# FDTD Analysis on Extraction Efficiency of GaN Light-Emitting Diodes With Microsphere Arrays

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Abstract—The improvement of light extraction efficiency of InGaN light-emitting diodes (LEDs) using microsphere arrays with various refractive indices was analyzed. Finite-difference time-domain (FDTD) simulations show that the use of microsphere ( $d_{
m microsphere}=500$  nm) arrays with refractive indices of 1.8 and 2.5 led to increase in light extraction efficiency of InGaN LEDs by 1.9 times and 2.2 times, respectively. The enhancement in light extraction efficiency is attributed to the decrease in the Fresnel reflection and increase in effective photon escape cone due to graded refractive index and curvature formed between microsphere and free space. The maximum enhancement of light extraction efficiency of InGaN quantum well LEDs was achieved by employing the refractive index matched anatase-TiO<sub>2</sub> microsphere arrays. The effects of microsphere diameters on the light extraction efficiency were also investigated and 2.4 times enhancement was achieved by employing 400-nm refractive index matched TiO<sub>2</sub> sphere arrays.

*Index Terms*—III-nitride, light-emitting diodes (LEDs), light extraction efficiency, matched refractive index, microspheres.

#### I. INTRODUCTION

THE III-Nitride materials have an important use for addressing device technologies applicable in solid state lighting [1]–[8], thermoelectrics [9], [10], diode lasers [11], [12], and solar cells [13]. Among them, GaN based light-emitting diodes (LEDs) have drawn a lot of attention in recent years for a variety of applications in flat-panel displays, mobile electronics, automobiles, traffic signals, large outdoor displays, and general lighting. However, for the next generation of applications of high-efficiency LEDs, further improvement of external quantum efficiency of LEDs is required. The external quantum efficiency depends on the internal quantum efficiency and light extraction efficiency [14]. The advances in active region optimization and growth methods had led to improvement in internal quantum efficiency in recent years [15]-[19]. However, the light extraction efficiency of conventional LED is still low due to large refractive index contrast between GaN ( $\sim 2.5$  in the visible region) and free space. Therefore, various methods

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have been employed to improve the light extraction efficiency of LEDs: 1) surface roughening [20]–[24]; 2) sapphire microlenses [25]; 3) oblique mesa sidewall [26]; 4) nanopyramid [27]; 5) photonic crystals [28]–[32]; 6) graded refractive index [33]; 7) self-assembled lithography p-GaN patterning [34]; 8) GaN micro-domes [35], [36]; and 9) TiO<sub>2</sub> micro-pillars [37]. The surface roughening approach utilizes chemical etching, which cause non-uniform surface. The photonic crystals and sapphire microlens approaches require the use of e-beam lithography or holography lithography [25], which leads to more expensive and/or complex fabrication process. Therefore, other low-cost and large area scalable method is highly desirable for implementation for low-cost and practical LEDs technologies.

Previously, we have demonstrated the use of SiO<sub>2</sub> microsphere arrays and SiO<sub>2</sub>/PS microlens arrays, deposited via rapid convective deposition (RCD) method, led to improvement in light extraction efficiency in III-Nitride LEDs [38]-[41]. The use of RCD method [38], [40] led to the ability for deposition of large area (wafer scale) microsphere (and/or microlens) arrays structures on top of LED device structures. Recently, this colloidal lithography method had been used as imprinting template for forming concave microstructure arrays for light extraction enhancement in GaN-based LEDs [42] and organic-based LEDs [43]. The selection of  $SiO_2$  as the microspheres in our previous works [38]-[41] had been primarily motivated from the ease in obtaining the silica-based spheres with wide range of dimensions commercially. However, the material choices (i.e., refractive indices) and dimensions of the spheres are design parameters that need to be optimized for maximizing the light extraction efficiency of nitride-based LEDs. In addition, the selection of spheres with various refractive indices and dimensions will also affect the far-field radiation pattern of the LEDs over wide angular distribution.

