Modification of internal quantum efficiency and efficiency droop in GaN-based flip-chip light-emitting diodes via the Purcell effect

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Abstract: The Purcell effect in GaN-based flip-chip (FC) light-emitting diode (LED) structures is investigated numerically using finite-difference time-domain simulations. Depending on the thickness of the p-GaN layer, the variation of the Purcell factor of FC LEDs is obtained to be as high as 20%, which results in the relative modification of the internal quantum efficiency (IQE) as large as 8% and 2.5% for the unmodified IQE of 0.4 and 0.8, respectively. Since the influence of the Purcell effect becomes more conspicuous as the IQE decreases, the Purcell enhancement can be advantageously used to mitigate the efficiency droop problem to some extent. When the Purcell effect is positively applied to the blue LED with the peak IQE of 0.8 and the droop ratio of 29.1%, the peak IQE and the droop ratio are found to be improved to 0.82 and 26.3%. This small but non-negligible effect on IQE is expected to be importantly adopted for industry development of high efficiency LEDs.

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References and links


1. Introduction

Over the last decade, there has been remarkable progress in the development of high-efficiency blue light-emitting diodes (LEDs) based on InGaN/GaN materials for general lighting applications [1–3]. However, GaN-based LEDs suffer from a phenomenon commonly referred to as “efficiency droop” [4–6]. The internal quantum efficiency (IQE) of LEDs typically peaks at a few A/cm² and then droops with increasing current density. Although the origin of this efficiency droop is not completely understood yet, Auger recombination [7–9], reduced active volume [10], electron leakage [11, 12], and carrier delocalization [13, 14] have been proposed as droop-causing mechanisms in InGaN LEDs. These processes imply that the nonradiative recombination rate increases much faster with increasing current density than the
radiative recombination rate. Therefore, most works for mitigating the efficiency droop have focused on reducing the nonradiative recombination.

Another strategy to reduce the efficiency droop is to increase the radiative recombination rate over the nonradiative recombination rate. For example, the radiative recombination rate can be increased greatly by surface plasmon (SP) coupling of light emitted from InGaN quantum wells (QWs), which is expected to increase IQE and to reduce efficiency droop [15–19]. However, due to the nonradiative energy transfer from QWs to metallic structures, efficient light extraction of SP-coupled light out of the LED chip is challenging and the development of practicable SP-coupled LEDs has not been demonstrated yet. The increase in the radiative recombination rate of the SP coupling results from the Purcell effect which states that the spontaneous emission (SE) rate can be enhanced or suppressed depending on the local density of states around emitters [20]. The relative enhancement of the SE rate is often called the Purcell factor, which is denoted as $F_P$ in this paper. When $F_P$ is higher than 1, the radiative carrier lifetime of carriers is reduced, which leads to an increase in the IQE of LEDs.

The SE rate can also be modified in a flip-chip (FC) or vertical LED structure. The FC LED structure basically consists of n-GaN/InGaN/p-GaN epitaxial layers placed on a high-reflectance p-type electrode. The high-reflectance reflector of the FC LED is expected to alter the SE rate of light by modifying the local density of states around QWs via the Purcell effect. In FC LEDs, light emitted directly from the QW interferes with light reflected from the mirror. The SE rate will be enhanced if the reflected field returns to the emitter in phase, and the SE rate will be suppressed if it is out of phase. The modification of the SE rate by the presence of a high-reflectance mirror was demonstrated long time ago, and the SE rate was shown to be enhanced or suppressed substantially depending on the distance between the high-reflectance mirror and the emitter [21–23]. Therefore, the FC LED structure having a high-reflectance mirror near QWs is also expected to exhibit a sizable Purcell effect and subsequent IQE modification. However, there have been few studies on the Purcell effect in GaN-based FC LED structures. Shen et al. studied the optical cavity effect in InGaN/GaN FC LED structures and observed strong dependence of light extraction efficiency (LEE) on the distance between the metallic mirror and a QW [24]. However, the modification of IQE by the Purcell effect was not investigated in detail.

