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Analysis of light extraction properties of AlGaN-based flip-chip ultraviolet light-emitting diodes by the use of self-assembled SiO₂ microsphere array

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ABSTRACT

Light extraction efficiency ($\eta_{\text{extraction}}$) remains as a big challenge for high-efficiency deep-ultraviolet (UV) light-emitting diodes (LEDs) due to the large refractive index contrast at the AlN(sapphire)/air interface. Various surface patterning approaches such as microdome design and patterned sapphire substrates have been proposed to address the low $\eta_{\text{extraction}}$ issue. Nevertheless, these previously proposed methods all involved additional complicated fabrication steps and the polarization-dependent analysis for these devices has not been investigated experimentally.

In this work, we investigate the feasibility of using 700-nm SiO₂ microsphere array on 280 nm flip-chip UV LEDs to improve the $\eta_{\text{extraction}}$. Angle- and polarization-dependent electroluminescence measurements have been performed to compare the 280 nm LEDs with and without the SiO₂ microsphere array. The UV LED with microsphere array showed enhancement for transverse-electric (TE)-polarized light intensities at small angles while decreased intensities at large angles with respect to c-axis, as compared to the device without SiO₂ microspheres For instance, up to 7.4% enhancement is observed at $\theta = 0^{\circ}$. However, for transverse-magnetic (TM)-polarized light, the intensities largely remain the same at small angles while decrease at large angles. Cross-sectional near-field electric field distribution from three-dimensional finite-difference time-domain simulation has confirmed that the use of SiO₂ microspheres array resulted in scattering of photons at the sapphire/SiO₂ microspheres interface, which eventually leads to enhanced TE-photons extraction at small-angles. From simulation, the light radiation patterns from the UV LED with SiO₂ spheres are reshaped to a small-angle-favored pattern without reducing the total output power, showing great consistency with the measurement results.

Keywords: Microsphere, UV LEDs, AlGaN, Light Extraction Efficiency, Polarization

1. INTRODUCTION

Ultraviolet light in the emission range of 200 nm - 300 nm has a variety of potential commercial applications[1]. However its most promising attribute may be its ability to effectively and reliably destroy bacteria and other harmful microorganisms. Compact, portable, and efficient UV light sources have been proven to be powerful tools for rapid sterilization of surfaces and instruments in medical installations and could also be implemented as means to purify drinking water in developing regions[1]–[3]. UV LEDs are of great interests for these specific applications due to their compact size, modularity, robustness, and long lifespan, which stand in contrast to conventional UV light sources such as mercury vapor lamps, which are bulky, inefficient, and produce hazardous mercury waste[1], [4]. Modern UV LEDs see very limited implementation in these applications however, due primarily to their low external quantum efficiency (η_{EQE})[1], [5]–[7]. Although carrier injection efficiency ($\eta_{\text{injection}}$) and radiative recombination efficiency ($\eta_{\text{radiative}}$) are also of concerns, light extraction efficiency ($\eta_{\text{extraction}}$) is often the key limiting factor in the realization of high-efficiency UV LEDs, and in many cases less than 10% of photons produced by the light emitting structure can be extracted. This is due primarily to the large refractive index contrast between the semiconductor surface/sapphire and air[1]. Specifically, AlGaN-based UV LEDs are often grown on sapphire substrates, and light extraction from flip-chip devices is achieved through the backside of the device, in accordance with Snell's law, light passing from a high index medium such as sapphire to low index medium such as air will have a small critical angle and consequently a narrow escape cone, allowing only a

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small fraction of the emitted light to escape from the device. In addition, the polarization of light emission from UV LED influences device light extraction efficiency as well. Specifically, the light polarization will switch from transverse-electric (TE) to transverse-magnetic (TM) at shorter emission wavelength and the TM-photons are more difficult to out-couple from the top (bottom) of the device[1], [8].

