# FDTD simulation of Photonic crystal enhanced OLED

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*Abstract: Organic light emitting diode devices (OLED) have potential applications in flat panel displays, flexible displays and illumination devices. In this paper the effect of a photonic crystal structure in the glass substrate on the emission characteristics is investigated by means of FDTD simulations..*

## Introduction

In this paper a photonic crystal structure (PC) based on air holes in a glass substrate is designed. It has a TE band gap but TM waves do not have a forbidden band. By a 3D FDTD simulation using periodic boundary condition (PBC), this structure was excited by a dipole in the center of the structure at the interface of the hole transport layer (HTL) and the electron transport layer (ETL). The near-field out-coupled light is recorded for the case with and the case without photonic crystal. It is shown that for the structure with photonic crystal the light emission in OLED is suppressed.

## Photonic Crystal Design

The aim of the photonic band gap structure is to diminish the guided modes in the OLED layers. The dispersion relation is obtained by solving the matrix problem. It should be noted that the analysis assumes an infinite 2D periodic structure with a photonic band gap [1]. A photonic crystal with periodic holes in a dielectric substrate is characterized by lattice constant, radius of holes, dielectric constants of substrate, and photonic crystal factor which is the ratio of a hole surface area to its unit cell surface area. A combination of these variables can lead to desirable dispersion characteristics of photonic band gap. A glass substrate with $\varepsilon_r$=2.25 and infinitely long cylindrical air holes are used in our analysis. The 2D triangular photonic crystal is a structure with a diameter of the air holes of 195nm and a lattice constant of 265nm which is equivalent to photonic crystal factor equal to 0.49 (Figure. 1). The dispersion diagram of a 2D photonic crystal structure is shown in the figure. 2. It has a TE (electric field in parallel

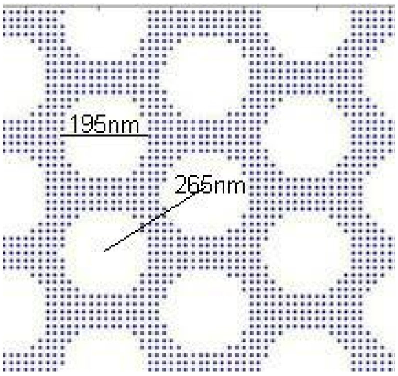


**Figure 1 Photonic Crystal in Glass (ε=2.25) with Air holes**

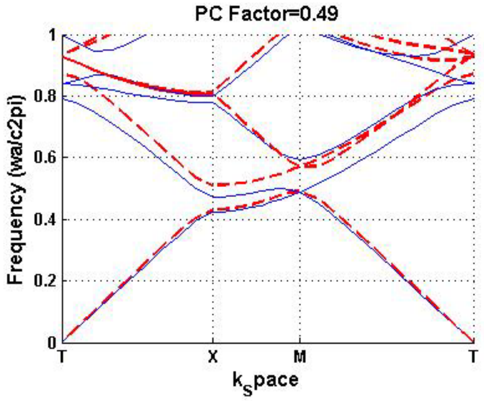


**Figure 2 Dispersion Diagram of the Photonic Structure**

with rods) band gap which is illustrated by dashed lines in the dispersion diagram. TM waves do not have a forbidden band, (Figure. 2). So the 2D structure can trap TE waves travel in the glass substrate and decrease the out coupling beam angle.

