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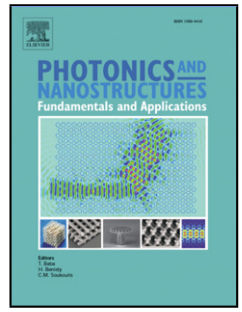

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Effects of Optical Absorption in Deep Ultraviolet Nanowire Light-Emitting Diodes

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Highlights

Summary and Significance

Aluminum gallium nitride (AlGaN) holds significant promises for deep ultraviolet (DUV) light-emitting diodes (LEDs) and laser diodes (LDs) for wide applications including bio-medical and analytical instrumentation, fluorescence sensing, curing, phototherapy and water/air/surface purification and disinfection. Several efforts have been made to develop high efficiency DUV LEDs using such material. However, the performance of DUV LEDs has been fundamentally limited by the large dislocation density and the extremely inefficient *p*-type doping, resulted to the low efficiency and low output power. Moreover, the realization of efficient nanowire LEDs has been limited in the UV ranges because of the performance degradation with increasing Al

composition due to the extremely low EQE, which is directly related to the UV light absorption in the Ga(Al)N p-contact layer and, the unique transverse magnetic polarization properties of high Al composition AlGaN quantum wells(QWs). Although the light extraction efficiency (LEE) of current UV LEDs is limited at <10%, using nanowire structures could overcome the poor performance of such UV emitting devices.

Though, the LEE of UV LEDs have been enhanced by nanowire structures, the strong material absorption are not negligible especially at the short wavelength range such as deep UV. The performances of GaN based LEDs falls short of what is expected due to material absorption. In this paper, we have further looked into this UV LEDs research to study the light absorption in UV LEDs which is an important foundation for the design and development of high-efficiency UV photonics. The significance of this study is the role of material absorption in the periodic nanowire deep UV LEDs. While the emission of the guided modes can be avoided and redirected into radiated modes utilizing nanowire structures, the light extraction can be decreased by light absorption due to absorptive materials which should be considered for deep UV LEDs. Finite-difference time-domain (FDTD) analysis is thoroughly conducted in order to elucidate the role of material absorption and how this reduces the LEE of GaN based UV LEDs for various parameters such as the radius and spacing of the nanowires. The FDTD calculations predicted the UV LED design with the specific nanowire radius and spacing can be utilized to develop the high efficiency III-nitride UV LEDs. Our results show a high LEE of ~34% can be achieved for deep UV emission at 240nm. Moreover, UV nanowire LEDs with random structure can exhibit LEE of ~19% which is comparable or higher than that of high efficiency planar UV LEDs.

Abstract: We report our study on the effect of optical absorption in nanowire ultraviolet light-emitting diodes (LEDs) using three-dimensional finite difference time domain simulation. Utilizing nanowire structures can avoid the emission of guided modes inside LED structure and redirect the trapped light into radiated modes. The optical loss due to material absorption can be decreased by reducing light propagation path inside the LED structure, and consequently enhance the light extraction efficiency (LEE). Nanowire form factors including size, and density play important roles on the LEE of ultraviolet (UV) nanowire LEDs. In this paper, the nanowire spacing and diameter are considered in simulation to reach maximum LEE. Our results show an unprecedentedly high LEE of ~34% can be achieved for deep UV emission at 240nm. Moreover, UV nanowire LEDs with random structure can exhibit LEE of ~19% which is comparable or higher than that of high efficiency UV thin-film LEDs.

Keywords: light-emitting diodes, ultraviolet, nanowire, FDTD, absorption, photonic integrated circuits