To address this issue and improve the $\eta_{\text{extraction}}$ of UV LEDs, various nanostructuring approaches have been proposed[1], [4]–[7], [9]–[11]. One possible solution is to change the angle between the photon emission direction and the surface normal by using encapsulation[1], photonic crystal structure[7], front side and back side surface roughening, patterned sapphire substrate[4], [9] and nanowire structure[11]. Several research groups also tried to collect the light emitted in the opposite directions toward the p-AlGaN layer for the bottom-emitting UV LEDs by using UV-reflective metal and UV-transparent P-AlGaN layer[5], [7], [10]. Up to 20% η_{EQE} has been reported by employing these techniques recently[10]. However, all of those include complex and expensive fabrication processes. Instead, a low-cost, large-yield and easy controlled approach by using microsphere arrays to improve device light extraction efficiency has been developed and demonstrated for visible LEDs[12]–[16]. Specifically, self-assembled two-dimensional close-packed SiO₂ microsphere arrays are coated on top/bottom of the devices, serve to scatter light emitted from the active region of the LED, allowing light which would normally be subject to total internal reflection to escape the device into air. The use of intermediate refractive index materials such as SiO₂ or polystyrene to form this nanostructured array also serves to reduce Fresnel reflection, further improving the light extraction efficiency of the device. As a result, up to 1.85 times light extraction efficiency enhancement can be realized. However, this concept has not been demonstrated in deep-UV regime, where photons with different polarizations should be considered separately[12]–[16].

Therefore, in this work, we used both experimental and simulation approaches to test the feasibility of increasing light extraction efficiency through the use of a self-assembled, close-packed monolayer of SiO₂ microspheres for deep-UV LEDs. A flip-chip UV LED with emission wavelength of 280 nm was examined. The light extraction characteristics from the LEDs were examined by an angle-dependent electroluminescence (EL) setup and compared with those of UV LEDs without microsphere arrays. Due to the lower refractive index from SiO₂ as compared to sapphire substrate and the sphere shape of the SiO₂ array, the transverse-electric (TE)-polarized light intensities are enhanced at the small angles with respect to the c-axis. In addition, here we also employed a finite-difference time-domain (FDTD) method to theoretically study device near-filed electric field distribution and light radiation properties. The results show great consistency with the measurement results, confirming the use of SiO₂ microsphere arrays could enhance device intensities at small angles.

2. EXPERIMENTAL RESULTS AND DISCUSSION

2.1 Device details and experimental setup

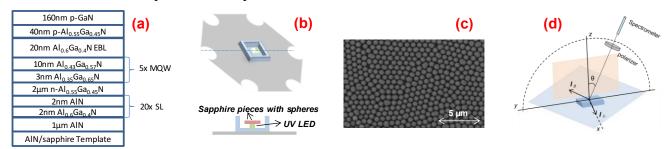


Figure 1. (a) Schematic of 280-nm UV LED heterostructure (b) Experimental setup for measurement of light emission from the LED device, showing the commercial UV LED beneath sphere coated sapphire. (c) SEM image of the close-packed microsphere array deposited on sapphire. (d) Schematic representation of the angle dependent EL setup used to measure light extraction and far field radiation patterns of the device.

The schematic of the 280-nm UV LED structure is shown in Figure 1 (a). The sample was grown on AlN/sapphire substrate, consisting of a 2-nm Al_{0.6}Ga_{0.4}N/2-nm AlN superlattice (SL) buffer layer, a 2-μm n-Al_{0.55}Ga_{0.45}N layer, a five-period 3-nm Al_{0.35}Ga_{0.65}N/10-nm Al_{0.43}Ga_{0.57}N multiple quantum well (MQW) active region and a 40-nm p-Al_{0.55}Ga_{0.45}N with 160 nm p-GaN layer. After the growth, the epitaxial structure was fabricated to be a flip-chip LED and mounted on a commercial device holder. To study the use of a self-assembled, close-packed monolayer of SiO₂ microspheres for deep-UV LEDs, we prepared several double-side polished sapphire pieces with SiO₂ microspheres coating on the surface and placed the sphere coated sapphire onto the UV LED sample, as shown in Figure 1 (b). Figure 1 (c) shows the scanning

electron microscopy (SEM) image of the 700-nm close-packed monolayer of SiO₂ microspheres. The UV LED samples with sapphire piece on top were then measured by an in-house angle-dependent EL measurements setup, as shown in Figure 1(d). Specifically, the sample was placed at the center of the stage while the optical fiber, which is connected to the spectrometer, was fixed on a rotatable stage. By rotating the fiber holder, the EL spectra at different angles can be collected and further translated into light radiation pattern.

