Simulation of InGaN/GaN light-emitting diodes with Patterned Sapphire Substrate

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***Abstract*-Blue InGaN/GaN multiple quantum well (MQW) light-emitting diodes (LEDs) with patterned sapphire substrate (PSS) are simulated by the APSYS software. Approach of combining finite-difference time-domain (FDTD) method and ray tracing technique is applied to perform light extraction. The simulation results show that PSS dramatically increases extraction efficiency of light power, in agreement with experiment. It is found that extraction efficiency can be maximized by changing the shape of PSS. This work presents a new approach to combine electrical simulation with FDTD and raytracing for both accuracy and efficiency in 3D TCAD simulation of GaN-LED.**

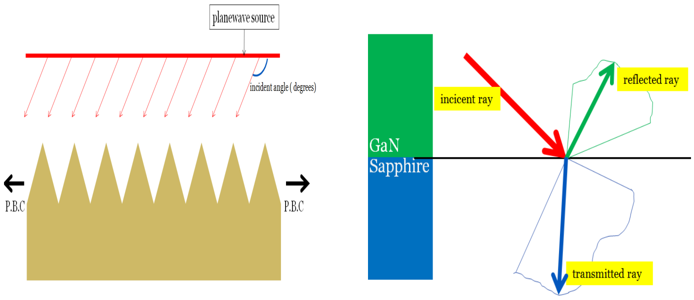
Ⅰ. INTRODUCTION

Gallium-nitride-based (GaN-based) multiple quantum well (MQW) light-emitting diodes (LEDs) have been applied to many energy-saving fields such as out-door full-color displays, high performance back-lighting for liquid crystal displays [1][2]. However so far, the external quantum efficiency (EQE) of MQW LEDs is still not large enough compared with what is expected [3]. The EQE is a product of carrier injection efficiency (CIE), internal quantum efficiency (IQE) and light extraction efficiency (LEE), and each term in the product is the focus of researches. CIE and IQE can be improved by specific designs such as electron blocking layer (EBL) [4], ITO as current spreading layer [5] and the last quantum barrier $In_{0.03}Ga_{0.97}N$ for improving IQE [6]. To improve LEE, the techniques of surface roughening [7], nanoprinting [8] have been used but not effectively [3]. In the past few years, GaN based-LEDs grown on patterned sapphire substrate (PSS) have attracted more and more interest from researchers [9][10]. The PSS reduces threading dislocation density in GaN epi-layers as well as enhances LEE of LEDs due to increased light escape probability [11]. Several types of PSS have been successfully applied to fabrication of high-efficiency LEDs [12] [13]. Also, comparison of the LED EQE between un-patterned sapphire substrate (u-PSS) and PSS has been carried out experimentally [14][15]. However, theoretical analysis of LEE on PSS LEDs is a major challenge. Ray tracing (RT) technique has been applied to LEE analysis for u-PSS LEDs previously. For PSS LEDs, some simplified RT methods were proposed in recent years but all were based on geometric optics [16][3]. When PSS size becomes comparable with wavelength of light emitted by LEDs, wave properties of light must be considered. In this work, we carried out 2D/3D simulation of InGaN/GaN MQW LED with PSS by the APSYS software. Light extraction processing is implemented by a new RT method which combines both geometric and wave behavior of light emitted from MQW. By properly changing shape of PSS, optimized LEE has been achieved.

Ⅱ. THEORETICAL MODELS

The APSYS software [17] self-consistently combines carrier transport and self-heating. Various mechanisms which are critical for LED analysis, such as self-consistent quantum well based spontaneous emission, non radiative recombination and injection current overflow have been included in the software. The transport model includes drift and diffusion of electrons and holes, Fermi statistics, built-in polarization and thermionic emission at heterointerfaces. An efficient RT module in APSYS proves to be especially useful for the study of light extraction. MEEP, a finite-difference time-domain (FDTD) simulation software package developed at MIT, was also included in APSYS using special data interface.

FDTD simulation calculates angular distribution of reflection and transmission coefficients with different incident angles to PSS interface. Fig. 1(a) shows the schematic of FDTD simulation. Light emitted by LED is treated as plane wave on PSS with an incident angle. Periodical boundary condition (P.B.C.) is considered.



Then in RT simulation, when an incident ray hits PSS interface, *Fresnel* conditions will not be applied. Effective reflection and transmission coefficients are imported from FDTD results. In other words, PSS interface is considered as a

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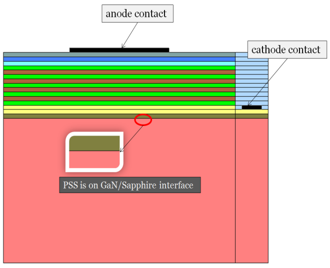
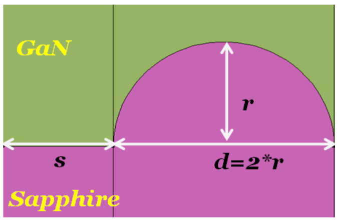
special interface with wave behavior. Fig. 1(b) presents the schematic of applying FDTD results on PSS in RT simulation. The reflected ray points in a direction with probability based on the angular profile of reflected radiation in the FDTD calculation. The refracted ray is handled in the same way.

