Simulation of the light extraction efficiency of nanostructure light-emitting diodes*

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The light extraction efficiencies have been calculated for various InGaN/GaN multiple quantum well nanostructure light-emitting diodes including nanopillar, nanorough of P-GaN surface, coreshell and nano-interlayer structure. From the calculated results we can see that the light extraction efficiency is remarkably improved in the nanostructures, especially those with an InGaN or AlGaN nano-interlayer. With a 420-nm luminescence wavelength, the light extraction efficiency can reach as high as 65% for the InGaN or AlGaN nano-interlayer structure with appropriate In or Al content while only 26% for the planar structure.

Keywords: light extraction efficiency, InGaN/GaN multiple quantum well, nanostructure

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1. Introduction

The direct wide-bandgap gallium nitride (GaN) and other III-nitride semiconductors have attracted increasing attention as they are widely used in many optoelectronic devices such as light-emitting diodes (LEDs) and blue laser diodes.[1]Over the last decade, InGaN/GaN based LEDs have attracted great attention due to their wide applications such as in traffic lights, indoor/outdoor displays, back lighting in liquid-crystal displays and solid-state lighting. However, despite an impressive commercial success, the light extraction efficiency is still low because of the total reflection in the interface between GaN and air. For a conventional planar LED structure, approximately only $1/4n^2$ ($n = 2.4$ is the refractive index of GaN) of the light from the active region can radiate through the top and bottom surface of the devices because of guided modes in which light is totally reflected between the device surfaces.[2] Therefore, enhancing the light extraction efficiency is one of the most important factors for the development of GaN based LEDs, and several methods have been reported to improve the light extraction efficiency such as surface-textured, photonic crystal and patterned sapphire substrates.[3−10] Recently, due to the great advantages of nanostructures over bulk materials, such as the 3D confinement effect, a large sidewall surface, strain relaxation and dislocation reduction, they have acquired many applications in devices such as super-bright LEDs, full colour displays, high efficiency laser diodes and detectors.[11,12] Additionally, it has been widely accepted that fabricating nanostructures on the LED wafer can offer a higher light output efficiency than conventional planar LEDs.[13,14] Due to the large sidewall surface of nanostructure, much of the light generated in the active layer can directly emit into the air through the sidewall of the nanostructure.[15−17]

In this report, the raytrace method is used to numerically calculate the light extraction efficiency of different nanostructures including nanopillar, nanotextured P-GaN surface, coreshell and nano-interlayer structures. It is found that the light extraction effi-

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ciency can be remarkably enhanced in the nanostructures.

2. Device structure and simulation parameters

We simulate the light extraction efficiency of an LED with different nanostructures using the raytrace method, which is based on the Monte Carlo method.

The GaN-based LED structures in our calculation were grown on a *c*-axis sapphire substrate and consist of a 3.0-μm N-type GaN: Si layer, a five periods InGaN/GaN MQW active layer, where the total thickness is about 200 nm and a 0.2-μm thick P-type GaN: the Mg layer is on the top. The simulation parameters are listed in Table 1. For convenience of calculation, in our simulation model we prescribe that the bottom surface of the P-GaN and the top surface of the N-GaN are the surface sources, thus the multiple-quantum well (MQW) layer can be ignored. The wavelength used in the calculation is 420 nm .

Table 1. The simulation parameters of the nanopillar LED.

Materials	Thickness/μm	Refractive index	Absorption coefficient/mm
P-GaN	0.2	2.5	10
N-GaN	3	2.5	10
Sapphire	300	1.76	0.001

3. Results and discussion

For comparison, we first calculate the light extraction efficiency ($\eta_{\text{extraction}}$) of a conventional planar LED structure. From the simulated results (not shown here) we obtained that the conventional LED has only a light extraction efficiency of 26%. In what follows, the light extraction efficiency of several different nanostructures will be calculated.

3.1. Calculation of the nanopillar structure

As is known, the sidewall of the nanopillars provides a larger surface area and more pathways by which the generated photons can escape. Much of the light from the active region that cannot radiate through the top or bottom of the device may be emitted through the sidewall of the nanopillars. Therefore, a nanopillar LED structure is considered to be a useful structure to enhance the light extraction efficiency of an LED. In the following simulation, we assume that the InGaN/GaN MQW active layer is embedded in the nanopillars; the height of the nanopillars and the refractive index of GaN for simulation are assumed to be 600 nm and 2.5, respectively. The schematic structure of nanopillar LEDs in the simulation is shown in Fig. 1(a) with a duty cycle of 4.4:1. We calculated the nanopillars with diameters varying from 50 nm to 250 nm, with the duty cycle fixed at 4.4:1 and the dependence of $\eta_{\text{extraction}}$ on the nanopillar diameter is shown in Fig. 1(b). From the calculated results, we can find that as the diameter of the nanopillar decreases, the light extraction efficiency is enhanced. For ae nanopillar diameter of 50 nm, the light extraction efficiency of a nanopillar LED can reach as high as 50%. We know that a nanopillar with a smaller diameter has a larger surface volume ratio, so the light emitted from the smaller nanopillars can go out through the sidewall more easily than that from the larger ones. This is why the LED with smaller nanopillars has a higher light extraction efficiency. We also calculated the dependence of $\eta_{\text{extraction}}$ on the duty cycle