In this work, we present the numerical simulation studies based on finite-difference time-domain (FDTD) method for analyzing the light extraction efficiency of III-Nitride LEDs employing microsphere arrays with various refractive indices and dimensions. Specifically, the light extraction characteristics of III-Nitride LEDs with anatase-TiO<sub>2</sub> and amorphous-TiO<sub>2</sub> microsphere arrays were compared with those of III-Nitride LEDs with SiO<sub>2</sub> microsphere arrays. The refractive indices of anatase-TiO<sub>2</sub> and amorphous-TiO<sub>2</sub> microsphere arrays are higher than that of SiO<sub>2</sub> microsphere, which will lead to the improved extraction characteristics for III-Nitride LEDs employing the TiO<sub>2</sub> microsphere arrays. The comparison of the light extraction efficiency enhancement for LEDs employing lower refractive index sphere SiO<sub>2</sub>, medium refractive index sphere amorphous-TiO<sub>2</sub>, and higher refractive index sphere

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Fig. 1. Schematic side view of the simulated microsphere LED device, and the corresponding SEM images of 100-nm-SiO<sub>2</sub> sphere arrays.

anatase-TiO<sub>2</sub> with various diameters will be presented. In contrast of the microsphere arrays LEDs, the fabrication of the microlens arrays can be formed by embedding the microsphere arrays with polystyrene (PS) materials (i.e., SiO<sub>2</sub>/PS microlens arrays [38]–[41]). However, the current study will only be limited to the light extraction efficiency optimization in GaN-based LEDs employing only microsphere arrays with various materials, refractive indices, and diameters.

#### **II. FDTD ANALYSIS OF LIGHT EXTRACTION EFFICIENCY**

The InGaN/GaN multiple quantum wells (MQWs) LED device structure analyzed in this study is shown in Fig. 1. The n-GaN template was grown on sapphire substrate and followed by the growth of active region with total thickness of 12 nm. Then 0.1  $\mu$ m p-doped GaN layer was grown on top. Afterwards, the hexagonal close-packed (HCP) microsphere arrays were deposited on top of LED by employing rapid convective deposition (RCD) method [38]–[42]. The deposition of the microspheres or nanospheres can be performed with high uniformity in close-packed 2-D hexagonal pattern, and the scanning electron microscopy (SEM) of the 100-nm diameter nanosphere arrays was shown in Fig. 1. Our prior works had demonstrated the deposition of micro/nanosphere arrays with diameters ranging from 100-nm up to 1- $\mu$ m performed consistently on the devices [38]–[43].

The LED devices were treated as 3-D structures solved by taking into consideration the appropriate boundary conditions for ensuring efficient computation time. The 3-D FDTD method requires a large amount of memory and computation time. Therefore, the size of the simulation volume has to be reduced. Perfect matched layers (PML) boundary conditions were applied on the boundaries in order to avoid unnecessary reflection of light at the boundaries of domain as well as reduce the domain size. To reduce the size of the calculation, we have taken the simulation domain to be 5.5  $\mu$ m × 5.5  $\mu$ m. The thickness of n-GaN reduced to 0.1  $\mu$ m and sapphire substrate was reduced to 0.2  $\mu$ m.

A single dipole source within a finite computational domain was chosen and positioned in the center of x-y plane and also in the center of the InGaN/GaN active layer in the vertical direction. In addition, inhomogeneous mesh was used during the



Fig. 2. Ratio of light extraction efficiency of microsphere array LEDs with various refractive indices to that of planar LED.

simulation; the grid size was 10 nm in the bulk and 2.4 nm in the interface. The refractive index of GaN and InGaN layer is set as 2.5 and 2.6, respectively. The absorption coefficient of InGaN was chosen to be 2000  $\text{cm}^{-1}$  [15]. The emission wavelength used in all our computation is set as  $\lambda = 500$  nm. The light extraction efficiency was calculated as the ratio of the optical output power radiated through the microlens array to the total output power generated in the InGaN/GaN MQWs active region. Two detection monitors were implemented for measuring the electric field radiated from the dipole and near-field electric field on the top surface of the LEDs. The first monitor was formed to surround the dipole, in order to measure the total output power generated in the QW active region. The second monitor was placed 200-300 nm away from the top surface of the LEDs for measuring the near field electric field  $[E(x, y, z_{\text{monitor}})]$  radiated from the device. The far-field electric field  $[E(r, \theta, \phi)]$  was obtained by performing the Fourier Transform on the near-field electric field  $[E (x, y, z_{\text{monitor}})]$ . The light extraction efficiency for LEDs is calculated by taking the ratio of the total power extracted from the LEDs, which was obtained by integrating the far-field power density over all solid angle, with the total power radiated the dipole as measured at the first monitor.