1. Introduction

GaN based LEDs are among the most promising next generation of solid state light sources which exhibit several advantages such as long lifetime, energy saving, compact size and environment friendly [1-10]. GaN based LEDs are applicable for various photonic applications with respect to their wavelength emission from deep UV to near infrared by tuning the compositions of their device active regions, consequently, altering the material band gap energy [11-15]. Recently, UV LEDs represents a potentially large market/customer base on water/air/surface purification and disinfections, and many other areas. The primary markets for these devices include bio-medical and analytical instrumentation, fluorescence sensing, curing, phototherapy and water/air/surface purification and disinfection [16-19]. To realize high performance LEDs, their external quantum efficiency (EQE), which is directly proportional to the multiplication of internal quantum efficiency (IQE) and LEE, must be improved. Several efforts have been made to develop high efficiency deep UV LEDs using III-nitride material. However, the performance of deep UV LEDs has been fundamentally limited by the large dislocation density and the extremely inefficient *p*-type doing, resulted to the low efficiency and low output power. In this regard, GaN based nanowire LEDs have recently emerged as the promising alternative that leads to boosting the IQE of UV LEDs due to several advantages including low defect densities, and low strain-induced polarization fields, and more effective in *p*-type doping [20, 21]. We have recently demonstrated high performance LEDs by employing several unique nanowire LED structure such as tunnel injection [22], core-shell nanowire LEDs [23], AlGaN nanowire deep UV LEDs [24], and AlN nanowire deep UV light sources [20]. The realization of efficient nanowire LEDs has been limited in the UV ranges because of the performance degradation with increasing Al composition due to the extremely low EQE, which is directly related to the UV light absorption in the Ga(Al)N *p*-contact layer [25] and, the unique transverse magnetic (TM) polarization properties of high Al composition AlGaN quantum wells (QWs) [26, 27]. Although the LEE of current UV LEDs is limited at <10% [28, 29], using nanowire structures could overcome the poor performance of such UV emitting devices. Moreover, due to the large surface to volume ratio, the LEE is expected to be tremendously improved in nanowire LED devices. "We have recently reported the enhanced LEE of AlGaN UV LEDs by using nanowire structures [24] in which emission wavelength at 280nm was considered."

Though, the LEE of UV LEDs have been enhanced by nanowire structures, the strong material absorption are not negligible especially at the short wavelength range such as deep UV (<280nm). The performances of GaN based LEDs falls short of what is expected due to material absorption. The material absorption is determined by the imaginary part of the dielectric constant which leads to the lower LEE due to the light being absorbed inside the UV LEDs. Photons emitted from active region may be either trapped or absorbed inside the UV LEDs. This shows that improving LEE and diminishing light absorption of UV LEDs have thus become the recent focus of researches [30-32]. The nanowire structures, which have large surface to volume ratio, can reduce the material absorption and enhance the LEE in III-nitride UV LEDs due to increased light escape probability and decreased light propagation path inside nanowires.

In this paper, we focus our study on the material absorption and LEE enhancement in III-nitride deep UV LEDs. Finite-difference time-domain (FDTD) analysis [33-35] is thoroughly conducted in order to elucidate the role of material absorption and how this reduces the LEE of GaN based UV LEDs for various parameters such as the radius and spacing of the nanowires. The FDTD calculations predicted the UV LED design with the specific nanowire radius and spacing can be utilized to develop the high efficiency III-nitride UV LEDs.

2. AlGaN periodic nanowire UV LEDs

Figure 1 shows the schematic of AlGaN based UV LED structure which is considered during the FDTD analysis. The LED structure includes an *n*-AlGaN layer, a multiple quantum well (MQW) active region, a *p*-AlGaN layer, and a *p*-GaN contact layer. Such nanowire arrays can be grown using the methods described elsewhere [36-38]. Additionally, selective area growth is considered as a matured technique for achieving highly uniform periodic nanowire arrays with precisely controlled radius and spacing [39, 40].

The nanowires geometry play an important role in directing the generated photons from active region to the air. In our simulation, the spatial grid sizes in the FDTD simulation were automatically assigned by Lumerical adaptive meshing [41, 42]. Compared to experiment results, some inconsistencies in the simulations can be induced considering the smaller device size which is adopted in the simulations due to limitations in computational resources. The simulated nanowire UV LED domain is 2.5μm x 2.5μm. The perfect matched layers (PMLs) were employed as the absorbing boundaries all around the structures to avoid the undesired reflection of boundaries [43-45]. Although, the AlGaN MQW emit light in both transverse electric (TE) and transverse magnetic (TM) polarizations, the TM emission is dominant in AlGaN UV LEDs and increases significantly with increasing Al composition [46, 47]. The electric field directions are perpendicular and parallel to the c-axis for TE and TM polarizations, respectively. At short wavelengths ~240 nm, the optical emission of AlGaN LEDs is largely TM polarized. Therefore, the high LEE in deep UV nanowire LEDs is made possible by exploiting the lateral side emission properties of nanowires at the TM polarization. The significantly enhanced LEE from lateral sides of the nanowire structure is attributed to the mode coupling through the nanowires. When the coupled modes are formed, light propagates horizontally through the nanowires and can be readily extracted. The lateral side LEE is defined as the ratio of the output power observed around the side surfaces of the LEDs to the total power generated by the QW active region.

