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Numerical Investigation of Purcell Enhancement of the Internal Quantum Efficiency of GaN-based Green LED Structures

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GaN-based green light-emitting diode (LED) structures suffer from low internal quantum efficiency (IQE), known as the "green gap" problem. The IQE of LED structures is expected to be improved to some extent by exploiting the Purcell effect. In this study, the Purcell effect on the IQE of green LED structures is investigated numerically using a finite-difference time-domain simulation. The Purcell factor of flip-chip LED structures is found to be more than three times as high as that of epi-up LED structures, which is attributed to the high-reflectance mirror near the active region in the flip-chip LED structures. When the unmodified IQE is 20%, the relative enhancement of IQE can be greater than 50%, without utilizing the surface-plasmon coupling effect. Based on the simulation results, the "green gap" problem of GaN-based green LEDs is expected to be mitigated significantly by optimizing flip-chip LED structures to maximize the Purcell effect.

Keywords : GaN, Light-emitting diode, Quantum efficiency, Purcell effect
OCIS codes : (230.3670) Light-emitting diodes; (310.6805) Theory and design; (160.6000) Semiconductor materials

I. INTRODUCTION

The efficiency of GaN-based blue light-emitting diodes (LEDs) has been improved to a level that is allowing solid-state lighting to rapidly replace conventional lighting technologies [1-3]. The external quantum efficiency (EQE) of InGaN/GaN blue LEDs has been demonstrated to be >80% [4]. On the contrary, GaN-based green LEDs still suffer from low efficiency. The EQE of InGaN/GaN LEDs with emission wavelengths from 530 to 600 nm has been reported to be <30%, which has been termed the "green gap" problem [5-7]. The "green gap" problem results from the low internal quantum efficiency (IQE) of InGaN quantum wells (QWs) with high indium content, which is attributed to the decrease in crystal quality and increase in internal polarization fields with increasing indium content. Recently it has been reported that the increase in nonradiative recombination rate with increasing indium content results from the random fluctuation of indium concentration that is natural in InGaN alloy [7]. Indium fluctuations could also result in reduced effective active volume of InGaN QWs, which leads to low IQE [8, 9]. This implies that increasing IQE by improving QW crystal quality may have its limitations in GaN-based green LEDs.

One strategy to increase the IQE is to increase the radiative recombination rate by using the Purcell effect. The Purcell effect is based on Fermi's Golden Rule, where the spontaneous-emission rate depends on the local density of states and the strength of electromagnetic modes around the emitters [10]. When the spontaneous emission rate is enhanced, the radiative carrier lifetime in QWs is reduced, which leads to an increase in the radiative carrier recombination rate and hence the IQE of LEDs. In fact, a large Purcell effect has been expected from surface-plasmon (SP)-coupled LEDs [11-14]. However, due to the nonradiative energy transfer from QWs to metallic structures, efficient extraction of SP-coupled light out of the LED chip has been challenging, and the development of practical SP-coupled

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LEDs has not been demonstrated yet [15, 16].

The spontaneous emission rate can also be modified in a flip-chip (FC) or vertical LED structure. The FC or vertical LED basically consists of *n*-GaN, InGaN multiple quantum well (MQW), and *p*-GaN epitaxial layers placed on a high-reflectance electrode reflector [17-19]. The high-reflectance mirror near the MQW layers can alter the spontaneous emission rate by modifying the local density of states around the QWs [20-22]. The relative enhancement of the spontaneous emission rate is often called the Purcell factor, which is denoted as F_P in this paper.

It has been shown that F_P can be calculated numerically using a finite-difference time-domain (FDTD) simulation [22-25]. Recently, the Purcell effect in InGaN blue LEDs has been numerically investigated, and the increase of IQE and substantial reduction of IQE droop have been reported [22]. However, the improvement of the IQE of a blue LED with unmodified IQE of 80% was calculated to be only ~2% when the Purcell effect was employed [22]. In this paper, the Purcell effect on the IQE of green FC LEDs is investigated using an FDTD simulation. Since the Purcell effect becomes increasingly dominant as the IQE decreases, green LEDs with low IQE are expected to show higher IQE enhancement via the Purcell effect, compared to blue LEDs.

