Photonic crystal used to increase extraction efficiency of ZnO light-emitting diodes

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Abstract—Low extraction efficiency following a low angle of total internal reflection at the output surface of simple light-emitting diodes (LEDs) considerably limits their performance and reduces their possible applications. From among various methods used to enhance extraction of radiation from LEDs manufactured from high index-of-refraction materials, an application of photonic crystals seems to be quite effective and relatively simple technologically. In the present paper, the FDTD approach is used to study the performance of a ZnO LED. As compared with a simple planar ZnO LED structure, the application of an optimized photonic crystal enables in this case an enormous increase in extraction efficiency by more than thirteen times.

ZnO is currently receiving the highest attention because of its possible application in short-wavelength light-emitting diodes (LEDs) (see e.g. [1]-[3]). This material seems to be superior over nitrides because of its better thermal stability, resistance to oxidation, commercial availability of large and high quality native or lattice-matched substrates and a strong exciton binding energy, which can ensure an efficient exciton emission at high temperatures. But, at the same time, because of its high refractive index n_{ZnO} of 2.02 [4] leading to a relatively low angle of a total internal reflection of 29.5^0 at the ZnO/air interface (narrow photon escape cone), photon extraction efficiency η_{ext} for a simple planar homo-junction ZnO LED is very low.

There are many methods used to enhance light extraction from such LEDs. In principle, they may be divided into methods applying strong reflectivities from diode bottom surfaces and/or methods increasing an escape cone. From among them, an application of a photonic crystal seems to be the most promising one. This method has been used many times in nitride LEDs (see e.g. [5]), but surprisingly, it has not been applied in ZnO LEDs. Therefore the main goal of this paper is to test the application of a photonic crystal to enhance light extraction in these devices.

A very simple optical LED structure, composed of only two uniform layers of ZnO and sapphire (n_S=1.77 [6]), is considered as a planar ZnO LED. The PC ZnO LED additionally contains a two-dimensional (2D) hexagonal photonic crystal (PC) in the upper part of the ZnO layer (Fig. 1). The calculation domain is of smaller size than the real device to overcome numerical challenge associated with reaching the desired calculation accuracy after a reasonable calculation time. The Maxwell equations are solved with the aid of the FDTD approach [7]. For high numerical accuracy, a grid size of only 20nm has been applied, essentially smaller than the wavelength and the smallest feature of the model. The PC lattice constant a is used as a length unit. The thicknesses of the ZnO and sapphire layers are assumed to be equal to a and $1.5a$, respectively, the depth of the PC columns is equal to $0.5a$ and the sizes of the calculation domain are equal to $2.5a$ and $5a$. The diameter of the PC column is equal to d=$2r$. The PC lattice constant a is changed from 0.4μm to 1.4μm by 0.2μm. Perfectly Matched Layers (PML) [8] are assumed at both the upper and the bottom boundaries of the calculation domain. It means that radiation reaching these surfaces is completely absorbed. Perfect mirrors, on the other hand, are assumed at four sides of the calculation domain creating a periodic boundary condition, which means that, in lateral directions, the LED structure is considered to be infinite. Radiative recombination is reduced to one dipole oscillator located at the beginning (0,0,0) of the coordinate system. Its emission spectrum is assumed to be of the Gaussian form centered at a wavelength of 375nm and with a full-width at half maximum of 8nm.

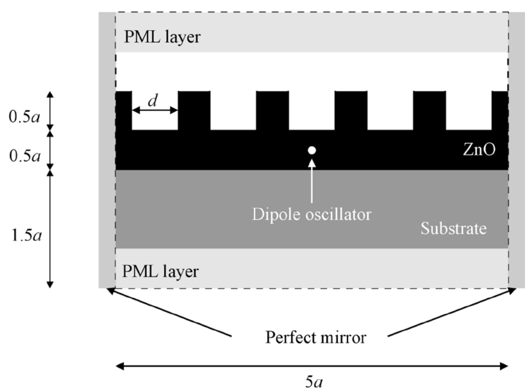

Fig. 1. The FDTD calculation domain.

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Emission spectra of the radiation emitted through the upper LED/air surface are shown in Fig. 2 for both the simple planar LED and one of the PC LEDs. As one has seen, this kind of emission has been considerably enhanced by the application of a photonic crystal. However, it should be noted that even more radiation is then leaving the ZnO layer through its bottom surface. It follows from a relatively high angle of total internal reflection at the ZnO/sapphire boundary equal to as much as about 60.7^0, because the values of refractive indices of sapphire (1.77) and ZnO (2.02) are very close to each other. Therefore the photon escape cone is much narrower for the ZnO/air boundary than that for the ZnO/sapphire boundary. This fact, in the case of the planar ZnO LED, leads to a considerably higher photon penetration of the sapphire layer than its emission through the LED upper surface. In PC LEDs, the emission of photons is considerably increased (Fig. 3) but it is still lower than their penetration of the sapphire layer. The above improvement of the photon extraction through the upper surface of the GaN PC LED is much lower (e.g. from only about 63% reported in [9] to 350% reported in [10]), because the GaN index of refraction of 2.42 [11] is distinctly different from that of sapphire (1.77), which leads to a much narrower escape cone at the GaN/sapphire boundary.