When the material absorption is considered in AlGaN UV LEDs utilizing imaginary part of refractive index, the LEE is estimated to be 34%, which is 30% lower than that of structure without considering material absorption. Such phenomena is a direct reflection of material absorption in this simulation.

To provide a comprehensive understanding of LEE from nanowire UV LEDs, the contour plots constructed by LEEs with and without material absorption, and light loss due to material absorption were derived and presented in Figure 2. In this regard, the variation in both nanowire radius and spacing between nanowires was introduced. The radius ranges of 42 – 58 nm, and spacing ranges of 155 – 210 nm were considered in this simulation. Shown in Figure 2(a), the maximum LEE of 34%, which was calculated for the spacing of ~195 nm and nanowire radius of ~44 nm at wavelength of 240 nm. This is confirmed by the particle swarm optimization (PSO) process which is a population of random solutions [48]. It searches for the best solution by updating generations. In our study, a swarm includes 5 particles which represent a potential solution to LEE. The solution converged in 10 iterations, which means we perform the total number of 50 simulations.

The low side LEE (blue area) can be described by photonic bandgap of periodic nanowire arrays which inhibit the light propagation through the structure. For some maximum LEEs such as the spacing ~173 nm and radius of the nanowires ~50 nm, very high light absorption can be seen in Figure 2(b) due to longer path lengths of light propagation which leads the light stays more time inside the semiconductor and increase the light absorption. Consequently, it is highly required to shorten the light propagation path inside the nanowires which is applicable by smaller radius nanowires. Moreover, the observed light extraction enhancement can be from the large nanowires surface which reduce the total internal reflection and decrease the absorption of the material by the shorten propagation distance.

Comparing Figures 2(c) and (a), it reveals that the diminished LEE is attributed to light absorbed by absorptive material in nanowires. The simulation results approved that the material absorption is one of important factors which deteriorate the nanowire LEDs output power evidently.

Figure 3 shows the simulated mode profiles with the optimized nanowire spacing and diameter. It is seen that light can be mostly extracted from sides of device and it is nearly half for the LED with absorptive material compared to lossless LED. The evanescent fields can be extended and produce a strong light propagation through the nanowires; thus, the LEE of the nanowire UV LEDs is significantly increased. Figure 3(b) presents the simulated mode profiles for the UV LED with material absorption which has lower intensity compared to that of UV LED without material absorption, illustrated in Figure 3(a). To clearly distinguish the difference between Figures 3(a) and (b), the simulated mode profiles with same intensity scale are provided in Figure 3(c). The light intensity for the structure with absorption is less than half compared to the lossless structure.

3. Dependence of LEE on the position of nanowires and size of LED devices

The LEE also depends on the device size. In order to gain further understanding of the relation between LEE and device size, we have performed simulation on devices with areal sizes in the ranges of $2.5\times2.5\ \mu m^2$ to $10\times10\ \mu m^2$. Illustrated in Figure 4(a), it is found that LEE is slightly decreased by increasing the device size, and the maximum LEE for device different device sizes decreases from ~34% to ~18%. It is obvious that the LEE is less sensitive to the device size than other parameters such as nanowire radius and spacing.

For practical applications, it is necessary to understand the dependence of the LEE on small variations of nanowire properties due to the fabrication tolerances. The LEE is calculated for twenty different random structures as shown in Figure 4(b). First, the spacing and radius of the nanowires are fixed at 195 nm and 44 nm, respectively. Then we introduced a ±10% random variation in the nanowire radius and spacing between nanowires. With such a random distribution, we observed that the average LEE for the nanowire devices with and without absorption are 19% and 41% respectively.