II. SIMULATION METHOD

For the numerical simulation of this study, a three-dimensional FDTD method with a perfectly matched layer (PML) boundary condition is employed [26]. We consider two types of LED structure: FC and epi-up. Figure 1 shows a FDTD computational domain for these two LED structures. The LED structures basically consist of an *n*-GaN layer, a InGaN/GaN MQW active region 20 nm thick, an AlGaN electron-blocking layer 10 nm thick, and a *p*-GaN layer. The thickness of the *n*-GaN layer is assumed to be 1 m; the *n*-GaN thickness was found to have little influence on the Purcell factor, once it is thicker than ~500 nm. For the FC LED, the *p*-GaN layer is placed on an Ag reflector. Both FC and epi-up LED structures are assumed to be enclosed by epoxy resin. The refractive indices of GaN, epoxy, and Ag are set to 2.45, 1.55, and $0.12 + 3.2\,i$ respectively [27]. For normal incidence, reflectance at the *p*-GaN/Ag interface of the FC LED is 93%, and that at the *p*-GaN/epoxy interface of the epi-up LED is 5%.

In the simulation, a point dipole source is positioned at the center of the computational domain in the horizontal direction and at the center of the active region in the vertical direction, as shown in Fig. 1. In the source spectrum, the spectral envelope of emitted light is Gaussian in shape, for which the center wavelength and full width at half maximum of the spectrum are chosen to be 530 and 25 nm respectively. The dipole source is polarized in the direction parallel to the QW plane for the excitation of transverse electric modes. In the FDTD method, the spontaneous emission rate is proportional to the total dipole radiation energy, which is obtained by integrating the Poynting vector over time and over the enclosing surfaces [24, 25]. F_P can be determined as follows: First, the total dipole radiation energy is calculated for a homogeneous material, without cavity or reflector structures. Next, the total dipole radiation energy is calculated for the case of the actual LED structure. Finally, F_P is determined by dividing the total radiation energy of the dipole source in the LED structure by that of the dipole source in homogeneous GaN material. In this work, F_P for the FC and the epi-up LED structures is calculated as the thickness of *p*-GaN varies. Since F_P is mainly influenced by the distance from the *p*-GaN surface to the QW, strong dependence of F_P on *p*-GaN thickness is anticipated.

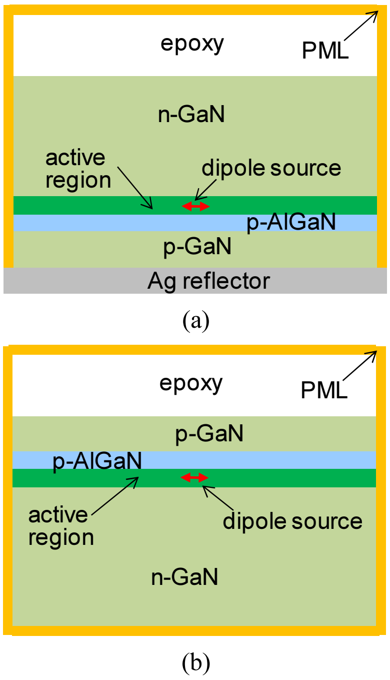


FIG. 1. Schematic cross-sectional view of the FDTD computational domain of simulated LED structures: (a) flip-chip (FC) LED having an Ag reflector; (b) epi-up LED encapsulated by epoxy. The simulated LED structures are surrounded by PML boundaries.

III. RESULTS AND DISCUSSION

Figure 2 shows simulated F_P for FC and epi-up LED structures, as a function of the *p*-GaN layer thickness. Since the Purcell effect results from the interference between the light emitted from the QW and the light reflected from the mirror, F_P varies periodically with *p*-GaN thickness. The periodicity of the *p*-GaN thickness is ~110 nm, which corresponds to half of the wavelength of green light inside the GaN. For a thin *p*-GaN layer <30 nm thick, F_P of the

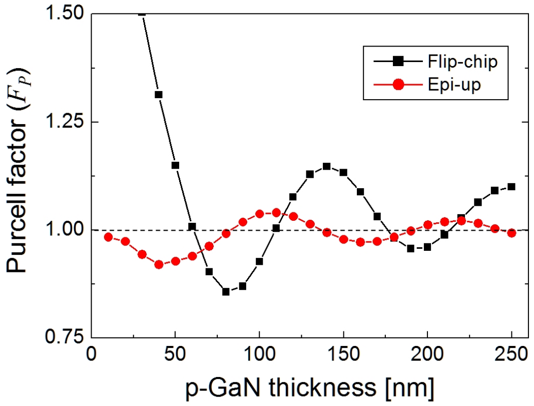


FIG. 2. Purcell factor F_P of flip-chip and epi-up LED structures, as a function of the *p*-GaN thickness.

FC LED increases rapidly with decreasing *p*-GaN thickness, which is attributed to the SP coupling of light at the Ag reflector. However, as mentioned, practical utilization of the SP resonance is challenging, due to too thin of a *p*-GaN layer and the dissipation of light at Ag. Therefore, a practical *p*-GaN thickness greater than 100 nm is considered here.

