm. The layer structure of the simulated UV LED is illustrated in Figure 1(a) which consist of 500 nm thick sapphire substrate, 200 nm AlN buffer layer, 100 nm n-AlGaIn layer, 50 nm thick AlGaIn layer to represent the MQW active region, 15 nm p-AlGaIn electron blocking layer (EBL), 10 nm p-AlGaIn layer and 20 nm p-GaN contact layer. The thickness of the sapphire substrate, AlN buffer layer and n-AlGaIn layer used in this study is much thinner than actual UV LED devices^{8,20} so as to reduce the consumption of large amount of memory and decrease the required computation time. A metallic layer that acts as a perfect mirror is attached to the bottom of the LED to reflect all photons incident upon it. Microdome-shaped array with microdome diameter, D , height, H , and spacing, S , is arranged in hexagonal pattern on the patterned sapphire substrate, as depicted in Figure 1(b).

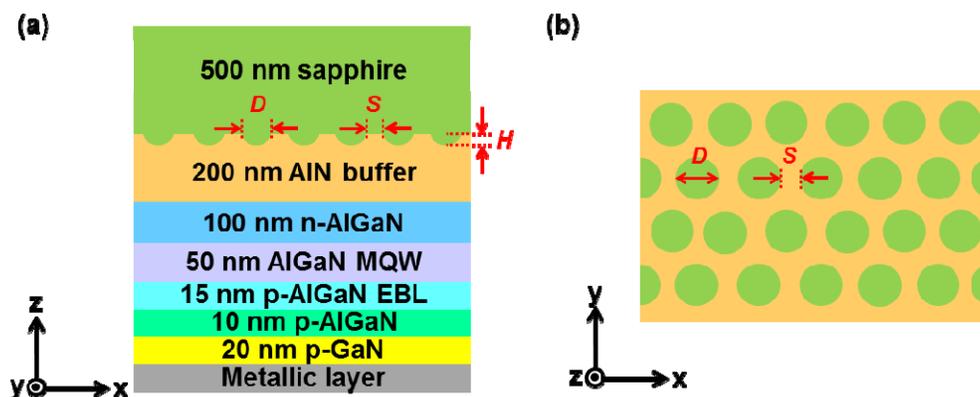


Figure 1. (a) Schematic side view of simulated AlGaIn-based flip-chip UV LED structure with microdome-shaped array patterning on patterned sapphire substrate. The diameter, spacing and height of the microdome are labeled as D , S , and H respectively. (b) Top view showing the microdome-shaped array on patterned sapphire substrate arranged in hexagonal pattern.

The refractive indexes and absorption coefficients for AlN, GaN and sapphire are taken from Refs. [8,21,22]. Linear extrapolation between AlN and GaN is used in calculating the refractive indexes and absorption coefficients for p-AlGaIn layers and AlGaIn active region where the Al-content for the corresponding emission wavelength are determined from Ref. [23]. The simulation domain is set to $5\ \mu\text{m} \times 5\ \mu\text{m}$ with non-uniform grid size (10 nm in the bulk and 5 nm at the edge). Perfectly matched layer (PML) boundary condition is applied to the lateral and top boundaries and perfect electric conductor (PEC) boundary condition is applied to the bottom boundary. A single dipole source is placed at the center of the AlGaIn MQW active region where TE-polarization is defined as the major electric field travels in the in-plane direction (parallel to the x and y directions labeled in figure 1) while TM-polarization is represented by the major electric field travels in the out-of-plane direction (parallel to the z direction labeled in figure 1). One power monitor is placed at distance λ away from the sapphire top surface to measure the light output power radiated out of the LED. The $\eta_{\text{extraction}}$ is calculated as the ratio of the light output power measured by the output power monitor to the total power dissipated by the dipole source in the active region^{8,20}.