In this paper, the Purcell effect in blue FC LED structures is investigated using numerical simulations based on the finite-difference time-domain (FDTD) method. Although the SE is a quantum-mechanical phenomenon whose rate is described by the Fermi’s golden rule, it was shown that the SE rate could also be calculated with the classical dipole radiation power using Maxwell’s equations [25, 26]. The FDTD simulation has been frequently employed for calculating the Purcell effects in wavelength-scale optical structures [25–30]. In this study, $F_P$ of the FC LED structure is calculated, and its effect on IQE and efficiency droop is investigated.

2. Methods of simulation

In the numerical simulation of this study, the 3-D FDTD method based on Yee’s algorithm with a perfectly-matched layer (PML) boundary condition is employed [31]. In the FDTD method, the SE rate is proportional to the total dipole radiation energy, which is obtained by integrating the Poynting vector over time and over the enclosing surfaces [25, 26]. The Poynting vectors of radiating electromagnetic fields are calculated near the PML layers surrounding the computational domain.

We consider three types of LED structures: a reference LED without reflective interfaces, a FC LED having an Ag reflective electrode, and an epi-up LED enclosed by epoxy. Figure 1 shows the FDTD computational domain for three LED structures. These LED structures basically consists of a thick n-GaN layer, 20-nm-thick InGaN/GaN active region, a 10-nm-thick AlGaN electron-blocking layer, and a p-GaN layer. The reference LED is assumed to have a very thick p-GaN layer, hence no Purcell effect is expected. The thickness of the n-GaN layer is sufficiently thick that the n-GaN layer has little influence on the Purcell effect. In this work, $F_P$ for the FC and the epi-up LED structures is calculated as the p-GaN thickness.
varies. Since $F_P$ is mainly influenced by the distance from the p-GaN surface to the QW, strong dependence of $F_P$ on the p-GaN thickness is anticipated.

The FC LED structure having a flat-top n-GaN surface can be regarded as a planar cavity structure [24, 32]. A standing wave effect can be observed in a cavity structure when the wavelength matches well with the cavity length. However, the simulated structures do not include the n-GaN surface as shown in Fig. 1. That is, the Purcell effect of this work can be observed without the cavity structure, which implies that the Purcell effect investigated in this work is not the same as the standing wave effect in a cavity. In the FC LED structure shown in Fig. 1(b), the Purcell effect due to the SP coupling of light with the Ag reflector can also be observed when the thickness of p-GaN is within a few tens of nanometers. For sufficiently thick p-GaN layer (>50 nm), the SP effect is expected to be negligible and the Purcell effect purely due to the high reflectance mirror will be observed.

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 InGaN/GaN active region in the vertical direction. That is, a single QW structure is assumed in the active region in most simulations. The Purcell effect in MQW structures will also be discussed later. In the source spectrum, center wavelength and full-width at half maximum are chosen to be 450 and 20 nm, respectively. The dipole source is polarized in the horizontal direction for the excitation of transverse-electric modes. In order for obtaining $F_P$, the dipole radiation power is calculated for the reference LED structure in the first place. Next, the dipole radiation power for the FC and the epi-up LED structures is calculated. Then, $F_P$ is determined by dividing the dipole radiation power of the FC or epi-up LED structure by that of the reference LED. In Fig. 1, the power detection plane for calculating the dipole radiation power is shown as yellow dotted area. However, the position of the detection plane is not important since the total emission power is calculated in the $F_P$ simulation.

The refractive indices of GaN, epoxy, and Ag are set at 2.5, 1.5, and $0.14 + 2.47\ i$, respectively [33]. Then, the reflectance of the interface between p-GaN and Ag in the FC LED is ~90% and that of the interface between p-GaN and epoxy in the epi-up LED is ~6% for normal incidence. The space resolution in the computational domain is ~5 nm, which gives good accuracy in calculating the SE rate.

