Nanostructured super-period gratings and photonic crystals for enhancing light extraction efficiency in OLEDs

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Abstract

The focus of this study is to improve the light extraction efficiency and directionality of the OLED using a photonic crystal. First, the single period dielectric structure was optimized for red, green and blue wavelengths. The results showed an increase in directionality to an angle of approximately ±15 degrees. This is promising since the angle needed for comfortable viewing is considered to be ±20 degrees. Then the superperiod structure was designed and simulated for red and blue wavelengths. There was a further increase in directionality to ±20 degrees. The transmission spectrum for both wavelengths was also affected at multiple regions, as proposed in the superperiod design. Further work entails more superperiod simulations with changes to parameter values, including consideration of four possible dipole positions.
1. Background

Organic light emitting diodes are LEDs whose electroluminescence layer is composed of a thin film of organic compounds. The very basic OLED structure consists of the substrate, anode, organic layers (conductive and emissive) and the cathode, as seen in Figure 1. When a voltage is applied to the OLED, electrons are injected by the cathode into the emissive layer and holes are injected by the anode into the conductive layer. Recombination of electrons and holes occurs at the interface between the organic layers, resulting in a release of energy in the form of a photon of light [2].

What makes OLEDs so unique and exciting to the field of nano optics is their ability to generate their own light, rather than modulate transmitted or reflected light. The organic layers are also very thin, on the order of 15 nm to 600 nm making the device lightweight and more flexible. This allows OLEDs to be formed on substrates of various shapes and sizes. They also consume low power, with no need for a backlight like in LCD technology. It is thought that if OLEDs are implemented over many typical devices, such as cameras, televisions, and lamps, the overall energy consumption will be greatly reduced, making OLEDs a definite “green” resource. Another key advantage is their high contrast since they can support the full spectrum of visible light. The light is emitted in a Lambertian pattern such that it is equally bright over a large angle, making it more comfortable for the human eye. Other important advantages include their high speed refresh rates, and wide operating temperature range [3]. However, OLEDs also face a few disadvantages. They have short lifetimes of about 14,000 hours. OLEDs are also susceptible to water as the organic layers can become easily damaged. A more pressing issue, however, is the poor internal light extraction efficiency.

The light emitted in the active region of the OLED is classified into three modes each accounting for some percentage: direct transmission to the air (20%), the glass total internal reflection (30%), and the high refractive index (organic/ITO) guided mode (50%). The 50% that is trapped is waveguided in these layers and usually escapes through the side and edge of the substrate [4]. Many studies have shown that a means of extracting some of this trapped energy is
through the implementation of a photonic crystal (PhC). The periodic dielectric structure of the PhC allows photons (as waves) to propagate through the structure. When the period of the PhC is equal to the cavity wavelength of the guided mode (in the ITO layer), the guided waves are coupled to the radiation mode in the normal direction [4,5]. Thus, by coupling a PhC structure to the organic and ITO layers of an OLED, it is possible to guide some of the trapped energy out. This is the principle goal of this study, but is conducted using computational electromagnetic tools and other compatible software in analyzing results.

2. Theory and Design

The basic idea behind the computer simulations of the OLED with PhC structure is to have a dipole source turn on and off instantly and view the radiation profile of the emitted light.

*Simulated OLED Structure*

The OLED structure with the additional photonic crystal layer is shown in Figure 2. The thicknesses indicated were provided by the company for which this study is being conducted. The glass is the substrate and around 1500 nm in thickness, the silicon nitride PhC layer depth is 200 nm, the following silicon nitride layer is 600 nm, the ITO (anode) is 200 nm, the organic layers are 180 nm, and then there is a metallic cathode. The cathode was assumed to be 100% reflective. Further specifications regarding the indexes of refraction and the thicknesses are shown in Table 1 provided in the Appendix.

*Photonic Crystals and the Superperiod Concept*

Two different photonic crystal structures were investigated in this study: the single period and dual period. The single period PhC has already been optimized for various uses in other studies. However, it was still necessary to computationally optimize the single period PhC since it is the basis for the dual period structure. The reason for the dual period is that the single period does not enhance the efficiency by much, only about 50% over the current emission, bringing to a total of 30%, as seen in previous studies. The idea behind the dual or super period structure is to
enhance the emitted light from multiple regions of the spectrum for a more balanced emission. If two distinct single period PhC structures are each optimized for a different wavelength and these structures are superimposed, then the collected emission from the superimposed structure should enhance both wavelengths. Another way to understand the superperiod concept is as a dielectric structure with two or more periods. If a single period is tailored for a specific wavelength, then two different alternating periods must target two different wavelengths. Theoretically, this should both increase the efficiency as well as the directionality of the emitted light.

