Position dependence of extraction efficiency in organic light-emitting diodes with photonic crystal structure

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We demonstrate by finite-difference time-domain simulations that a one-dimensional (1D) photonic crystal (PC) structure between glass substrate and indium tin oxide layer can improve the light extraction efficiency of organic light-emitting diodes. The extraction efficiency depends on the emitters' positions varying laterally in a unit cell of PC. The highest efficiency is obtained when the emitters are under higher refractive index strips. Efficiency decreases when the emitters shift to lower refractive index strips. Simulations for both transverse magnetic and transverse electric modes indicate that when emitters are close to the middle of the higher refractive index strips, the guided wave transmits with less divergence and inhibited reflection because of the guiding effect of higher refractive index strips. A modified method that considers the position effects is proposed to calculate the extraction efficiency more precisely.

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Organic light-emitting diodes (OLED) have elicited much attention in the fields of lighting and flat panel displays because of their advantages such as low power consumption, wide viewing angles, high contrast ratio, short response time, and low cost[1,2]. To boost OLED application, out-coupling efficiency and lifetime need to be further improved. Although the internal quantum efficiency of OLED can reach almost 100% with the use of phosphorescence emitters, the out-coupling efficiency remains minimal due to the total internal reflection and waveguide effects. Based on Snell's Law, only about 20% of the total generated light can escape without extra methods, whereas about 30% of the light is trapped in the glass substrate due to the total internal reflection at the interface between the glass and the air; about 50% of the light exists as waveguide modes in the indium tin oxide (ITO) layer, organic layers, and in areas near the electrode[3]. Random textures, ordered microlens arrays, and rough substrate surface have been employed on the top surface of the substrate to minimize total internal reflection and to extract the light trapped in the glass substrate; the effectiveness of these methods has been theoretically and experimentally proven[4,5]. Incorporating a polymeric diffraction grating fabricated directly on top of the ITO electrode is effective in out-coupling the light near the cathode[6,7]. Constructing a photonic crystal (PC) or other periodic structures between the ITO layer and glass substrate is an efficient method to extract the waveguide modes in organic and ITO layers[8−11].

The finite-difference time-domain (FDTD) method is widely used in designing and optimizing PC structures. Numerous dipoles are generated in the active layer and evenly distributed on the plane of an OLED. Therefore, a large quantity of dipole emitters should be placed in the organic layers for the simulations to obtain accurate results. Nevertheless, this strategy is not practicable for FDTD simulations because of two reasons. On one hand, numerous sources will make the calculation too complicated to carry out. On the other hand, they will lead to nonphysical interference patterns and result in undesirable errors. In most cases, FDTD simulations are performed with only one dipole source placed in the middle of the device for convenience[12,13]. Unfortunately, such procedure will cause overestimated results[14].

This letter aims to study and highlight the variations of extraction efficiency with the sources' positions and modify the existing calculation method to achieve more accurate results.

We employed one-dimensional (1D) FDTD simulations to study how photonic crystal extracts light from ITO and organic layers and how the source's position affects the waveguide modes in OLED. Figure 1 shows the basic device structure for the simulations. In this research, the organic layer thickness is 100 nm, the ITO layer thickness is 50 nm, and the refractive indexes are 1.7 and 1.75. These parameters were set in accordance to common OLED structures. The PC is assumed to be constructed by etching the glass and then depositing the ITO. Therefore, the low and high refractive indexes of PC are 1.5 and 1.75, referring to glass and ITO, respectively. A continuous wave (CW) point source with a vacuum wavelength of 550 nm was placed in the organic layers. Given the computer's memory limitation, the size (about 2×2 (mm)) of a real OLED is too large for direct FDTD calculations. Instead, an 11-period PC-OLED was used with the boundary conditions set to be anisotropic perfectly matched layers in both X and Z directions, which means light is almost totally absorbed without pseudo reflection caused by the truncation of the simulation zone. Through verification via FDTD simulations, the deviation of the relative efficiency is found to be less than 5% with an increase in the number of periods.