![Fig. 1. FDTD computational domain of the simulated LED structures. (a) Reference LED having a thick p-GaN layer, (b) flip-chip (FC) LED having an Ag reflector, and (c) epi-up LED encapsulated by epoxy. The simulated LED structures are surrounded by PML boundaries. The yellow dotted area represents the power detection plane.](image)

### 3. Results and discussion

#### 3.1 Simulation of the Purcell factor

In Fig. 2, $F_P$ for the FC and the epi-up LED structures is plotted as a function of the p-GaN thickness. Since the Purcell effect results from the self-interference effect of light emitted from the QW due to reflection from the reflecting surface, $F_P$ varies periodically with the p-GaN thickness [22–24]. As a result, the periodicity of the p-GaN thickness is ~90 nm, which corresponds to the half wavelength inside GaN material. Since the interference effect is
averaged over angle and wavelength, the amplitude of $F_P$ variation decreases slowly as the p-GaN thickness increases. Therefore, $F_P$ will converge to one when the p-GaN layer is very thick. The amplitude of the $F_P$ variation for the FC LED is much larger than that of the $F_P$ variation for the epi-up LED. For thin p-GaN thicknesses of <30 nm, $F_P$ of the 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 before, practical utilization of the SP resonance is challenging due to the too thin p-GaN layer and the dissipation of light at Ag.

When the p-GaN thickness is larger than 50 nm, the influence of SP is negligible and the Purcell effect purely comes from the modification of optical density of states due to the interface of LEDs. For the FC LED, the local peaks of $F_P$ are obtained when the p-GaN thickness is 110 and 200 nm, and the local valleys of $F_P$ are obtained when the p-GaN thickness is 60 and 150 nm. $F_P$ of the FC LED varies up to ~20% while that of the epi-up LED varies by less than 8%, indicating that the reflectance at the interface has a significant influence on $F_P$.

Fig. 2. Purcell factor ($F_P$) of flip-chip and epi-up LED structures as a function of the p-GaN thickness.

3.2 IQE modification by the Purcell effect

The rate equation for carriers under steady state is simply written as

$$\frac{\eta J}{qV} = R_r + R_{nr},$$  \hspace{1cm} (1)

where $q$, $I$, $\eta$, and $V$ are elementary charge, injection current, carrier density, injection efficiency, and the volume of QW active layers, respectively. $R_r$ and $R_{nr}$ are radiative and nonradiative recombination rate, respectively. Then, the IQE of the reference LED is given by

$$\eta_0 = \frac{R_r}{R_r + R_{nr}}.$$  \hspace{1cm} (2)

The IQE versus current can be obtained using Eqs. (1) and (2).

When the Purcell effect is included in the rate equation model, the injection current and IQE are modified as follows for fixed $R_{nr}$.

$$\frac{\eta J'}{qV} = R'_r + R_{nr},$$  \hspace{1cm} (3)

$$\eta' = \frac{R'_r}{R'_r + R_{nr}}.$$  \hspace{1cm} (4)
where $R_r'$ is the radiative recombination rate modified by the Purcell effect. Since $F_P$ is the ratio of the bulk SE rate to the modified SE rate, $R_r'$ equals to $R_r$ multiplied by $F_P$.

$$R_r' = F_P R_r.$$  

(5)

By using Eqs. (1)-(5), the modified injection current and IQE are obtained as a function of $\eta_0$ and $F_P$.

$$I' = [1 + (F_P - 1)\eta_0]I,$$

(6)

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

(7)

Equation (6) implies that, when $F_P$ is larger than 1, more current needs to be injected due to the increased radiative recombination rate. Equation (7) implies that the modified IQE increases with $F_P$ as expected. From Eqs. (6) and (7), the relation of IQE versus current modified by the Purcell effect can be obtained.

The modified IQE $\eta'$ for the FC and the epi-up LED is calculated using Eq. (7). Figure 3 shows $\eta'$ as a function of the p-GaN thickness when $\eta_0$ is 0.4, 0.6, and 0.8. It should be noted that the IQE modification in Fig. 3 is obtained under the condition that $R_{nr}$ is fixed while injection current for each data point varies with $\eta_0$ and $F_P$ according to Eq. (6). The variation of $\eta'$ with the p-GaN thickness is basically similar to that of $F_P$ as shown in Fig. 1. The IQE variation of the FC LED is much larger than that of the epi-up LED. Large increase in IQE for a thin p-GaN layer <30 nm is observed due to the high $F_P$. However, too thin p-GaN layer cannot be practically employed in LED structures and the SP coupling effect may degrade LEE as will be shown later. Therefore, the p-GaN thickness of larger than 100 nm is mainly considered here.