When the *p*-GaN thickness is greater than 50 nm the influence of SPs is negligible, and the Purcell effect results purely from the modification of the optical density of states due to the interface of the LED. The amplitude of the F_P variation for the FC LED is more than three times as great as that for the epi-up LED. The local peak of F_P for the FC LED is as large as 1.15, while that for the epi-up LED is less than 1.05, when the *p*-GaN thickness is >50 nm. This indicates that the reflectance at the interface has a significant influence on F_P. The amplitude of F_P variation decreases slowly as the thickness of *p*-GaN increases. For the FC LED, the local peaks in F_P are obtained at *p*-GaN thicknesses of 140 and 250 nm, while for the epi-up LED they are observed at 110 and 220 nm. The difference in the *p*-GaN thickness for peak F_P between FC and epi-up LEDs originates from the phase shift during reflection at the Ag reflector of the FC LED. Although F_P of ~1.15 for the FC LED is much smaller than the F_P that can usually be obtained by SP coupling, it could provide a substantial increase in the IQE of green LEDs, as will be shown later.

The IQE of a homogeneous, reference LED structure without Purcell enhancement can be written as

$$\eta_0 = \frac{R_r}{R_r + R_{nr}}, \tag{1}$$

where R_r and R_{nr} are respectively the radiative and non-radiative recombination rates. When a dipole source is placed in the FC LED structure, the IQE modified by the Purcell effect is written as

$$\eta' = \frac{R_r'}{R_r' + R_{nr}'}, \tag{2}$$

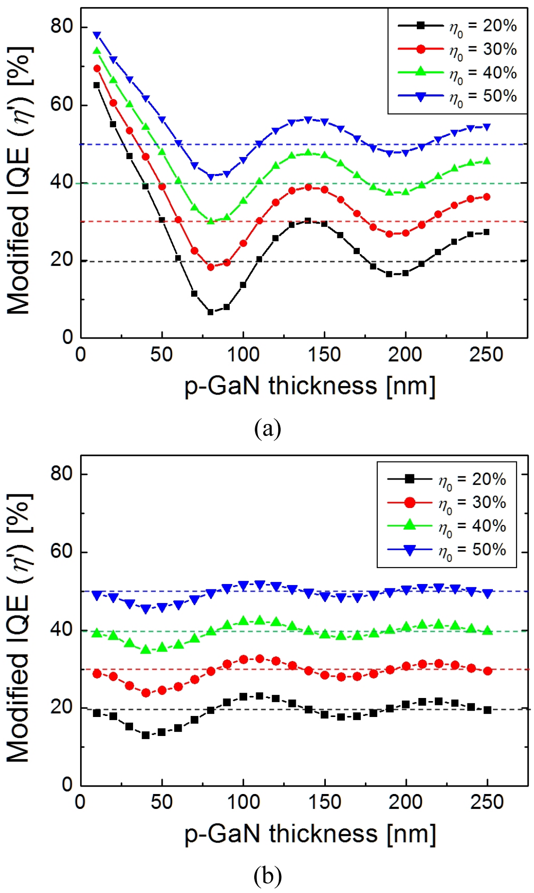
where R_r' is the radiative recombination rate modified by the Purcell effect. Then F_P is expressed as

$$F_P = \frac{R_r'}{R_r}. \tag{3}$$

Using Eqs. (1)-(3), the modified IQE η' is obtained in terms of η_0 and F_P as in the following [22]:

$$\eta' = \frac{F_P \eta_0}{(F_P - 1)\eta_0 + 1}. \tag{4}$$

Using Eq. (4), the modified IQE η' is calculated for the FC and epi-up LEDs. Figure 3 shows η' as a function of the *p*-GaN thickness when η_0 is 20%, 30%, 40%, or 50%. The variation of η' with *p*-GaN thickness is basically similar to that of F_P shown in Fig. 2. The IQE variation of the FC LED is much larger than that of the epi-up LED. A large increase in IQE is observed for the FC LED with a thin *p*-GaN layer <50 nm, which is attributed to the SP coupling effect, as mentioned. For the FC LED structure with *p*-GaN thickness of 140 nm, the modified