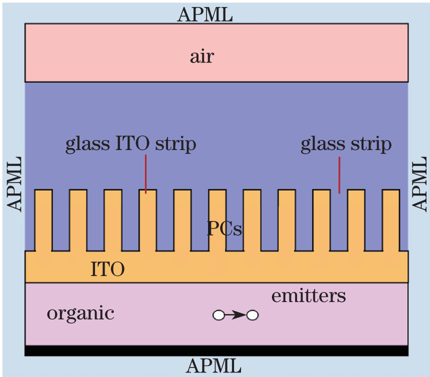

Fig. 1. Cross-sectional view of an OLED device with 1D photonic crystal structure.

An observation line with a length identical to the wafer's width was placed in front of the device along the Z direction to catch output light. The mesh step of X direction and Z direction is 3 nm. The time step is 6.67×10^{-18}s, and all of the simulations run for 15 000 steps, which is long enough for the energy to pass the observation line completely. The permittivity of the bottom Al electrode is obtained by using the Lorentz–Drude model[15].

The extraction efficiency produced by the photonic crystal is related to three factors: depth, period, and duty cycle. To achieve better performance, the parameters were first optimized through traditional FDTD simulations. Without loss of generality, we performed the optimization in transverse magnetic (TM) mode. The depth of the PC was optimized with the period and the duty cycle set to 450 nm and 50%, respectively. The dependence of relative efficiency (extraction efficiency of the device with PC over that without PC) of PC-OLED on the depth of the PC layer is shown in Fig. 2(a). The relative efficiency increases with the PC depth; the value is largest when the depth is 100 nm, after which it decreases. Therefore, 100 nm was picked and applied as the PC depth in the subsequent optimization. Figuer 2(b) shows the relative efficiency as a function of the duty cycle for various periods. The duty cycle was chosen to be between 0% to 100% in 10 steps, and the period varied from 300 to 900 nm with a step of 100 nm. Results indicate that at each given period, the relative efficiency increases with the duty cycle and reaches the maximum, after which it decreases. The same tendency with PC period is also depicted. The largest relative efficiency is obtained with a period of 700 nm and a duty cycle of 50%. The parameters obtained thus far are the local optimal solutions, not the global optimal solutions. Enumerating all the combinations is difficult because all the parameters are related to each other. The local optimal result is sufficient for the following simulations without loss of physical meaning.

Figure 3 shows the field distributions of OLEDs without PC, with PC for an emitter in the center, and with PC for an emitter 350 nm away from the center. The simulation results of the TM modes are shown in Figs. 3(a)-(c), whereas those of the transverse electric (TE) mode are shown in Figs. 3(d)-(f). Figure 3(a) clearly shows that the emitted light of OLED without PC is divided into two parts: output light in the center, with incident angles smaller than the critical angle between the air and the substrate, and trapped light divergent with incident angles larger than the critical angle. When a PC structure is added into the OLED device with source placed in the middle, more light is concentrated in the light cone and the light trapped in the device is greatly reduced, as illustrated in Fig. 3(b). However, in Fig. 3(c), when the emitter is 350 nm away from the higher refractive index center, the light is more divergent from the center, indicating that more light is trapped in the substrate. The simulations of the TE mode show similar phenomena in Figs. 3(d)-(f). The TM polarization light output relative efficiency of the PC-OLED with point sources varying in a pitch is shown in Fig. 4. The result agrees with the light field distributions in Figs. 3(a)-(c). The extraction efficiency is highest when the light source is at the center under the high refractive index material of PC. When the position shifts to the lower refractive index, the extraction efficiency decreases to less than that without PC.

The 1D PC considered in this research is composed of periodical alternative ITO and glass strips. The ITO strips act as waveguides along the X direction due to the total internal reflection between the ITO and the glass. Thus, the light from the emitters could function as waveguide modes in ITO strips. When the light source is placed under the middle of the ITO strips,

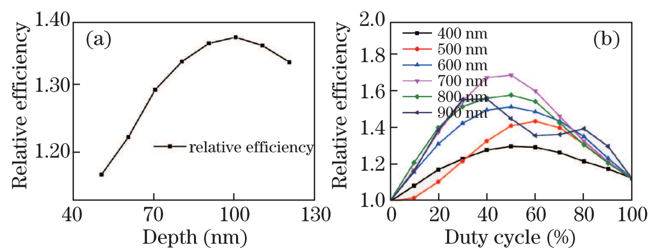

Fig. 2. Variations of relative efficiency with (a) PC depth, (b) PC's period and duty cycle.