In the FC LED structure, the IQE at the p-GaN thickness of 110 nm for $\eta_0$ of 0.4, 0.6, and 0.8 is increased to 0.431, 0.63, and 0.82, respectively. That is, a small but non-negligible increase in IQE can be achieved by appropriately choosing the p-GaN thickness of the FC LED. Note that the local minimum of IQE is also observed. For the FC LED, structure, the IQE at the p-GaN thickness of 150 nm for $\eta_0$ of 0.4, 0.6, and 0.8 is decreased to 0.376, 0.576, and 0.782, respectively. That is, there is another possibility that the IQE decreases by the Purcell effect when the p-GaN thickness is inappropriately chosen. In the epi-up LED, the variation of IQE with the p-GaN thickness is much smaller compared with the IQE variation in the FC LED as shown in Fig. 3(b). For the p-GaN thickness from 90 to 130 nm, $\eta'$ of the epi-up LED varies from 0.806 to 0.795 when $\eta_0$ is 0.8, and it varies from 0.41 to 0.393 when $\eta_0$ is 0.4. Therefore, the Purcell effect on IQE modification is almost negligible in the epi-up LED structure.

![Fig. 3. Modified IQE as a function of the p-GaN thickness when the IQE of the reference LED ($\eta_0$) is 0.4, 0.6, and 0.8. (a) FC LED, (b) epi-up LED](image-url)
Note that the relative variation of $\eta'$ with the p-GaN thickness increases as $\eta_0$ decreases. Here, we define the relative IQE modification as $(\eta' - \eta_0)/\eta_0$. Figure 4(a) shows the relative IQE modification for the FC LED as a function of the p-GaN thickness when $\eta_0$ is 0.4, 0.6, and 0.8. For the p-GaN thickness from 50 to 200 nm, the amplitude of relative IQE modification varies by 5 to 15% for $\eta_0$ of 0.4 while it varies by only 2 to 5% for $\eta_0$ of 0.8. In Fig. 4(b), the relative IQE modification is plotted as a function of $\eta_0$ when the p-GaN thickness is 110 and 150 nm which respectively corresponds to the peak and the valley of the IQE modification. One can clearly see that the relative IQE modification decreases or increases linearly with $\eta_0$. This implies that one can expect large modification of IQE via the Purcell effect when the IQE of the LED is low. This effect can be advantageously used to improve the IQE of yellow-green LEDs. The external quantum efficiency (EQE) of LEDs with emission wavelengths from 530 to 600 nm has been reported to be <30% due to low IQE of materials in this spectral [34, 35]. This so-called “green gap” problem can be improved by making good use of the Purcell effect in FC LED structures. However, IQE would decrease even worse if the p-GaN thickness is chosen to be 60, 150, or 240 nm.

![Fig. 4.](image)

**3.3 Purcell effect on IQE droop**

Another important implication of the result of Fig. 4 is that the Purcell effect can be used to mitigate the efficiency droop problem to some extent. Suppose that the p-GaN thickness of the FC LED corresponds to the local peak of $\eta'$. Since the IQE enhancement by the Purcell effect becomes more conspicuous as IQE decreases, the droop rate will be slowed down as current density increases. That is, the reduction of IQE droop is expected in addition to the overall increase in IQE. In order to confirm this droop-reduction effect, the IQE curve, which is the relation of IQE versus current density, is calculated including the Purcell effect.