Figure 4(c) shows the simulated mode profiles with the random nanowire spacing and radius. It is seen that some local cavities are formed which confine and localize light inside the UV LED structure. It should be noted that the LEE of 19% is still nearly two times higher than deep UV LEDs which is previously reported with maximum external quantum efficiencies of <10%. With well-controlled growth and fabrication process, it is expected that the LEE of deep UV LEDs can become comparable to that of high efficiency visible LEDs.

4. Conclusion

We have presented the design of periodic nanowire deep UV LEDs and investigated the role of material absorption using 3D FDTD simulation. While the emission of the guided modes can be avoided and redirected into radiated modes utilizing nanowire structures, the light extraction can be decreased by light absorption due to absorptive materials. Through a comprehensive investigation of different parameters including the nanowire size, density as well as the LED device size, we have shown that an unprecedentedly high LEE of ~34% can be achieved. Although we have considered periodic nanowire UV LEDs with high LEE, UV LEDs with random structure can exhibit ~19% which is comparable to that of high efficiency planar UV LEDs. With a properly designed nanowire structures, the UV light absorption can be reduced, resulted in the enhanced LEE in III-nitride deep UV LEDs. This study provides important information for the design of high performance optoelectronic devices operating in the deep UV wavelength regime.

Acknowledgments

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Figure Captions:

Figure 1: The 3D schematic of GaN based UV LED structure including an *n*-AlGaN layer, a multiple quantum well (MQW) active region, a *p*-AlGaN layer, and a *p*-GaN layer.

Figure 2: The contour plots show light extraction efficiencies with the radius ranges of 42 – 58 nm, and spacing ranges of 155 – 210 nm for (a) the structure with material absorption, (b) light power loss due to material absorption, (c) the structure without material absorption.

Figure 3: The simulated mode profiles with the optimized nanowire parameters for the spacing ~195 nm and radius of the nanowires ~44 nm for the UV LED (a) without and (b) with material absorption, (c) the simulated mode profiles with same intensity scale.

Figure 4: (a) Dependence of the light extraction efficiency on the various device sizes, (b) The light extraction efficiency for twenty different structures with random nanowire spacing and random nanowire radius, (c) the simulated mode profiles with the random nanowire spacing and radius.

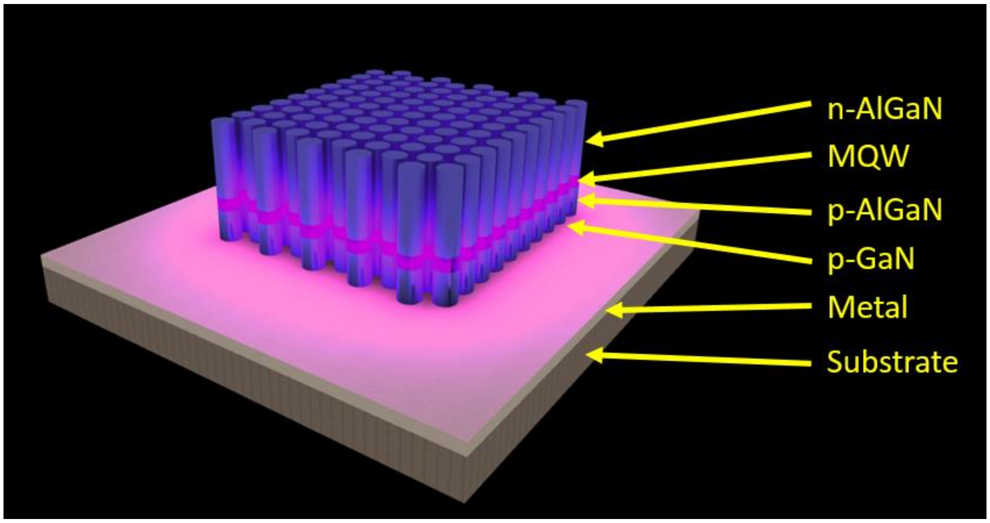
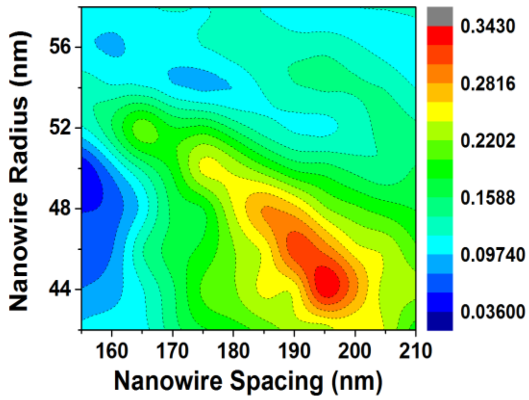