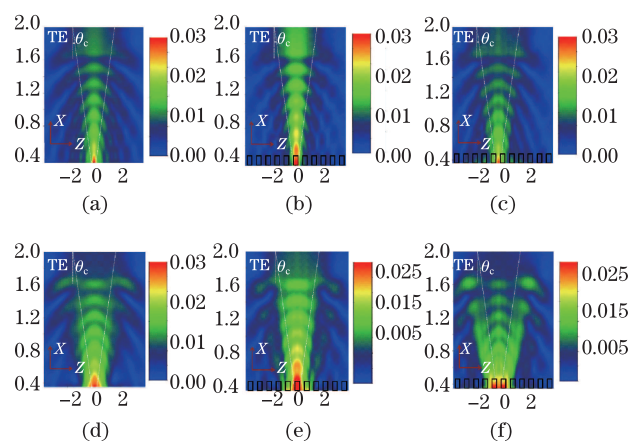

Fig. 3. Field distribution graphs. (a) Magnetic field of TM polarization without PC; (b) magnetic field of TM polarization with PC and the light source is in the center; (c) magnetic field of TM polarization with PC and the light source is 350 nm away from the center; (d), (e), and (f) the corresponding TE polarization (electric field) simulation results. The unit of the X and Z coordinates is μm. The symbol θ_c is the critical angle at the interface of the glass and the air. The area between the two white lines is the extraction light cone.

the emitted light could be coupled to the waveguide modes more efficiently because light is mostly confined in the core of higher refractive index in a waveguide[16]. Therefore, the guided waves are more concentrated in the extraction cone and transmit perpendicular to the substrate. Thus, more light is coupled out because of the reduction of reflection with smaller incident angles.

When the source is placed away from the middle under the higher refractive index material of the PC (i.e., ITO strips), the coupling efficiency of light to waveguide modes decreases, and so does the extraction efficiency[17]. When the source is placed under the lower refractive index material of the PC (i.e., glass strips), the efficiency further deteriorates, as shown in Fig. 3(c). By calculating via the traditional method, the relative efficiency of the PC-OLED with the source placed 350 nm away from the middle is 0.63, which means the efficiency is even lower than that without PC. The position of the source greatly influences the extraction efficiency of PC-OLED, so it merits special care.

To eliminate the mismatch of the simulation and reality, a new method that considers the influence of source's position is proposed to calculate the relative efficiency in a comprehensive manner. By verifying with FDTD simulations, we found that the variation is negligible when the source is at the same relative position in different periods. Therefore, only one period is considered for convenience. In the new method, the relative efficiencies of the device with the source placed at different distances relative to the middle position with a 100-nm step are first calculated. Based on these points, a fourth-order polynomial fitting function is selected for its high accuracy and small error. The original plot and the fitting curve are shown in Fig. 4. The fitting function is as follows:

Table 1. Fitting Results

Coefficient	Value
a_0	1.70
a_1	-8.96×10^{-5}
a_2	-3.11×10^{-5}
a_3	8.74×10^{-8}
a_4	-6.12×10^{-11}

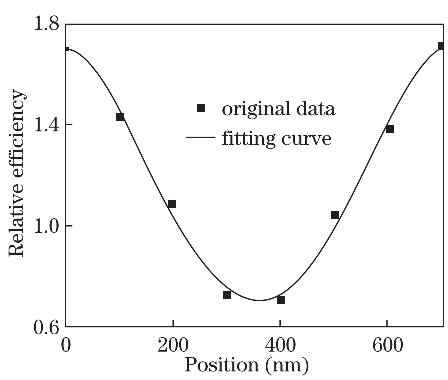

Fig. 4. Relative efficiency of the device with sources placed in different positions. The "position" is the distance between the source and the middle of the device. The line is the fitted curve with the fourth-order polynomial.