## Modeling of the Metallic Layer

The FDTD algorithm can extend to dispersive media using an auxiliary differential equation (ADE) [2], which operates on the frequency-domain equations. Metals exhibit dispersive properties at optical frequencies. Metallic elements are simulated using the Drude model, in which the complex frequency dependent current density is related to the electric field by:

$$J(\omega) = \frac{\varepsilon_0 \omega_p^2}{i\omega + 1/\tau} E(\omega) \tag{1}$$

Where $\tau$ is the relaxation time and the plasma frequency $\omega_p$ is defined as:

$$\omega_p = \sqrt{\frac{Ne^2}{m\varepsilon_0}} \tag{2}$$

In the time domain, this equation corresponds to:

$$J(t)/\tau + \frac{\partial J}{\partial t} = \varepsilon_0 \omega_p^2 E(t) \tag{3}$$

Using equation (4) the discrete time domain form of Ampere's law expanded about the time step n+1/2 can be determined as:

$$E^{n+1} = \left(\frac{1+\frac{dt}{2\tau}-\frac{\varepsilon_0\omega_p^2 dt}{2}}{1+\frac{dt}{2\tau}+\frac{\varepsilon_0\omega_p^2 dt}{2}}\right)E^n + \left(\frac{\frac{dt}{\varepsilon_0}\cdot\left(1+\frac{dt}{2\tau}\right)}{1+\frac{dt}{2\tau}+\frac{\varepsilon_0\omega_p^2 dt}{2}}\right)\nabla\times H^{n+1/2} - \left(\frac{2}{1+\frac{dt}{2\tau}+\frac{\varepsilon_0\omega_p^2 dt}{2}}\right)J_p^n \tag{4}$$

With:

$$J_p^{n+1/2} = \frac{J_p^{n+1} + J_p^n}{2} \tag{5}$$

## Numerical Simulation

The geometry of the photonic crystal enhanced OLED has been illustrated in figure.3. The structure is excited by a sinusoidal electric dipole at the HTL/ETL interface, with frequency corresponding to a wavelength $\lambda$=530nm for 4096 time steps (equivalent to about 32 periods). The dielectric parameters are given in Table 1.

**Table 1 Dielectric Parameters of OLED**

| **Material** | **Thickness (nm)** | **n@530nm** | **k@530nm** |
|---|---|---|---|
| **Air** | 0 | 1 | 0 |
| **Glass** | 300 | 1,5 | 0 |
| **Photonic crystal** | In Glass | D=195nm a=265nm | |
| **ITO** | 90 | 1,92 | 0 |
| **Org bottom** | 28 | 1,77 | 0 |
| **Emitter** | 0 | 0 | 0 |
| **Organic top** | 28 | 1,77 | 0 |
| **Ag** | 100 | $\omega_p$= 1.3703×$10^{16}$,<br>$\tau$=40×$10^{-15}$ | |