3. RESULTS AND DISCUSSION

As pointed out in previous studies, the polarization of light generated from AlGaIn-based MQW UV LEDs changes from TE-dominant to TM-dominant as the Al-composition increases^{17,18}. Since TM-polarized light is primarily propagates in the lateral direction, majority of the UV light will be trapped inside the conventional planar structure due to total internal reflection. For conventional flip-chip UV LEDs with flat sapphire substrates, the calculated TM-polarized $\eta_{\text{extraction}}$ is $\sim 0.12\%$ and $\sim 0.85\%$ for 230 nm and 280 nm respectively, and the calculated TE-polarized $\eta_{\text{extraction}}$ is $\sim 13\%$ for both 230 nm and 280 nm. In order to investigate the effect of microdome-shaped patterned sapphire substrate on the $\eta_{\text{extraction}}$ of mid and deep-UV LEDs, the ratio of $\eta_{\text{extraction}}$ for AlGaIn-based flip-chip UV LEDs with patterned sapphire substrates to those of conventional planar flip-chip structure with flat sapphire substrate are plotted in figure 2 as a function of microdome diameter (D). Figure 2(a) presents the $\eta_{\text{extraction}}$ ratio for the investigated UV LED structures emit at 230 nm and figure 2(b) shows the ratio of $\eta_{\text{extraction}}$ for the investigated UV LEDs emit at 280 nm. The microdome height (H) is fixed at 50 nm while the spacing between microdomes (S) is fixed at 100 nm.

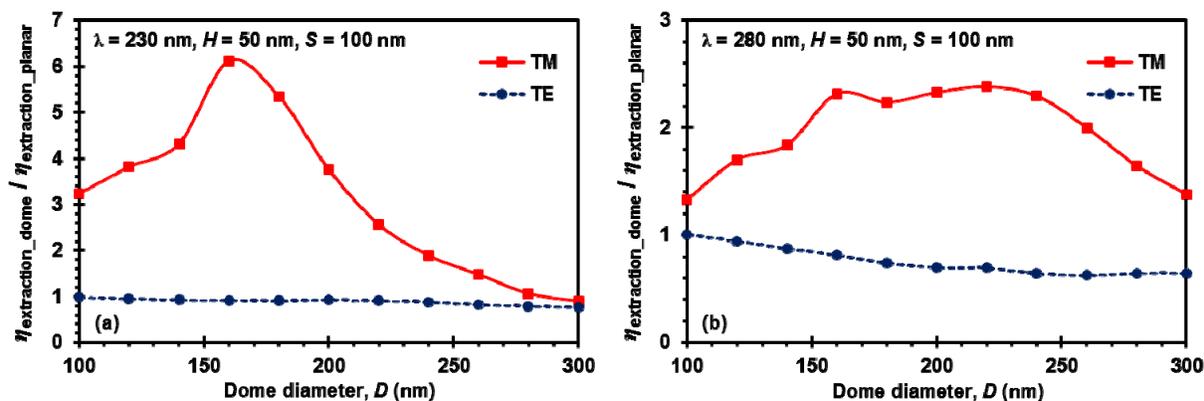


Figure 2. Ratio of light extraction efficiency for the investigated AlGaIn-based flip-chip UV LEDs with patterned sapphire substrates emit at (a) $\lambda = 230\ \text{nm}$ and (b) $\lambda = 280\ \text{nm}$ as a function of microdome diameter (D). The microdome height (H) is set as 50 nm and the spacing between microdomes (S) is fixed at 100 nm.

For both 230 nm and 280 nm UV LEDs, TM-polarized $\eta_{\text{extraction}}$ for the investigated AlGaIn-based UV LEDs with microdome-shaped patterned sapphire substrates demonstrated strong dependence on the microdome diameter as D changes from 100 nm to 300 nm. For 230 nm UV LEDs, up to ~ 3.2 -times enhancement in the TM-polarized $\eta_{\text{extraction}}$ is observed when $D = 100\ \text{nm}$ as compared to conventional planar flip-chip UV LED with flat sapphire surface. The TM-polarized $\eta_{\text{extraction}}$ ratio rises significantly to ~ 6.1 -times when D increases to 160 nm, and then drops to ~ 1.1 -times when D increases to 300 nm. For the case of mid-UV regime (280 nm), the TM-polarized $\eta_{\text{extraction}}$ ratio of ~ 1.3 -times is observed when $D = 100\ \text{nm}$ and peaked at ~ 2.4 -times when $D = 220\ \text{nm}$. Based on the results presented in figure 2, with $H = 50\ \text{nm}$ and $S = 100\ \text{nm}$, the optimum microdome diameter for the investigated UV LEDs is preferably to be smaller

than the emission wavelength. For example, for the investigated 230 nm UV LEDs, the $\eta_{\text{extraction}}$ ratio drops to below 2-times enhancement when the microdome diameter is larger than 240 nm while for the case of 280 nm, the decreasing trend observed at microdome diameter between 260 and 300 nm also demonstrated that microdomes with diameter larger than the emission wavelength will not help with large improvement in the light extraction. The analysis for microdome diameter beyond 300 nm will be included in future work.