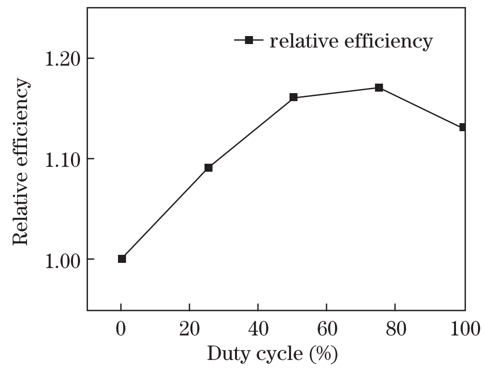

Fig. 5. Relative efficiency calculated using the new method varies with the PC's duty cycle (the period is 700 nm).

$$E_r(z) = a_0 + a_1 \cdot z + a_2 \cdot z^2 + a_3 \cdot z^3 + a_4 \cdot z^4, \quad (1)$$

where z is the source's position as defined above and $E_r(z)$ is the fitted relative efficiency with the source placed in position z. T is the length of a period of PC. The coefficients of the fitting function are listed in Table 1. Finally, based on the fitting line, the average relative efficiency E_r is calculated by

$$E_r = \frac{1}{T}\int_0^T E_r(z)d_z. \quad (2)$$

The final relative efficiency is 1.16, which is much lower than the result obtained when the source is placed in the middle of the device (1.71).

We applied the new method in calculating the relative efficiency over the duty cycle with PC period fixed at 700 nm (Fig. 5). The relative efficiency is much smaller when the influence of the emitter's position is considered. Furthermore, the maximum efficiency is achieved at a duty cycle of around 75% instead of 50%.

In conclusion, constructing a PC layer at the interface of ITO and substrate changes the direction of light transmission by the waveguide effect of ITO strips and improve the out-coupling efficiency of OLEDs. The energy distribution of PC-OLED simulated by 1D FDTD shows that the closer the emitter to a higher refractive index ITO pillar, the higher is its extraction efficiency. Taking the position dependence of extraction efficiency into account, a new method that is more in line with the actual situation is proposed. Finding the dependence of PC-OLED emission on the source's position is important in building a more accurate simulation model to investigate the extraction efficiency of PC-OLED.

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References

1. H. Sasabe and J. Kido, J. Mater. Chem. C **1,** 1699 (2013).
2. T. Nakayama, K. Hiyama, K. Furukawa, and H. Ohtani, "19.1: Invited Paper: Development of Phosphorescent White OLED with Extremely High Power Efficiency and

Long Lifetime" in SID Symposium Digest of Technical Papers **38,** 1018 (2007).
3. C. F. Madigan, M. H. Lu, and J. C. Sturm, Appl. Phys. Lett. **76,** 1650 (2000).
4. J. Yang, Q. Bao, Z. Xu, Y. Li, J. Tang, and S. Shen, Appl. Phys. Lett. **97,** 223303 (2010).
5. D. S. Mehta and K. Saxena, in *Proceedings of Asian Society for Information Display* 198 (2006).
6. J. H. Jang, M. C. Oh, T. H. Yoon, and J. C. Kim, Appl. Phys. Lett. **97,** 123302 (2010).
7. U. Geyer, J. Hauss, B. Riedel, S. Gleiss, U. Lemmer, and M. Gerken, Appl. Phys. Lett. **104,** 093111 (2008).
8. A. Kumar, R. Strivastava, M. N. Kamalasanan, and D. S. Mahta, Opt. Lett. **37,** 575 (2012).
9. B. Wang, L. Ke, and S. J. Chua, J. Cryst. Growth **288,** 199 (2006).
10. B. K. Hong, H. K. Yu, I. Lee, K. Kim, S. Kim, and J. L. Lee, Adv. Mater. **2010,** 22 (2010).
11. A. Kumar, R. Strivastava, P. Tyagi, M. N. Kamalasanan, and D. S. Mahta, Org. Electron. **13,** 2879 (2012).
12. Q. Y. Yue, W. Li, F. M. Kong, and K. Li, Adv. Mater. Sci. Eng. **2012,** 985762 (2012).
13. M. Le, R. Yan, and Q. Wang, Semicond. Photon. Technol. **12,** 10 (2006).
14. Y. J. Lee, S. H. Kim, J. Huh, G. H. Kim, Y. H. Lee, S. H. Cho, Y. C. Kim, and Y. R. Do, Appl. Phys. Lett. **82,** 3779 (2003).
15. E. D. Palik, *Handbook of Optical Constants of Solids* (Academic, Orlando, 1985).
16. A. W. Snyder and J. Love, *Optical Waveguide Theory* (Springer, Berlin, 1993).
17. B. E. Little and W. P. Huang, Prog. Electromagn. Res. **10,** 217 (1995).