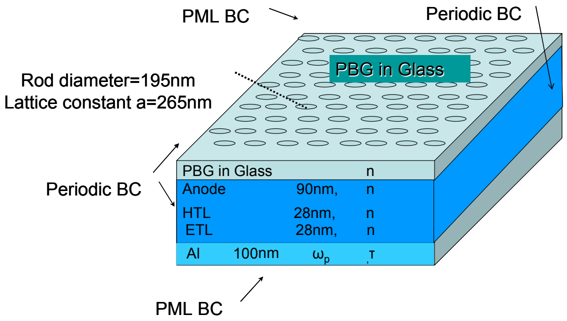


**Figure 3 Simulation Space and OLED structure**

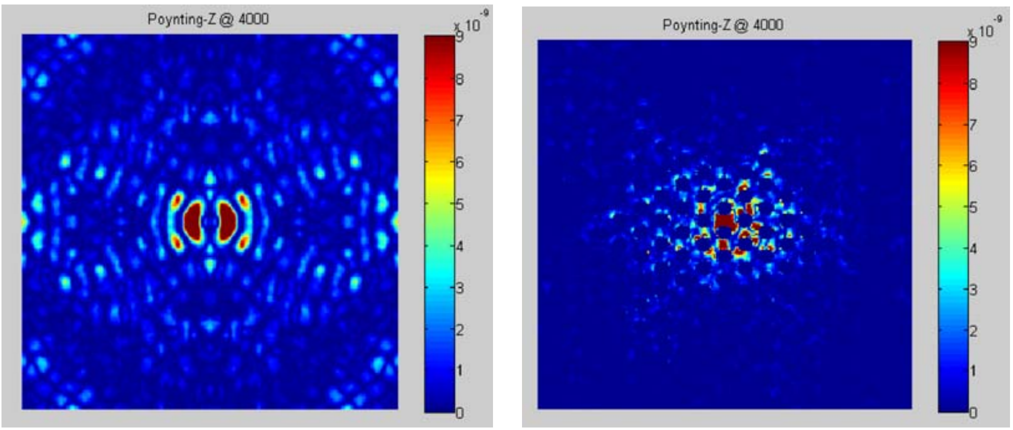
The simulation volume is X=250×dx, Y=250×dy where dx=dy=dz=λ/32. dt=dx/4/c. The periodic boundary condition (PBC) is used for the four sides of the volume and the perfectly matched layer (PML) boundary condition for top and bottom . The structure is analyzed with photonic crystal and without photonic crystal. The near-field plot of the z component of poynting vector in the OLED without photonic crystal is shown in figure. 4a. In figure. 4b the near-field plot of the z component of poynting vector is shown for the structure with photonic crystal.

## Simulation Results

Average of energy related to the z-component of the Poynting in the OLED versus radial distance from the place of dipole has been calculated (Figure 5).

$$\textbf{Average of Energy in One Period of Radiation} = \frac{\iint\limits_{r=R} \int\limits_{t=3968}^{t=4096*dt} P(x,y,t)dt\ \ dxdy}{\pi R^2} \qquad \textbf{(6)}$$

It is obvious that in one period of oscillation more energy is confined near the location of the dipole in the photonic crystal enhanced OLED (Figure. 5). The ratio of the extracted energy of enhanced OLED over the simple OLED is illustrated in figure 6 as a function of the radial distance from the dipole.



**(a)** **(b)**

**Figure 4 z-component of the near-field Poynting vector in an OLED at time step 4000 (a) without photonic band gap (b) with photonic band gap**

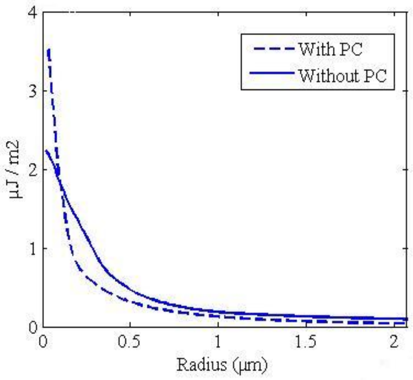


**Figure 5 Average of the z-component of the Poynting in the OLED versus radial distance from the place of dipole**

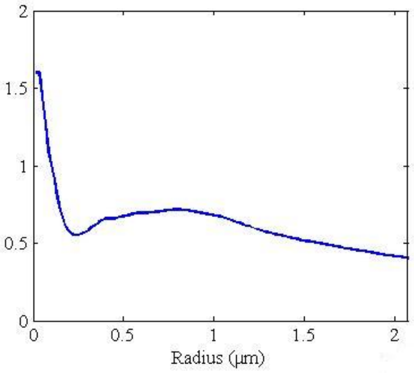


**Figure 6 Ratio of the averaged (over a circle with given radius) z-component of the Poynting vector of the enhanced OLED over the original OLED.**

## Conclusions

Optical extraction of a photonic band gap enhanced OLED was simulated by 3D FDTD method. The metallic layer is modeled as a dispersive material. It is shown that photonic band gap enhancement confines the near-field emission and increases the contrast of the OLED.

## References:

[1] John D. Joannopoulos, Robert D. Meade, Joshua N. Winn, Photonic Crystals: Molding the Flow of Light, Princeton University Press, 1995

[2] Allen Taflove, Susan C. Hagness, Computational Electrodynamics: The Finite-Difference Time-Domain Method, Artech House Publishers, 2005