On the contrary, for TE-polarized emission, the patterned sapphire substrates with microdome diameter ranges between 100 and 300 nm for the investigated 230 nm and 280 nm UV LEDs are resulting in more TE-polarized photons trapping that diminish the extraction of TE-polarized photons out of the LED structure. For the case of 230 nm UV LEDs, the TE-polarized $\eta_{\text{extraction}}$ is less affected by the various microdome diameters where more than 0.9-times TE-polarized $\eta_{\text{extraction}}$ ratio can still be obtained from the investigated 230 nm UV LEDs. As opposed to the case of 230 nm, the TE-polarized $\eta_{\text{extraction}}$ ratio for the investigated 280 nm UV LEDs drop significantly from ~ 1 to ~ 0.63 as D increases from 100 nm to 300 nm. The purpose of patterned sapphire substrate is to enhance the light scattering effect for the LED structure, where it can help to scatter the light out of the structure, or scatter the light back into the structure²⁴. In order to result in larger $\eta_{\text{extraction}}$, the fraction of scattered light out of the structure needs to be larger than the fraction of the scattered light into the structure. For the results presented in figure 2, the design of the patterned sapphire substrate investigated in this work acting more like a reflector that inhibits the light extraction through the sapphire substrate. Further investigation on various microdome dimension, for example, various H , S and D , is necessary in order to enable the microdome-shaped patterned sapphire substrates to act as extractor for both the 230 nm and 280 nm flip-chip UV LEDs and result in larger TE-polarized $\eta_{\text{extraction}}$.