**Parameters to consider in the general Photonic Crystal Structure Design**

- **Lattice parameter, \(a\):** distance between adjacent cells (holes). This value stays constant for a single design. All other parameters are coded accordingly, as seen in the code provided in the Appendix. For example, if \(a = 600\) nm or unit value “1”, then the height of the PhC layer of 200 nm is considered to be \(0.3333 \times a\). Thus, the ratio of the parameter values stays the same with changing lattice parameter values.

- **Hole depth:** set at 200 nm for both single period and dual period. This was based on optimal designs provided in a previous study [4,5].

- **Hole radius:** set at 100 nm for single period and varied for the dual period design.

- **Dipole source placement**
  - Single period: optimal placement is at the center of the structure, or lattice coordinate point (0,0,0)
  - Dual period: four possible placements. Each need to be investigated to determine the optimal position.

**Single Period Structure**

The following PhC structure is based on the work of Yong Hee Lee et al. whose group found the optimal parameters for the single period to be those listed below the figure [4].

![Figure 3: Single period PhC structure](image)

[r = 100 nm, Dipole at (0,0,0), h = 200 nm, a = 600 nm]
**Dual Period Structure**

The design used in the simulations is a general dual period grating with two hole radii, and two periods. The lattice parameter and hole depth remained the same at 600 nm and 200 nm respectively.

![Figure 4: Dual period PhC structure](image)

The values of $b_1$ and $b_2$ are the two important parameters of this design. Ideally, by adjusting $b_1$ and $b_2$, we can deterministically choose two regions of the visible spectrum that may be influenced. For the simulation results, $b_1$ was 200 nm and $b_2$ was 400 nm.

**Measuring extraction efficiency and directionality**

The following are some aspects to consider when evaluating PhC efficiency and directionality:

1. The *Far Field Projection* is of interest because it graphically represents the specific symmetry related to the original photonic crystal pattern inscribed in the OLED, resulting in the angular variation of light intensity and color. It also gives a sense of the directionality of the light [5].

2. The *Total Emitted Power* is measured for each dipole source, if more than one is placed in the structure. It can be normalized to the total power an ideal dipole would radiate in a homogeneous material to give a sense of the efficiency of the OLED with the PhC [5].

**Software**

Two softwares (Lumerical Solutions and MEEP) were considered for the simulations. Both use FDTD (finite difference time domain) methods as they have several advantages for computational electromagnetics. On MIT’s MEEP website, they explain the use of FDTD clearly as “a widely used technique in which space is divided into a discrete grid and then the fields are
evolved in time using discrete time steps—as the grid and the time steps are made finer and finer, this becomes a closer and closer approximation for the true continuous equations, and one can simulate many practical problems essentially exactly” [7].

1. **Lumerical Solutions**: commercial software that was initially used to realize the superperiod concept. The free version of this software limited the number of parameters available to optimize the design [6].

2. **MEEP**: This software was developed at MIT to model electromagnetic systems. Every aspect of the OLED and PhC can be specified and relevant outputs can be extracted from the simulations. The simulations are visual representations of the near field radiation from the emitted light [7].

3. **MATLAB** was used to convert the data from the near field to the far field using the fourier transform. MEEP resulted in about 80 images depicting the radiation of light from the OLED. Of these, about 10 consecutive images which demonstrated the points in time where the emission was most balanced were converted to data files and time averaged for use in the MATLAB fourier transform code.

**Simulation Time**

The extraction efficiency for individual wavelengths was calculated by changing the pulse center frequency (fcen) of the Gaussian dipole source. \( f_{cen} = \frac{a}{\lambda} \) demonstrates the simple relationship between the lattice parameter \( a \), the wavelength \( \lambda \), and fcen.

Simulation time is dependent on both fcen and df (the pulse width). By setting fcen and adjusting df accordingly, the simulation is ensured to run for several seconds after the dipole turns off, capturing the radiated emission in a series of time shots.