Figure 1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52
48
44
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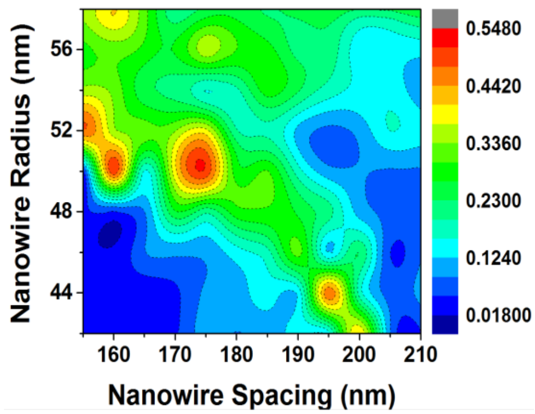
0.1588
0.09740
0.03600

(a)


Nanowire Radius (nm)
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52
48
44
160 170 180 190 200 210
Nanowire Spacing (nm)
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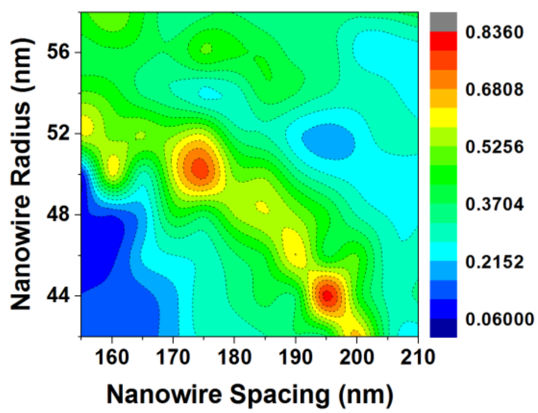
0.2300
0.1240
0.01800

(b)

Figure 2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52
48
44
160 170 180 190 200 210
Nanowire Spacing (nm)
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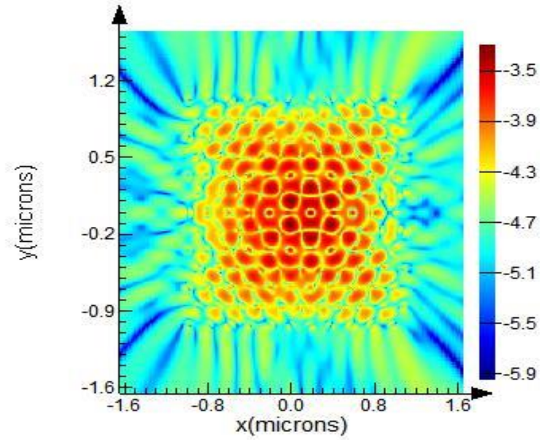
0.5256
0.3704
0.2152
0.06000

(c)

Figure 3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-0.9
-1.6
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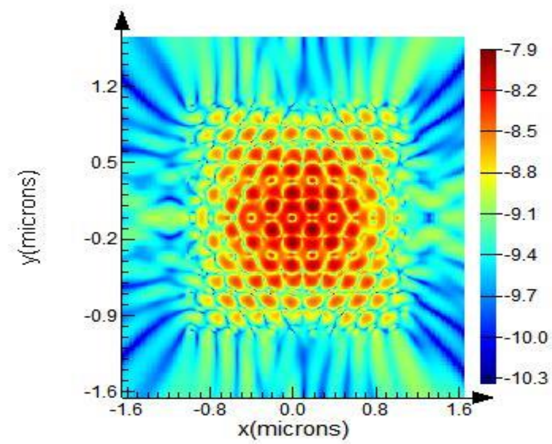
-0.8
0.0
0.8
1.6
x(microns)
-3.5
-3.9
-4.3
-4.7
-5.1
-5.5
-5.9