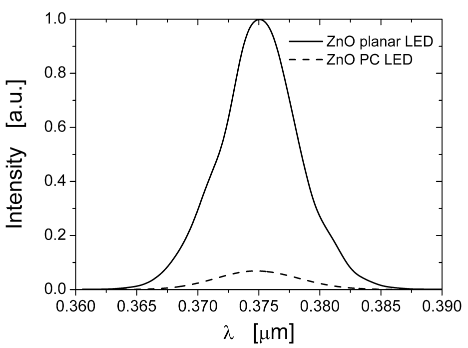

Fig. 2. Spectra of the radiation emitted by the ZnO planar LED and by the ZnO PC LED (a=1.2μm, r/a=0.3).

The main simulation results are shown in Fig. 3, presenting an improvement of the extraction efficiency η_{ext} obtained in the ZnO PC LEDs as compared with the ZnO planar LED as a function of the PC lattice constant a and the radius r of the PC columns. For PC columns not penetrating each other, r/a should not exceed 0.5. On the other hand, r/a is equal to zero for the planar LED. As one can see, to obtain the highest enhancement of light extraction efficiency in the considered ZnO PC LED, its optimal PC should have r/a between 0.3 and 0.4 and a should be equal to 1.2μm. Then this improvement is expected to be higher even than 1200%.

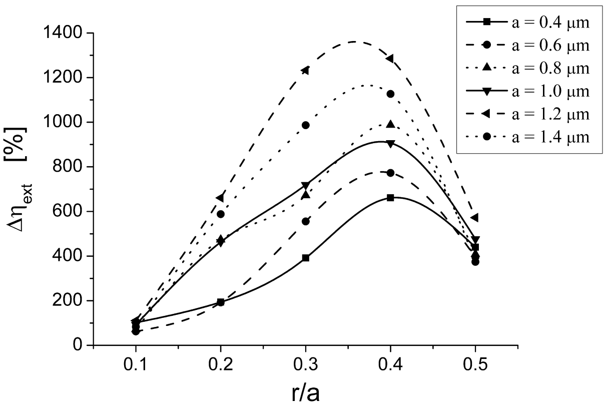

Fig. 3. An improvement $\Delta\eta_{ext}$ of the photon extraction in ZnO PC LED as compared with the ZnO planar LED. a – PC lattice constant, r - radius of PC columns.

In PC LEDs, there are three possible physical mechanisms responsible for the enhancement of light extraction:

1) the photonic bandgap effect,
2) the diffraction effect,
3) the scattering effect.

In the first effect, the propagation of some photons in lateral directions is forbidden because of an existence of the photonic bandgap. Then their extraction along the PC columns seems to be enhanced [12]-[13]. This mechanism has been found not to exist in GaN PC LEDs, because their PC bandgap corresponds to significantly shorter wavelengths than the emission one [9]. A similar situation is probably also in ZnO PC LEDs. It is believed that the second possible mechanism above may be associated with a modification of the incident angle at the ZnO/air boundary by the diffraction of a PC Bragg grating [14].

The first two mechanisms above require a perfect PC structure, because the photonic bandgap and the Bragg scattering follows from a perfect periodic structure. Therefore some disordering of the PC lattice, i.e. an introduction of random column diameters and random column locations, has been intentionally introduced to an optical PC LED model to study its impact on light extraction. But, according to the calculations reported in [15], light extraction has happened to be nearly independent of an introduced disorder in the PC lattice, which excludes two first above mechanisms as possible reasons of improved light extraction. Therefore the remaining third mechanism, i.e. scattering of light by PC columns, was found as the most probable enhancement reason [16]. This conclusion has been additionally supported by the reported enhancement of light extraction induced simply by roughening the external upper LED surface [17]-[19]. Hence, it may be concluded, that the best method to increase light extraction from a LED surface is to give its photons multiple opportunities to find an escape cone.

In conclusion, the FDTD approach has been used to study the enhancement of light extraction from the ZnO LED obtained with the aid of a photonic crystal. It has been found that an optimized photonic crystal may cause a very considerable enhancement of photon extraction efficiency, much higher than in the case of GaN LEDs with photonic crystals.

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