**3. Results**

The extraction efficiencies for the Red (650 nm), Green (510 nm) and Blue (475 nm) wavelengths were observed as they are of most significance for display technology.
General Simulation Time shots (noPhC vs. PhC)

Wavelength = 600 nm

Figure 5: no PhC vs. PhC radiation over a series of time shots

General noPhC vs. PhC Directionality Results (for sample red wavelength)

Figure 6: Directionality (noPhC vs PhC)
Single Period Red Wavelength (650 nm)

Figure 7: (A) Far field distribution (B) Time avg emission (C) Near field (D) Far field
Plots are of simulation data pts vs. power output

Single Period Green Wavelength (510 nm)

Figure 8: (A) Far field distribution (B) Time avg emission (C) Near field (D) Far field
Plots are of simulation data pts vs. power output
Single Period Blue Wavelength (475 nm)

Figure 9: (A) Far field distribution (B) Time avg emission (C) Near field (D) Far field
Plots are of simulation data pts vs. power output

Sample Power Transmitted (Blue wavelength)

Figure 10: Transmitted power for single period PhC (blue). Normalized to power for no PhC.
Superperiod Red Wavelength Results

Figure 11: Superperiod results for Red wavelength. Increased directionality as seen in FF plot.

Figure 12: Transmission for superperiod (Red). Observe two additional peaks at 486 nm and 548 nm aside from the "red" peak.
Superperiod Blue Wavelength Results

Figure 13: Superperiod results for Blue wavelength. Similarly increased directionality.

Figure 14: Two small additional peaks at 447nm and 548nm. Note that 548 nm was similarly affected in the red wavelength.
**Discussion**

Initial simulation results for a wavelength of 600 nm, or a center frequency of 1 are seen in Figure 5. Observations of the radiated light at five different time shots for an OLED with and without a photonic crystal clearly show an increase in directionality with the dielectric structure. This is confirmed in the far field angular profiles for the OLED with and without PhC as seen in Figure 6. The directionality for noPhC is around ±7 degrees and for PhC it is about ±15 degrees. This is very promising as the angle sought for comfortable viewing for the human eye is around ±20 degrees. In general, the emission should lie somewhere within the ±30 degree cone.

The application of OLEDs is primarily colored displays, making the study of the emission of the red, green, and blue wavelengths imperative. In the single period emission profiles for RGB shown in Figures 7-9, we see four diagrams. The top left is the visual picture of the time averaged image of the emission. The near field (bottom right) is the power output at the surface of the substrate. The fourier transform of the near field results in far field power output (top right). Most important is the bottom left far field angular profile. In all three cases, the directionality was consistently around ±15 degrees. This is satisfactory for current simulations since it is hoped that the super period gratings enhance the directionality of the light. In Figure 10, a sample transmitted power plot is given for the blue wavelength for an OLED with and without a single period photonic crystal. The tuning of the structure to 475nm is definitely reflected in the transmission graph with a peak around this wavelength. The graph for the PhC is normalized to the results from without a PhC. The power output at the wavelength is about five times as great as the transmission without a PhC. The transmissions were very similar for the red and green wavelengths and were therefore not included. The single period results were computationally very promising, providing a strong basis for developing the superperiod and running simulations.

At present, the superperiod results have been calculated for red and blue wavelengths only. In both Figure 11 and 13 for the red and blue wavelengths, respectively, it is apparent that the directionality has significantly improved with the superperiod structure. The angle of emission is around ±20 degrees. However, it is the transmitted power that is of more interest in the superperiod. The idea of the superperiod is to improve the light extraction efficiency from multiple regions of the visible spectrum simultaneously. The physical structure of the
superperiod PhC used in these simulations is shown in Figure 4. Setting the center frequency to red or blue, we expect to not only see a peak at 650 nm or 510 nm but also two additional peaks resulting from the two periods in the structure of Figure 4. This is clearly reflected in the transmission results shown in Figures 12 and 14. For the red wavelength (Figure 12), the transmitted power had three peaks at 486nm, 548nm, and 650nm. For the blue wavelength (Figure 14), the transmitted power had three peaks at 447nm, 548nm, and 475nm. Interestingly, there is an overlap between the two results at 548nm. The discrepancy between the 447nm and 486nm peaks is not too significant since this could have been because the red wavelength peak of 475nm is too closely situated to a possible 486nm peak. This can be investigated by tuning the superperiod to frequencies higher than 600 and observing if the same two peaks are affected. This preliminary result is significant since it demonstrates that regardless of the tuning of the center frequency, two similar wavelength regions are affected, as expected in a superperiod structure.

Conclusions

The initial single period simulations and far field results for RGB were very promising, indicating definite enhancement in extraction efficiency with a PhC OLED. These optimized structures provided a basis for designing and simulating a particular superperiod structure. Preliminary far field results of the superperiod for red and blue showed an even more directional angular profile of around ±20 degrees. The transmission results for red and blue overlapped at two specific wavelength regions with small discrepancies. This is an important result as it confirms the possibility of the superperiod to influence more than one wavelength region.