The IQE curve can be obtained by using the well-known ABC carrier rate equation model [4–7]. $R_e$ and $R_{nr}$ in Eqs. (1) and (2) are expressed as

$$R_e = BN^2 \quad \text{and} \quad R_{nr} = AN + CN^2,$$

where $N$ is carrier density and the coefficients $A$, $B$, and $C$ represents Shockley-Read-Hall nonradiative recombination, bimolecular radiative recombination, and Auger nonradiative recombination, respectively. The IQE curve can be obtained from Eqs. (1), (2), and (8). It has been found that the IQE curve is uniquely determined from the peak value of IQE, $\eta_{\text{max}}$ and the current $I_{\text{max}}$ at $\eta_{\text{max}}$ [36, 37]. The relation between $\eta$ and $I$ is obtained by solving the following equation [37].

$$aI^2 + bI + c = 0,$$
where \( a = \eta^2 \), \( b = 2\eta_{\text{max}} I_{\text{max}} \left[ \eta^2 + \frac{4\eta_{\text{max}}^2 \eta}{(1-\eta_{\text{max}})^2} - \frac{2\eta_{\text{max}}^2 (1+\eta^2)}{(1-\eta_{\text{max}})^2} \right] \), and \( c = \eta_{\text{max}}^2 I_{\text{max}}^2 \).

The IQE curve for the reference LED without the Purcell effect is calculated from Eq. (9) assuming that \( \eta_{\text{max}} \) and \( I_{\text{max}} \) of the reference LED is 0.8 and 2 mA. Then, the modified IQE curves in the FC LED are calculated using Eqs. (6) and (7). Figure 5 shows the IQE curves for the p-GaN thickness of 110 and 150 nm along with the IQE curve for the reference LED. \( F_P \) at the p-GaN thickness of 110 and 150 nm was 1.14 and 0.9, respectively. In the reference LED, the IQE decreases from the peak value of 0.8 to 0.567 at 1000 mA. The FC LED with the p-GaN thickness of 110 nm exhibits overall increase in IQE along with reduced efficiency droop. In this case, the peak IQE is 0.82 and the IQE is decreased to 0.604 at 1000 mA. The relative increase in the peak IQE and the IQE at 1000 mA is 2.5% and 6.5%, respectively. The normalized IQE curves in Fig. 5(b) shows that the IQE droop is somewhat reduced in the FC LED with the p-GaN thickness of 110 nm.

In order to quantify the degree of IQE droop, the droop ratio is introduced as in the following [38, 39].

\[
\text{Droop ratio} = \frac{\text{peak IQE} - \text{IQE at 1000 mA}}{\text{peak IQE}}
\]

The droop ratio of the reference LED is 29.1% and that of the FC LED with the p-GaN thickness of 110 nm reduced to 26.3%. However, there exists opposite possibility that the IQE droop could be aggravated if the p-GaN thickness was inappropriately chosen. When the p-GaN thickness is 150 nm, the peak IQE is 0.783 and the IQE is decreased to 0.536 at 100 A/cm². The corresponding droop ratio is 31.5% in this case. The normalized IQE curve shows that the efficiency droop is a little increased in this p-GaN thickness. Therefore, depending on the p-GaN thickness, the peak IQE varies from 0.783 to 0.82 and the IQE droop ratio varies from 26.3% to 31.5%. The relative variation of the peak IQE is ~4.5% and that of the droop ratio is ~18%. These variations of IQE could be significant in the current LED industry. The result of Fig. 5 implies that choosing the proper p-GaN thickness is quite important in improving the IQE of the FC LED structure via the Purcell effect.

3.4 Purcell effect in MQW structures

Up to now, a single dipole source at the center of active region was considered. That is, Purcell effects for a single QW structure were investigated. In actual LED structures, MQW layers are typically employed in the active region. When a specific QW of MQWs
corresponds to the peak $F_P$, the position of other QWs will deviates from the peak $F_P$ position. Consequently, the average $F_P$ and IQE can be decreased in MQW structures. We calculate the average IQE with varying number of QWs when the distance from the Ag reflector to the center of MQWs, $d$ is fixed at 130 or 170 nm. Note that $d$ the p-GaN thickness plus 20 nm. When $d$ is 130 nm (170 nm), the center of MQWs corresponds to the peak (valley) of $F_P$. Here, it is assumed that the period of QWs is 10 nm and the radiative recombination rate in MQWs is homogeneous.