2.2 Experimental results and discussion

The sapphire pieces with and without the microspheres array were placed on the LED samples and compared under the same test conditions. From the EL spectra as shown in Figure 2 (a) inset, both devices show strong emissions at 280 nm. Figure 2 plots the integrated EL intensities as a function of current for the structures with and without microsphere arrays. At $\theta = 0^{\circ}$, the sample with microsphere array show 8% enhancement of the integrated EL intensity as compared to that from the structure without microsphere array. Further investigate the influence of the microsphere array on the light extraction efficiency of the UV LED, the EL intensities at different emitting angles were collected. Figure 2 (b) plots the light radiation patterns for the structures with and without the microsphere arrays. The results show at smaller angle ($\theta < 30^{\circ}$), the light intensities from the structure with microsphere array are larger than that from the structure without the microspheres while at larger angles ($30^{\circ} < \theta < 60^{\circ}$), the intensities decrease by the use of the microsphere arrays.

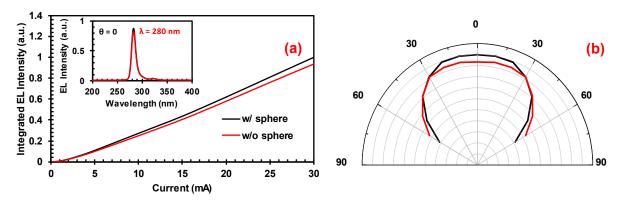


Figure 2. (a) Integrated EL intensity as a function of current for the structure with microsphere arrays (black) and without microsphere arrays (red) Inset: EL spectra of the structures with (black) and without (red) the 700-nm microspheres array at $\theta = 0^{\circ}$. (b) Light radiation pattern from the structures with microsphere arrays (black) and without microsphere arrays (red), showing the EL intensity enhancements at small angles $\theta < 30^{\circ}$.

3. PHYSICS AND SIMULATION RESULTS

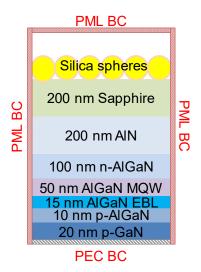
In accordance with Snell's Law, only a small fraction of the light emitted isotropically from a point source into a high refractive index medium such as sapphire, for which $n_{\text{sapphire}} = 1.82$, will be able to escape into air. The indices of refraction at 280 nm for materials used in fabrication of AlGaN-based UV LEDs are given in Table 1. The critical angle for light passing from sapphire into air is $\theta_c = 33.33^\circ$, which corresponds to an extraction efficiency of $\eta_{\text{extraction}} = 0.082$, as given by Equation 1.

$$\eta_{extraction} = \frac{1}{2}(1 - \cos \theta_c) \tag{1}$$

A light extraction efficiency of 0.082 is a severe hindrance to the implementation of these devices in any sort of application. Even if 100% internal efficiency could be achieved, less the 10% of the light produced by the device would be emitted. The high surface incidence angle required for light to escape means that much of the light produced ends up propagating in plane, and this phenomenon is complicated by the fact that the polarization of emitted light affects its interaction with the interface, with TM-polarized light far more likely to experience total internal reflection than TE-polarized light. The polarization of emitted light depends heavily on the band structure of the active region of the LED.

To investigate the physics of the influence of the microsphere arrays on the UV LED light extraction profiles, several FDTD simulations were performed and analyzed by the use of Synopsys R-soft. The three-dimensional device structure was built in the CAD module of the software package according to the cross-sectional depiction shown in Figure 3. Layer

thicknesses were defined and material constants assigned according to Table 1. A hexagonal close-packed array of SiO_2 spheres of variable defined diameter was located atop and adjacent to the sapphire layer. A perfect electric conductor (PEC) boundary condition was assigned to the free surface of the p-GaN layer to represent the metal current spreading layer which would exist in this location in a real device. All other simulation boundaries were assigned as perfectly matched layers (PMLs). The simulation domain was set to be 6 μ m x 6 μ m and a single isotropically emitting point source was used to produce 280 nm UV light. More simulation results can be found in Ref. [17]



λ = 280 nm	n	α (cm ⁻¹)
Sapphire	1.82	0
AIN buffer	2.42	0
n-AlGaN	2.49	10
AIGaN MQW	2.54	1010
AIGaN EBL	2.43	7
p-AlGaN	2.49	10
p-GaN	2.63	170544
SiO ₂	1.49	0