Future Work

The superperiod simulations were preliminary and can be redone for various parameterizations and wavelengths. Also to be investigated is the influence of different dipole positions on the extraction efficiency and directionality. Currently the dipole is at the center of the structure at lattice point (0,0,0) like in the single period. But the superperiod allows for more creative positions for the dipole and these must be studied as a possible factor in the parameterization.
Acknowledgements

I would like to thank Professor Chee Wei Wong and PhD student Ranojoy Bose for their help and guidance. In particular, Ranojoy Bose who wrote a majority of the MATLAB code for the fourier transform.

Criticism of Course

I enjoyed working as a part of the research aspect of this course. However, I think that if time permitted, I would have liked to work on a more traditional project for this course as well. It would be nice to see integration between the pure research and pure hardware aspects of experimentation. This is difficult to do in one semester and for that reason, two semesters might be more educational and more fulfilling for the student(s).

References


7. MEEP Software: http://ab initio.mit.edu
Appendix

1. Indexes of refraction and thicknesses

<table>
<thead>
<tr>
<th>OLED layer</th>
<th>Thickness</th>
<th>Index of Refraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Glass</td>
<td>900 nm</td>
<td>n = 1.5</td>
</tr>
<tr>
<td>SiNx</td>
<td>600 nm</td>
<td>n = 1.9</td>
</tr>
<tr>
<td>Anode/ITO</td>
<td>200 nm</td>
<td>n = 1.8</td>
</tr>
<tr>
<td>Organic</td>
<td>180 nm</td>
<td>n = 1.75</td>
</tr>
<tr>
<td>Cathode</td>
<td>Metallic layer</td>
<td>complex</td>
</tr>
</tbody>
</table>

2. MEEP Code

```
(define-param eps1 1) ; dielectric constant of Air (n_air = 1)
(define-param eps2 2.25) ; dielectric constant of Glass
(define-param a 1) ; lattice parameter 600 nm
(define-param eps3 3.61); SiNx
(define-param eps4 3.24); ITO
(define-param eps5 3.0625); Organic

(define-param r 0.165) ; radius of air holes 100nm
(define-param t1 0.33) ; glass rod height 200nm
(define-param h 1.5) ; Glass layer ??
(define-param h1 1) ; SiNx layer 600nm
(define-param h2 0.33) ; ITO Layer a = 600 nm
(define-param h3 0.3) ; Olayer 80nm + 100 = 180
(define-param dpml 1) ; PML thickness
(define-param sx 30) ; size of cell in x direction
(define-param sy 30) ; size of cell in y direction
(define-param sz 12) ; very large to avoid PML layer

(set! progress-interval 100)
(set! eps-averaging? false)
(set! geometry-lattice (make lattice (size sx no-size sz)))

(set! pml-layers (list (make pml (thickness dpml))))
;set! field-set-boundary fields Low Z Metallic);
(set! geometry
  (append
   (list (make block (center 0 0 2.23) (size sx sy 1.5) (material (make dielectric (epsilon eps2))))))
   (list (make block (center 0 0 .98) (size sx sy 1) (material (make dielectric (epsilon eps3)))))
)
(list (make block (center 0 0 0.315) (size sx sy .33) (material (make dielectric (epsilon eps4))))))

(list (make block (center 0 0 0) (size sx sy .3) (material (make dielectric (epsilon eps5))))))

(list (make block (center 0 0 -2.15) (size sx sy 1) (material metal)))

(geometric-objects-lattice-duplicates
 (list
   (make cylinder (center 0 0 1.65) (radius r) (height 0.33) (material (make dielectric (epsilon eps3))))
 ) 1 1 80)
)

(set-param! resolution 16)
(use-output-directory "PCfixed")

(define-param fcen 2) ; pulse center frequency
(define-param df 1) ; pulse width (in frequency)
(define-param nfreq 500) ; number of frequencies at which to compute flux

; false = transmission spectrum, true = resonant modes:
(define-param compute-mode? true)

(if compute-mode?
  (begin
    (set! sources (list
      (make source
        (src (make gaussian-src (frequency fcen) (fwidth df) ))
        (component Ey)
        (center 0 0 0)
        (size 0 0 0)
      )))

    ; (set! symmetries
    ;   (list (make mirror-sym (direction Z) (phase +1)) ; z-even
    ;     ; (list (make mirror-sym (direction Y) (phase +1)) )) ; y-even
    ;   ;(make mirror-sym (direction X) (phase -1)); x-odd
    ;))

    (run-sources
     (at-beginning output-epsilon)
     (after-sources (harminv Ex (vector3 0) fcen df)))
    (run-until (/ 10 fcen) (at-every (/ 0.1 fcen 1) (at-end output-dpwr) output-efield-y
      ;output-hfield-x
      ;output-hfield-y
     ))
  )
)