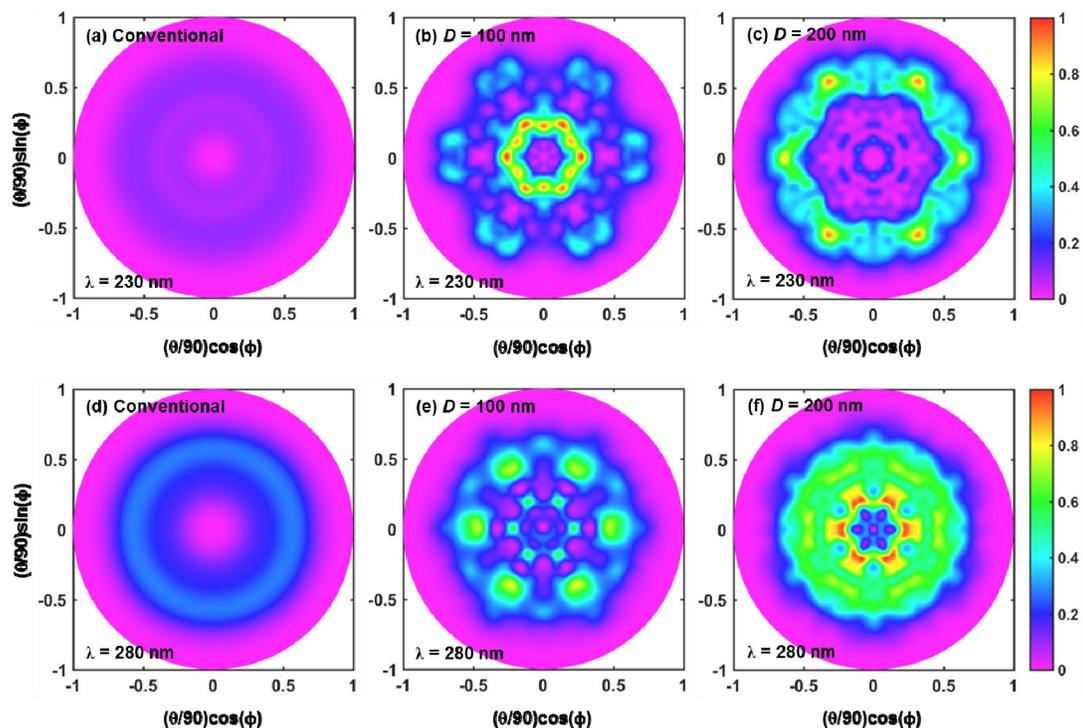


Figure 3. TM-polarization far-field radiation patterns of the investigated 230 nm [(a)-(c)] and 280 nm [(d)-(f)] UV LEDs with conventional flat sapphire substrate [(a) & (d)], $D = 100$ nm [(b) & (e)] and $D = 200$ nm [(c) & (f)].

In addition to enhancing the light extraction, periodic pattern on the sapphire substrate is also anticipated to help with randomizing and redirecting the light emission pattern. The TM-polarization far-field radiation pattern plots presented in figure 3 show that the microdome-shaped patterned sapphire substrates are providing strong scattering centers which result in noticeably different light radiation patterns for both the investigated 230 nm and 280 nm UV LEDs as compared to conventional planar flip-chip UV LEDs with flat sapphire substrates. In addition, the curvature surfaces introduced by the microdomes are increasing the photon escape cone in the structure which in turn result in

overall higher radiant intensity that eventually lead to improved TM-polarized $\eta_{\text{extraction}}$. For the investigated 230 nm UV LEDs with microdome-shaped patterned sapphire substrates, most of the light is being extracted out at both large angular (θ) and azimuthal (ϕ) directions, especially when D increases from 100 nm [figure 3(b)] to 200 nm [figure 3(c)]. Conversely, the investigated 280 nm UV LEDs with patterned sapphire substrates are exhibiting more uniform far-field emission pattern over a larger surface. Specifically, the light from the investigated 280 nm UV LEDs with $D = 200$ nm [figure 3(f)] can be extracted out in a relatively larger θ range as compared to UV LEDs with $D = 100$ nm [figure 3(e)]. The spread out distribution of high intensity radiation pattern observed for both the investigated 230 nm and 280 nm UV LEDs with patterned sapphire substrates is the reason that lead to larger TM-polarized $\eta_{\text{extraction}}$ than the conventional LEDs with flat sapphire substrates. The hexagonal symmetry radiation patterns observed from both the investigated 230 nm and 280 nm UV LEDs is due to the hexagonal arrangement of the microdome array.

As opposed to TM-polarization, the use of microdome-shaped patterned sapphire substrates for the investigated 230 nm and 280 nm UV LEDs are unfavorable for TE-polarized $\eta_{\text{extraction}}$. As illustrated in figures 4(a) and 4(d), the TE-polarized far-field radiation patterns for conventional 230 nm and 280 nm planar flip-chip UV LEDs with flat sapphire substrates exhibit Lambertian radiation patterns with θ dependent and symmetrically ϕ distribution. By the use of microdome-shaped patterned sapphire substrates with microdome diameter of 100 nm, the far-field radiation patterns with high intensity for both the investigated 230 nm and 280 nm [figures 4(b) and 4(e)] are primarily concentrated near the center region, which imply that such microdome design can be acting like an extractor. However, the effect is not as much as can be observed for the TM-polarization. As D increases to 200 nm, lower intensity distributions for both the 230 nm and 280 nm UV LEDs [figures 4(c) and 4(f)] are observed for light extraction through sapphire substrate, as the microdome-shaped patterned sapphire substrates are mainly acting as reflector that hinder TE-polarized light extraction through the sapphire substrates. Therefore, further investigation for various microdome dimension is required in order to allow the microdome-shaped patterned sapphire substrates to behave like an extractor that can help to enhance the TE-polarized $\eta_{\text{extraction}}$.