Table 1. Parameters of the materials used in the simulations

Figure 3. Schematic of the FDTD simulated structure (spheres not to scale)

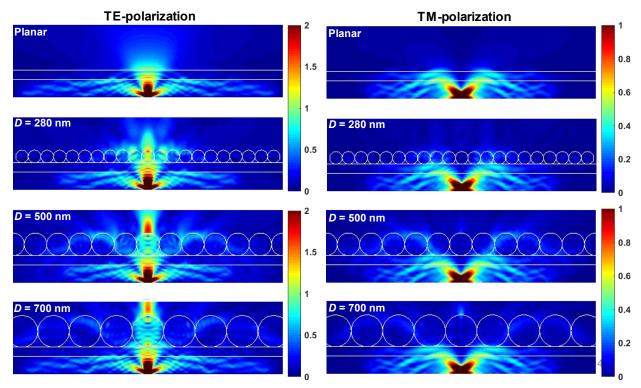


Figure 4. Cross-sectional electric field maps produced by FDTD simulation for the structures without spheres, with 280 nm spheres, 500 nm spheres and 700 nm spheres.

The simulation was completed for four distinct device structures, one with no SiO₂ spheres, and then with 280, 500, and 700 nm diameter spheres. The simulated cross-sectional electric fields from the four structures are presented in Figure 4. For the planar structure without SiO₂ spheres, the electric field from TE-polarized light shows large intensities at smaller angles while most of the E-fields are kept within the LED structure at larger angles which indicates the lambertian radiation pattern from the structure. For the structures with the spheres, the results show a marked increase in light emission intensity at smaller angles for TE-polarized light, while a slight decrease in intensity at intermediate angles is also evident. The SiO₂ spheres appear to act as resonant cavities, serving to amplify extraction of light normal to the surface of the sapphire. This can be seen most readily for the TE-polarized 500 nm SiO₂ spheres in Figure 4. TM-polarized light also appears to benefit from the addition of the sphere monolayer to the sapphire substrate. The cross-sectional electric fields shown in Figure 4 indicate enhanced light extraction at multiple angles, and for the 280 and 500 nm sphere arrays in particular.

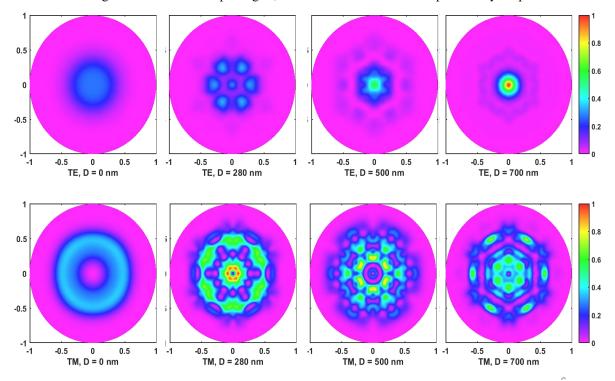


Figure 5. TE- and TM-polarized far-field patterns of the structures without spheres, with 280 nm spheres, 500 nm spheres and 700 nm spheres.

Figure 5 plots both TE- and TM-polarized far-field patterns of the structures. The results clearly show the large intensities enhancements at smaller angles as compared to the planar structure for the TE-polarized light, which show great consistency with the measurements results and the intensities reach the highest with the use of the 700 nm spheres. For TM-polarization, the donut-shape radiation patterns are observed for all the structures. Instead of the perfect donut shape for the planar structure, the spheres scatter the light and enhance the intensities only at several angles which are determined by the spheres size, while the intensities drop at other angles. The simulation results verify that the use of SiO₂ microspheres array resulted in scattering of photons at the sapphire/SiO₂ microspheres interface, which eventually leads to enhanced TE-photons extraction at small-angles.

4. SUMMARY

In summary, the feasibility of using 700-nm SiO₂ microspheres arrays on 280 nm flip-chip UV LEDs to improve light extraction efficiency was investigated in this study. Angle-dependent EL measurements have been compared for the LEDs with and without microspheres, showing light intensities are enhanced at small angles and decreased at larger angles with respect to the c-axis. Cross-sectional near-filed electric field and light radiation patterns from FDTD simulation confirm the use of microspheres array results in scattering of photons at the sapphire/SiO₂ interface and hence the light intensities enhancement at small angles.

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