![Fig. 6. Average IQE as a function of the number of QWs when the distance from the Ag reflector to the center of MQWs, $d$ is 130 and 170 nm. The IQE of the reference LED is 0.7 and the period of QWs is assumed to be 10 nm.](image)

In Fig. 6, the average IQE is plotted as a function of the number of QWs when $\eta_0$ is 0.7. With increasing number of QWs, the average IQE approaches the IQE of the reference LED and the Purcell effect becomes diminished for both p-GaN thicknesses. When the number of QWs is 8, even though the central QWs have a peak $F_P$, the first and the last QW corresponds to near the valley of $F_P$. Therefore, in LEDs having a large number of QWs, the Purcell effect will play only a minor role in the IQE and IQE droop. In order to expect a non-negligible Purcell effect, it is necessary to reduce the number of QWs or to optimally design the QW active region.

3.5 Purcell effect and LEE

Up to now, the variation of $F_P$ and IQE depending on the p-GaN thickness was investigated. In addition to the IQE, LEE can also be strongly dependent on the p-GaN thickness due to the cavity effect in FC LED structures [24, 32]. It is necessary to compare the p-GaN thickness dependence of the Purcell effect and the LEE of a FC LED. Figure 7(a) shows the FDTD computational domain for the LEE simulation. It is basically similar to the structure in Fig. 1(b). Here, the thickness of the n-GaN layer is assumed to be 3 $\mu$m, and the LED chip is encapsulated with epoxy. The radiation power is detected above the n-GaN surface as shown in Fig. 7(a), which is divided by the total dipole radiation power to obtain the LEE. The lateral dimension of the computational domain is 10 $\mu$m, sufficient to detect all escaped light in the detection plane.

Figure 7(b) shows the simulated result of LEE as a function of the p-GaN thickness along with the $F_P$ data calculated in Fig. 2. LEE varies periodically with large amplitude as the p-GaN thickness increases. The periodicity of the LEE variation is ~100 nm, similar to that of $F_P$ variation. In addition, the peak or valley positions of LEE and $F_P$ are also quite similar. That is, enhancement of IQE and LEE can be achieved almost simultaneously in FC LED structures. Note that the local peak of LEE at the p-GaN thickness of 10–20 nm is much smaller than the peak LEE at the p-GaN thickness of 100 nm while $F_P$ at the p-GaN thickness of 10–20 nm is quite high. As mentioned before, the high $F_P$ at this thin p-GaN layer is a result of SP coupling. However, LEE is not so high due to the dissipation of SP-coupled light at Ag. In this sense, the optimum choice of the p-GaN thickness will be 100 or 200 nm. As discussed in the previous sub-section, the amplitude of LEE variation with the p-GaN
thickness can be significantly reduced as the number of QWs increases. By careful design of QW active region and layer structures of FC LEDs, EQE is expected to be greatly improved through the simultaneous enhancement of LEE and IQE.

Fig. 7. (a) FDTD computational domain of a FC LED structure for the LEE simulation. (b) LEE (red) and $F_p$ (black) are plotted as a function of the p-GaN thickness

4. Conclusion

The effect of $F_p$ on the IQE modification in GaN-based FC LED structures was investigated using FDTD simulations. As the p-GaN thickness increases from 50 nm to 200 nm, the variation of $F_p$ was calculated to be as high as 20%. As a consequence of the Purcell effect, the relative IQE modification was obtained to be as large as 8% and 2.5% when the IQE of a reference LED is 0.4 and 0.8, respectively. Since the influence of the Purcell effect becomes more significant as the IQE of LEDs decreases, the Purcell enhancement can be advantageously used to mitigate the green gap and the efficiency droop problems of InGaN LEDs to some extent. The relative variation of the droop ratio could be as large as 18% depending on the p-GaN thickness. Although the influence of the Purcell effect becomes diminished as the number of QWs increases, the FC LED with higher efficiency and lower droop is expected to be achieved by optimizing the active layer structures for obtaining large Purcell effects.

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