## III. EFFECT OF REFRACTIVE INDICES ON LIGHT EXTRACTION EFFICIENCY OF MICROSPHERE ARRAY LEDS

To investigate the effect of the refractive index of microsphere arrays on the light extraction efficiency of III-nitride LEDs, light extraction efficiency of GaN LEDs with microsphere ( $d_{microsphere} = 500$  nm) arrays and planar LED were computed for various refractive indices. The ratios of the light extraction efficiencies of the LEDs with microsphere arrays to those of the planar LED are shown in Fig. 2. Light extraction efficiency increases with the increase in refractive index of microsphere, and ~2.2 times enhancement was achieved when the refractive index of microsphere matched with that of GaN. The enhancement started to decrease with further increase in the refractive index of the microspheres, which is expected to the increased light trapping in microspheres (for n > 2.5). To compare suitable microsphere materials applicable for the experi-



Fig. 3. Contour plot of far-field radiations of (a) planar LED, (b) LED with SiO<sub>2</sub> microsphere arrays, (c) LED with amorphous TiO<sub>2</sub> microsphere arrays, and (d) LED with anatase TiO<sub>2</sub> microsphere arrays.

ments, the following microspheres were investigated: 1)  $SiO_2$  $(n \sim 1.5)$ , 2) amorphous TiO<sub>2</sub>  $(n \sim 1.8)$ , and 3) anatase  $TiO_2$  (n ~ 2.5). The computational analysis indicated that the use of SiO<sub>2</sub> microsphere arrays ( $d_{SiO2} = 500$  nm) led to an increase of 1.7-times in the light extraction efficiency of the devices, which was in good agreement with the experiments ( $\sim 1.69$  times increase) [39] and the simulation results employing ray tracing method (1.75 times enhancement) [39]. Note that simulation results using FDTD method is much closer to the experimental results compared to that of using ray tracing method. By using amorphous and anatase TiO<sub>2</sub> microsphere arrays, the light extraction efficiencies of the LEDs increase by1.91-times and 2.19-times over that of planar LEDs. As the microsphere refractive indices increases beyond n > 2.5, the light trapping in the microspheres leads to reduction in the light extraction to free space.

The increase in the refractive indices of the microspheres up to  $n \sim 2.5$  provides minimal Fresnel reflection (between the GaN and spheres) resulting in efficient light capture in the spheres, which will then be extracted out efficiently by the increased escape cone from the strong curvature surfaces introduced by microsphere arrays.

As comparison,  $SiO_2$  film was deposited on the LEDs as antireflection coatings to reduce the Fresnel reflection and increase the light extraction efficiency. In the planar SiO<sub>2</sub> antireflection coating film, the Fresnel reflection within the light escape cone will be significantly reduced. However, the use of  $SiO_2$  planar antireflection film will not increase the critical angle of the structure ( $\theta_{\text{critical}} = 23.5^{\circ}$ ), of which is determined by the index contrasts of the GaN material and air (free space). Thus, the use of SiO<sub>2</sub> antireflection thin film will not increase the light escape cone, which results in only reduced Fresnel reflection within the existing escape cone ( $\theta_{critical} = 23.5^{\circ}$ ). In contrast, the role of the microsphere or nanosphere arrays is to provide strong scattering centers to extract light out beyond the critical angle, which in turn results in the increase in light extraction efficiency for the microsphere LEDs over LEDs with only planar SiO<sub>2</sub> anti-reflecting film.