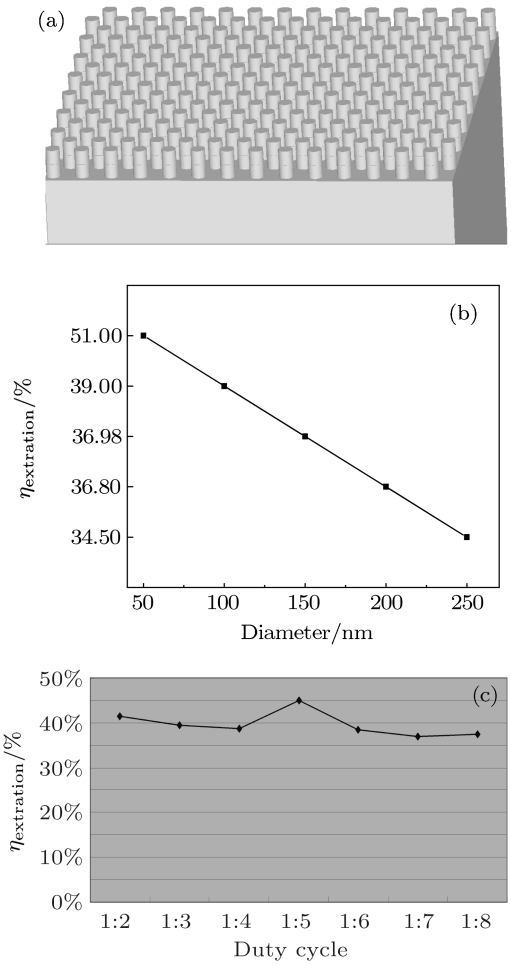


Fig. 1. (a) The schematic structure of nanopillar LEDs. (b) The dependence of $\eta_{\text{extraction}}$ on the nanopillar diameter.(c) The dependence of $\eta_{\text{extraction}}$ on the duty cycle of nanopillars with a given diameter of 200 nm.

of nanopillars with a given diameter of 200 nm, and found that with a duty cycle of 1:5, the $\eta_{\text{extraction}}$ can reach its maximum value of 45% with nanopillars of 200 nm, as shown in Fig. 1(c).

3.2. Calculation of coreshell structure

A P-GaN/MQW/N-GaN coreshell structure has large active layer area and surface area, which can provide a higher recombination efficiency and more pathways by which the generated photons can escape. We calculated the coreshell structure with a pillar height of 500 nm and diameter of 200 nm. As shown in Fig. 2, the P-GaN and MQW layers are coated on the N-GaN nanopillars. The light extraction efficiency for this structure is calculated to be 40.86%. We could deduce that the light extraction efficiency could be further improved by adjusting the dimension, density or height of pillars in this structure.

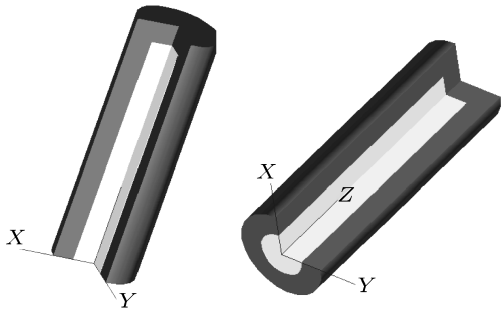


Fig. 2. The schematic structure of coreshell LEDs.

3.3. Calculation of the nano-textured structure

Surface texturization is another approach to enhancing the light extraction efficiency of LEDs due to the scattering of photons from the textured semiconductor surface. This process allows the photons generated within the LEDs to find the escape cone by multiple scattering from a rough surface without destroying the MQWs active region. For the nano-textured structure, very shallow nanopillars are fabricated only on the P-GaN layer. The schematic structure of a nano-textured LED is shown in Fig. 3(a). With a fixed height H of 80 nm of the nanopillars, the light extraction efficiencies of a nano-textured LED with different nanopillar diameters are calculated, and the dependence of $\eta_{\text{extraction}}$ on the diameter of the nanopillar is shown in Fig. 3(b). We find that $\eta_{\text{extraction}}$ can reach the maximum value of 35% while the nanopillar diameter is 250 nm.