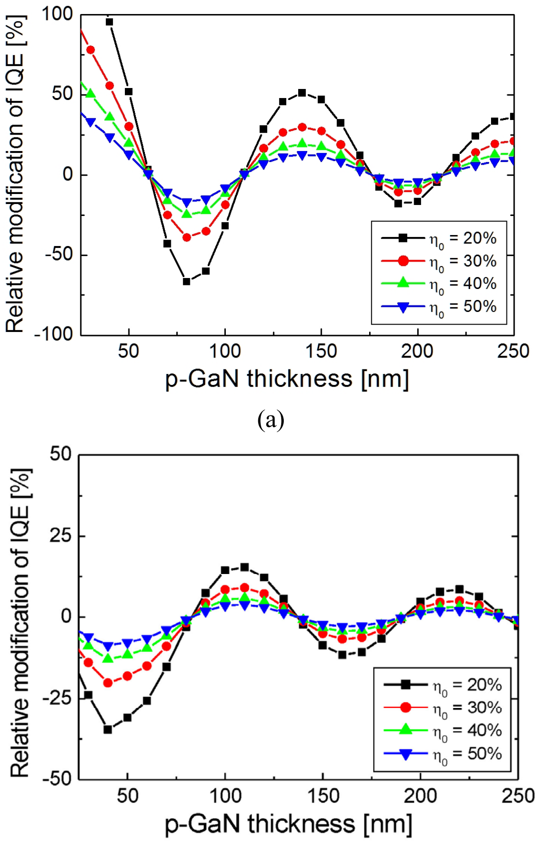
(a)

(b)

FIG. 3. Modified IQE as a function of the *p*-GaN thickness when the IQE of homogeneous material η_0 is 20%, 30%, 40%, or 50%, for (a) FC LED and (b) epi-up LED.

IQE (η') for η_0 of 20%, 30%, 40%, and 50% is increased to 30.3%, 39%, 47.7%, and 56.4% respectively. This means, for example, that the unmodified IQE of 20% can be increased to >30% via the Purcell effect for a green FC LED. For the epi-up LED, on the contrary, the variation of IQE with *p*-GaN thickness is much smaller than in the FC LED, as shown in Fig. 3(b). When the *p*-GaN thickness is 110 nm, η' for the epi-up LED for 0 of 20%, 30%, 40%, and 50% is increased to only 23%, 32.7%, 42.3%, and 51.9% respectively. Note the other possibility that the IQE decreases due to the Purcell effect, when the *p*-GaN thickness is inappropriately chosen. For the FC LED with *p*-GaN thickness of 80 nm, the modified IQE for η_0 of 20%, 30%, 40%, and 50% is decreased to 6.7%, 18.3%, 30%, and 41.7%, respectively.

Here we define the relative IQE modification as $(\eta' - \eta_0)/\eta_0$. Figure 4 shows the relative IQE modification for FC and epi-up LEDs as a function of *p*-GaN thickness when η_0 is 20%, 30%, 40%, and 50%. As one can see from Fig. 4, the amplitude of the relative IQE modification increases as η_0 decreases. For the FC LED with *p*-GaN thickness of 140 nm, the relative IQE modification for η_0 of 20%, 30%, 40%, and 50% corresponds to 51.2%, 29.9%, 19.2%, and 12.8% respectively. This result implies that the Purcell effect can have a significant influence on the IQE of FC LED structures especially when η_0 is low. The relative IQE modification of the epi-up LED is much lower than that of the FC LED. When the unmodified IQE is 20%, the relative modification of the FC LED is >50% for *p*-GaN thickness of 140 nm, while that of the epi-up LED is 15.5% for *p*-GaN thickness of 110 nm. Recalling that the relative IQE modification of a blue LED with η_0 of 80% was only ~2% when Purcell enhancement was employed [22], the IQE modification of a green FC LED by the Purcell effect is quite large. The large IQE modification for low-IQE LEDs implies that the Purcell effect in the FC LED structure can be advantageously used to improve the low IQE of contemporary green LED structures.



(a)

(b)

FIG. 4. Relative IQE modification as a function of the *p*-GaN thickness when η_0 is 20%, 30%, 40%, or 50%, for (a) FC LED and (b) epi-up LED.

IV. CONCLUSION

In this research, using FDTD simulations we theoretically investigated the modification of IQE in InGaN green LED structures as a result of the Purcell effect. The Purcell factor for the FC LED was found to be more than three times as high as that for the epi-up LED, owing to the high-reflectance reflector near the QWs for the FC LED structure. The local peak of the Purcell factor was obtained to be ~1.15 at a properly chosen *p*-GaN thickness, without utilizing the surface-plasmon coupling effect. Since the influence of the Purcell effect becomes increasingly significant as the IQE of an LED decreases, the Purcell enhancement can be quite advantageous to increase the IQE of green LEDs having low IQE. It was found that an IQE of 20% can be increased to >30% as a result of the Purcell effect, implying that InGaN green LEDs are expect to show much higher IQE enhancement than InGaN blue LEDs. Utilization of the Purcell effect in FC LEDs is expected to be a viable solution to mitigate the green-gap problem.

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