The comparison for the far-field radiation patterns for the planar LEDs, LEDs with SiO<sub>2</sub> microspheres, LEDs with amorphous TiO<sub>2</sub> microspheres, and LEDs with anatase TiO<sub>2</sub> microspheres was presented in Figs. 3 and 4 ( $d_{microsphere} = 500$  nm). The far-field radiation pattern for planar LEDs, as expected, ex-



Fig. 4. (a) Polar plot of far-field intensities of microsphere LEDs with various refractive indices, and (b) angular dependent power density of microsphere LEDs with various refractive indices.

hibited Lambertian radiation pattern with only angular ( $\theta$ ) dependent, while the symmetrically azimuthal ( $\phi$ ) distribution. Note that the far-field radiation pattern for 2-D hexagonal closepacked microsphere arrays LEDs exhibits both angular ( $\theta$ ) and azimuthal ( $\phi$ ) dependent, as shown in Fig. 3(b)–(d). The significantly higher intensity was also observed for far-field radiation pattern for microsphere LEDs for both the normal and large angular distribution, which in turn results in improved light extraction efficiency for these LEDs. Note that the comparison of the light extraction efficiency ratio for the microsphere LEDs and planar LEDs were carried out by taking the total output power integrated in all angular ( $\theta$ ) and azimuthal ( $\phi$ ) directions.

In order to provide a quantitative comparison, the far-field radiation patterns for these LEDs were plotted at a particular azimuthal direction of  $\phi = 0$  [as shown in Fig. 4(a)]. The angular dependent (in  $\theta$  direction) power density comparison data for microsphere LEDs and planar LED were also plotted for comparison purpose [as shown in Fig. 4(b)]. The microsphere LEDs exhibited significant increase in the far-field radiation patterns for all angular distribution. More importantly, the contribution of the large angular  $\theta$  component in the far-field radiation pattern is significantly increased for anatase TiO<sub>2</sub> microsphere arrays LEDs, which resulted in increase in power density extracted from this microsphere LEDs.

Note that the choice of the refractive indices of the materials (SiO<sub>2</sub>, amorphous TiO<sub>2</sub>, and anatase TiO<sub>2</sub>) strongly affects the radiation pattern, extraction value, and power density profile at large angular direction. The studies presented in Figs. 3 and 4 assume identical diameters for all the microspheres investigated. However, both the refractive indices and diameters of the spheres are important as optimization parameters in LEDs extraction.

### IV. EFFECT OF MICROSPHERE DIAMETERS ON LIGHT EXTRACTION OF MICROSPHERE LEDS

In order to further optimize the light extraction efficiency of LEDs with microsphere arrays, the effect of diameter of spheres on the light extraction efficiency of microsphere LEDs was also investigated [as shown in Fig. 5(a), (b), and (c)]. Fig. 5(a) shows the light extraction efficiency enhancement of LEDs with SiO<sub>2</sub> ( $n \sim 1.5$ ) microsphere arrays as a function of diameters of spheres at  $\lambda = 500$  nm. All the three microsphere LEDs exhibited strong dependence on the diameter for the microsphere arrays employed in the structures. The optimum dimensions for each type of sphere materials occur at different dimensions resulting in maximum allowed enhancement in the microsphere LEDs. The comparison of the light extraction efficiencies for microsphere LEDs were carried out with that of planar LEDs serving as reference LEDs.

For the case of SiO<sub>2</sub>-based microsphere LEDs, the maximum extraction enhancement of 1.85 times is expected for diameter of ~1  $\mu$ m. Large range of SiO<sub>2</sub> microsphere diameter exists for achieving extraction efficiency enhancement by ~1.6 times or higher. Specifically, the diameters in the range of 0.4  $\mu$ m up to 1.2  $\mu$ m are expected to result in relatively favorable increase in light extraction in LEDs.

For the case of amorphous TiO<sub>2</sub> microsphere LEDs, the increase up to 2.1 times is observed for LEDs using optimum diameter d ~ 0.8  $\mu$ m. The use of amorphous TiO<sub>2</sub> microspheres with diameters ranging from 0.4  $\mu$ m up to 0.9  $\mu$ m is expected to result in increased extraction efficiency by 1.9 times or higher.

By using the anatase TiO<sub>2</sub> microsphere arrays, the optimum diameter for this structure was obtained as  $d \sim 0.4 \ \mu m$ . The use of this optimum anatase TiO<sub>2</sub> microsphere arrays with  $d \sim 0.4 \ \mu m$  results in 2.4 times increase in light extraction efficiency over that of planar LEDs.

From our finding, the optimum diameter range for high extraction efficiency for each type of microsphere arrays reduces, as the refractive indices increases to  $n \sim 2.5 (n_{GaN})$ . However, the maximum light extraction enhancement for the LEDs can be obtained from the microspheres with the refractive index closest to  $n \sim 2.5$  (anatase TiO<sub>2</sub>).