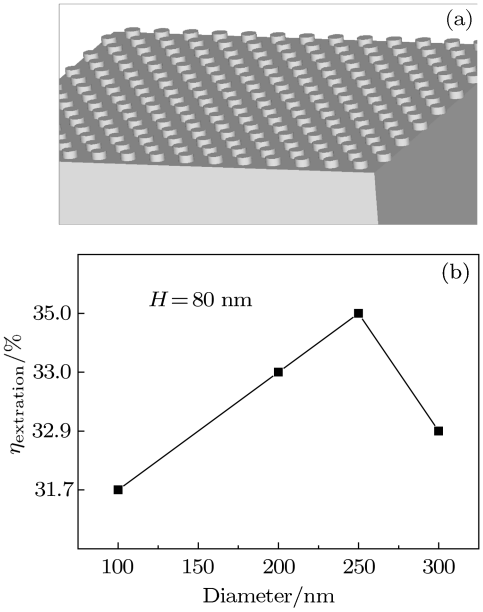


Fig. 3. (a) Schematic structure of nano-textured LEDs. (b) The dependence of light extraction efficiency on the dimension of the nano-textured pillar.

3.4. Calculation of structure with a nano-interlayer

Then, we simulate a structure with an InGaN or AlGaN nano-interlayer. The fabrication process is described as follows: first, GaN nanopillars were fabricated. Next, InGaN or AlGaN interlayers, which have a different refractive index from that of the GaN layer, were grown on the top and side surfaces of the GaN nanopillars. The nano-interlayer was coated over the entire surfaces of the GaN nanopillars. Finally, N-GaN, MQWs and P-GaN were grown in succesion, as shown in Fig. 4(a). The refractive index of the interlayer can be adjusted by the In content in InGaN or the Al content in AlGaN. The dependence of $\eta_{\text{extraction}}$ on the refractive index of the interlayer is shown in Fig. 4(b). We assume that the height and diameter of the nanopillars are 500 and 200 nm, respectively. The simulated results show that when $n = 2.2$ and $n = 2.7$ the light extraction efficiency can reach a maximum value of 65%. From the simulated results, we can see that the light extraction efficiency of the nano-interlayer structure can reach more than 65% through adjusting the In content in InGaN or Al content in AlGaN. Theoretically, a GaN LED with a nano-interlayer can achieve a higher light extraction efficiency than a conventional planar one, mainly because the perpendicular sidewall surface of the interlayer can break the parallel relationship between the layers in the conventional LED structure and could change the rays' transmission directions,

which can enhance the ratio of the rays emitted outwards. In addition, the refractive index difference between the InGaN or AlGaN interlayer and the GaN buffer layer can introduce a new interface, which can enhance the reflection probability of the rays emitted from the MQW active layer and thus enhance the light extraction efficiency of the LED. Thus, the light extraction efficiency is remarkably improved in nano-interlayer structure than that in a conventional planar structure.

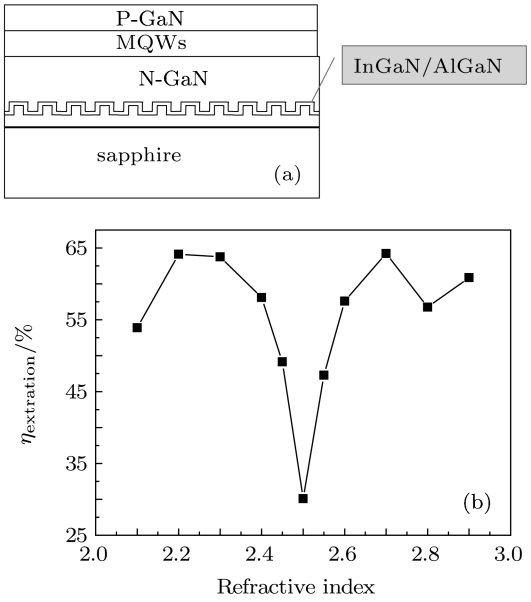


Fig. 4. (a) Schematic structure of nano-interlayer LEDs. (b) The dependence of light extraction efficiency on the refractive index of the interlayer.

From the above-mentioned calculation and analysis, we can conclude that the structure with a nano-interlayer has the highest light extraction efficiency. However, this structure is very difficult to grow and fabricate because of the different growth modes for the sidewall and the top surface of nanopillars. The growth in the nanopillar sidewall is featured by the nonpolar growth mode while on the top (0001) plane is by the polar growth mode.[18,19] Different growth modes result in different growth rates and In contents. Although the nano-interlayer structure performs well, several improvements of device growth and fabrication processing is still needed.

4. Conclusion

In conclusion, the raytrace method has been used to calculate the light extraction efficiency of different InGaN/GaN MQW nanostructures, including nanopillar, nanorough surface, coreshell and nano-interlayer structure. From the calculated results, we can see that the light extraction efficiency is remarkably improved in the nanostructure, especially in the structure with an InGaN or AlGaN nano-interlayer. With the 420-nm luminescence wavelength, the light extraction efficiency can reach as high as 65% by adjusting the In or Al content for the nano-interlayer structure while only 26% for the planar structure.

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