(a)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0.8
1.6
x(microns)
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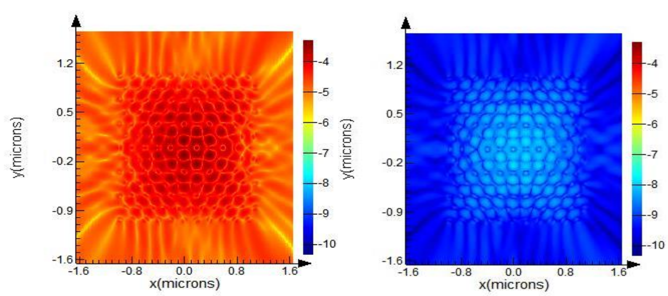
-9.7
-10.0
-10.3

(b)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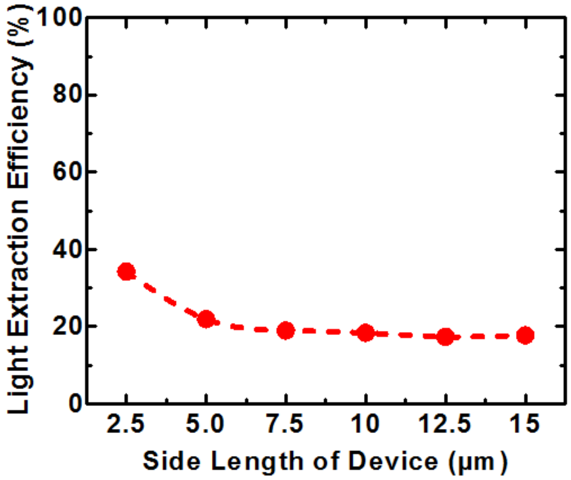
x(microns)
-4
-5
-6
-7
-8
-9
-10
y(microns)
1.2
0.5
-0.2
-0.9
-1.6
-1.6
-0.8
0.0
0.8
1.6
x(microns)
-4
-5
-6
-7
-8
-9
-10

(c)


Light Extraction Efficiency (%)
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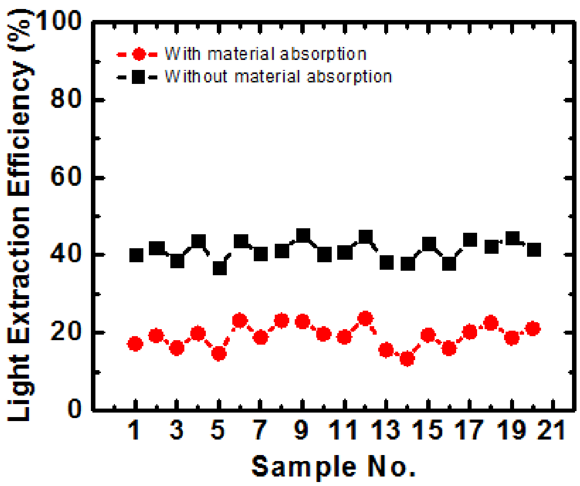
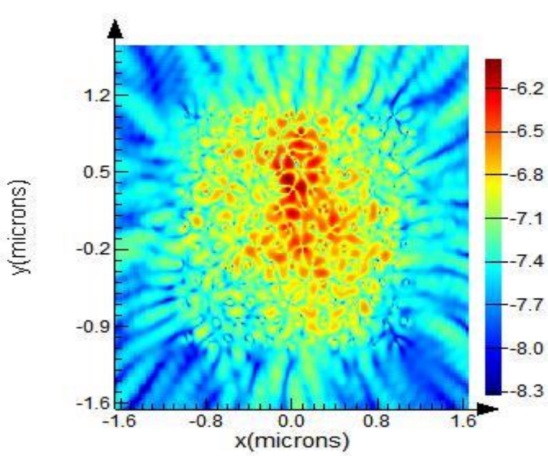
20
40
60
80
100
2.5
5.0
7.5
10
12.5
15
Side Length of Device (μm)
(a)

Figure 4


With material absorption
Without material absorption
Light Extraction Efficiency (%)
0
20
40
60
80
100
1 3 5 7 9 11 13 15 17 19 21
Sample No.
(b)


y(microns)
1.2
0.5
-0.2
-0.9
-1.6
-1.6
-0.8
0.0
0.8
1.6
x(microns)
-6.2
-6.5
-6.8
-7.1
-7.4
-7.7
-8.0
-8.3
(c)