The comparison of the far-field radiation patterns of the  $SiO_2$ and anatase  $TiO_2$  (as optimized material) microsphere arrays



Fig. 5. Ratio of the light extraction efficiency of microsphere LEDs with various diameters to that of planar LED: (a) LEDs with SiO<sub>2</sub> microsphere arrays; (b) LEDs with amorphous TiO<sub>2</sub> microsphere arrays and (c) LEDs with anatase TiO<sub>2</sub> microsphere arrays.

for various diameters were shown in Figs. 6 and 7. The comparison of the far-field patterns for both SiO<sub>2</sub> [Fig. 6(a)] and TiO<sub>2</sub> [Fig. 7(a)] microspheres were taken with azimuthal  $\phi = 0$  direction, in order to provide quantitative comparison between the two materials with various diameters. The comparison of the angular power density distributions for both SiO<sub>2</sub> and TiO<sub>2</sub> microsphere LEDs for various diameters were also shown in Figs. 6(b) and 7(b), respectively (with azimuthal  $\phi = 0$  direction).

In the case of SiO<sub>2</sub> microsphere LEDs [Fig. 6(a) and (b)], the microsphere diameters were varied from 0.1  $\mu$ m, 0.4  $\mu$ m, 0.5  $\mu$ m, 0.75  $\mu$ m and 1  $\mu$ m. The use of small SiO<sub>2</sub>microsphere (d<sub>SiO2</sub> < 0.1  $\mu$ m) leads to enhancement of light extraction at large angular component, while LEDs with larger sphere arrays (d<sub>SiO2</sub> > 0.5  $\mu$ m) results in significant increase in the output power in the normal direction. The large contribution of diffuse light output power can be attributed to the increased photon escape cone in the structure.





Fig. 6. (a) Far-field radiation patterns of  $SiO_2$  microsphere array LEDs with various  $SiO_2$  sphere diameters. (b) Angular dependent power density comparison of  $SiO_2$  microsphere array LEDs. The planar LED is included as reference.

In the analysis of the anatase-TiO<sub>2</sub>microsphere array LEDs [Fig. 7(a) and (b)], the diameters were varied from 0.25  $\mu$ m, 0.4  $\mu$ m, and 0.75  $\mu$ m. As shown in Fig. 7(b), the far-field radiation pattern for the anatase TiO<sub>2</sub> microsphere LEDs were strongly enhanced in comparison to that of planar LEDs. Similar to the SiO<sub>2</sub> microsphere LEDs, the use of smaller anatase TiO<sub>2</sub> spheres results in strong enhancement in the large angular emission. In contrast, the dominant component leading to enhancement in extraction efficiency for larger anatase TiO<sub>2</sub> spheres can be attributed to the stronger normal light emission.

## V. CONCLUSION

The effects of refractive indices, material choices, and sphere diameters were investigated for optimizing the far-field radiation patterns and light extraction in III-Nitride based LEDs with microsphere arrays. The analysis was carried out by using 3-D vectorial FDTD with PML boundary condition. The results show that the use of microspheres with high refractive index as favorably for achieving maximum light extraction efficiency in microsphere LEDs. Specifically, the use of anatase TiO<sub>2</sub> microsphere arrays is expected to result in more than 2.4 times increase in light extraction efficiency over that of planar LEDs. The optimum diameters of the spheres are found to strongly affect the radiation patterns and light extraction efficiency in microsphere LEDs. The use of smaller spheres results in significant enhancement in light extraction at large angular component, while the larger sphere appears to result in stronger enhancement in normal light emission. The current work is limited to the optimization of LEDs with microsphere arrays, and this

Fig. 7. (a) Far-field radiation patterns of anatase  $TiO_2$  microsphere array LEDs with various  $TiO_2$  sphere diameters. (b) Angular dependent power density comparison of anatase  $TiO_2$  microsphere array LEDs. The planar LED is included as reference.

finding will serve as useful guide for optimizing the light extraction in microsphere LEDs deposited by RCD method. Future works will also include the optimization of the microlens array LEDs, which can be formed by embedding the microsphere arrays with polystyrene (PS) materials (i.e., SiO<sub>2</sub>/PS microlens arrays [38]–[41]).

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