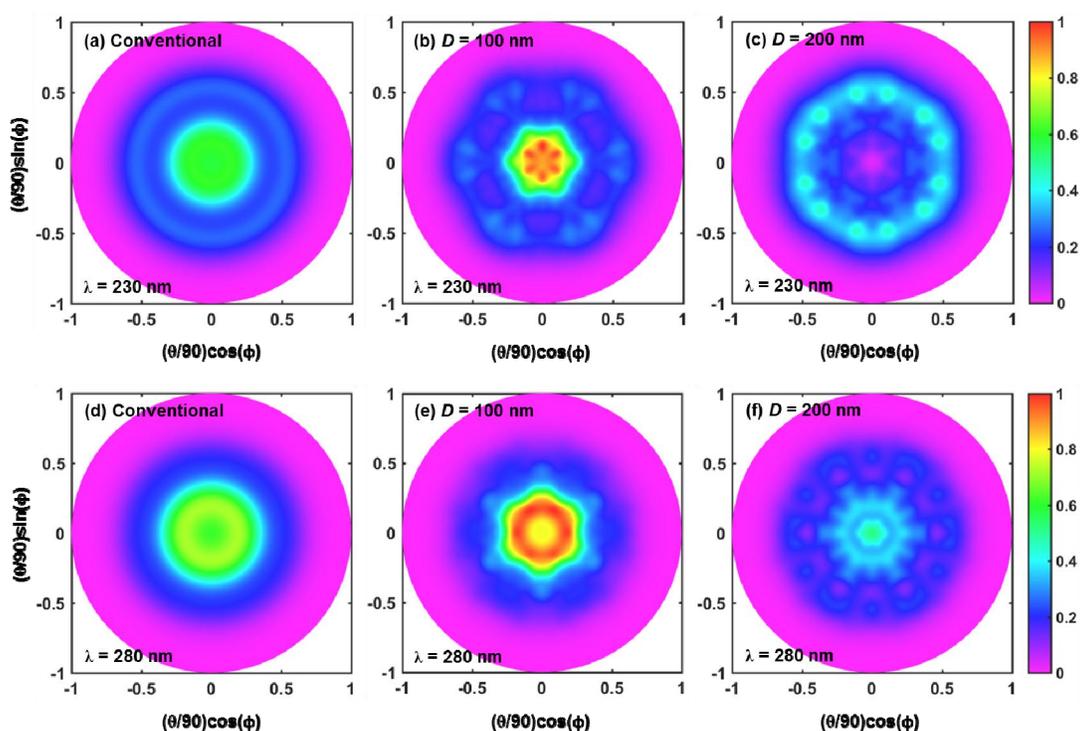


Figure 4. TE-polarization far-field radiation patterns of the investigated 230 nm [(a)-(c)] and 280 nm [(d)-(f)] UV LEDs with conventional flat sapphire substrate [(a) & (d)], $D = 100$ nm [(b) & (e)] and $D = 200$ nm [(c) & (f)].

4. CONCLUSION

In summary, the polarization dependence $\eta_{\text{extraction}}$ of 230 nm and 280 nm AlGaIn-based flip-chip UV LEDs with microdome-shaped patterned sapphire substrates has been investigated and compared in this work. The results show that microdome-shaped patterned sapphire substrate is particularly efficient in enhancing TM-polarized light extraction where up to 6.1-times and 2.4-times improvement in TM-polarized $\eta_{\text{extraction}}$ can be achieved for the investigated 230 nm and 280 nm UV LEDs respectively. For TE-polarization, the microdome-shaped patterned sapphire substrates for the investigated 230 nm and 280 nm UV LEDs are reflecting majority of the light back to the LED structure and result in very minimal TE-polarized $\eta_{\text{extraction}}$ through the sapphire substrates. Based on our simulation results, the microdome-shaped patterned sapphire substrate with $H = 50$ nm, $S = 100$ nm, and $D = 100 - 300$ nm are beneficial in enhancing TM-polarized $\eta_{\text{extraction}}$ for the investigated 230 nm and 280 nm UV LEDs. In particular, for the case of 230 nm, the significant enhancement in the TM-polarized $\eta_{\text{extraction}}$ in conjunction with the large TM-polarized spontaneous emission rate is expected to result in high η_{EQE} . On the other hand, further analysis on various microdome design is necessary for both the investigated 230 nm and 280 nm UV LEDs in order to enable the microdome-shaped patterned sapphire substrates to act as extractor for achieving higher TE-polarized $\eta_{\text{extraction}}$. Future work on optimizing the microdome design is still on-going, and is expected to serve as a guideline on designing microstructure patterned sapphire substrate for achieving high-efficiency mid- and deep-UV LEDs.

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