Ⅲ. LED DEVICE AND PSS STRUCTURE

The LED structure in this paper stands on a 200µm sapphire. The layer structure consists of 2µm un-doped GaN, 1µm n-doped (5×10^{18} cm^{-3}) GaN, four periods of un-doped $In_{0.11}Ga_{0.89}N$(4nm)/GaN(20nm) MQW active region, topped with 0.2µm p-type (8×10^{18} cm^{-3}) GaN cap layer. Fig. 3(a) shows the schematic structure of the LED with setting of contact positions.

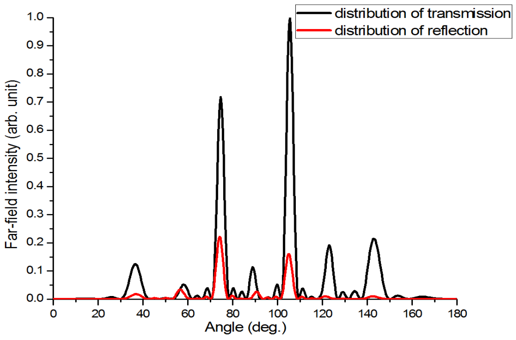
Unit structure of PSS is formed by a half circle (sphere in 3D view) with radius of *r* and distance of *s* to next unit, which is shown in Fig. 3(b). The unit structure will be periodically extended according to the P.B.C. in the FDTD simulation.





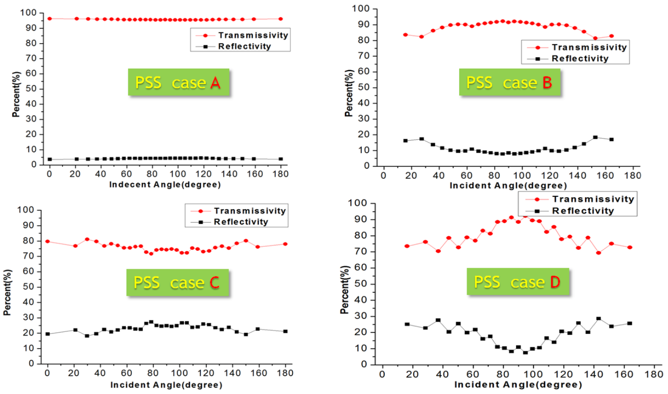
Ⅳ. RESULTS AND DISCUSSIONS

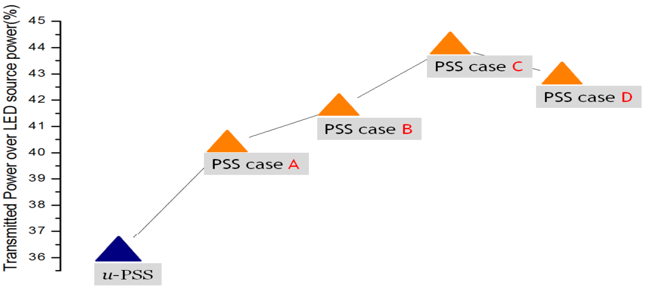
To investigate how PSS shape affects light extraction, we settled on four shapes of PSS unit with sizes ranging from much smaller to much larger than peak wavelength of the LED: case A, B, C and D with *r* =0.05µm, 0.2µm, 0.5µm and 1µm while *s* is fixed as 0.5µm, respectively. Fig. 3 illustrates a typical angular distribution of reflection and transmission coefficients for case C with incident angle of 15° .



Integration of each distribution curve gives total reflected power (reflectivity R) and transmitted power (transmissivity T). Fig. 4 shows the changing trends of R and T for the four cases.

RT simulation is finally carried out for the LED device with the four cases of PSS. Light sources of RT simulation are automatically located by getting results from opto-electrical simulation of APSYS software. RT simulation for u-PSS LED is also performed. Fig. 5 shows the percent of transmitted light power out of LED device. All PSS patterns used in this study yield a higher LED light power compared with u-PSS LED. Moreover, for PSS cases, as *r* increases, transmitted light power increases firstly and then drops down after a peak at *r*=0.5µm. This indicates that micro-structure width (2*r*) has a strong effect on LED light extraction.





Ⅴ. CONCLUSIONS

An LED with PSS has been accurately simulated by combining FDTD and ray tracing approaches and different PSS configurations has been compared. An important finding of this study is that for a specific PSS geometry, the peak of light extraction efficiency can be found at a PSS size. This work can be widely extended to investigations on any shape of PSS for the optimization of LED performance.

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