FDTD Modeling and Simulation of Organic Light Emitting Diode with Improved Extraction Efficiency using Moth-eye Anti Reflective Coatings

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Abstract: In this work modeling of two dimensional fluorescence based bottom emitting Organic Light Emitting Diode (OLED) using Moth eye Anti Reflective Coatings (ARC) is presented. The Finite Difference Time Domain (FDTD) mathematical modeling has been used to analyze the light extraction efficiency from fluorescence based Organic Light Emitting Diode (OLED). The OLED structure has been simulated by using 2D Moth-eye Anti Reflective coatings. The Finite Difference Time Domain (FDTD) method is used to model and simulate the OLED structure. An enhancement of Light Extraction Efficiency (LEE) has been achieved by inserting Moth-eye Anti Reflective coatings on the surface of the glass substrate which reduces reflection and increases the transmission. Comparative study is carried out between hexagonal photonic crystals and Moth eye Anti reflective coatings by placing these nanostructures on the substrate of OLED. The improvement in the far field intensity of OLED structure is achieved by optimizing the angular distribution of light through the substrate with moth eye anti reflective coatings.

1 INTRODUCTION

Organic Light Emitting Diode (OLED) is an luminescence based device which is formed using organic layers to produce light emission. The excitons excitation is achieved by driving voltage as dc source below 10 Volts (Tang and VanSlyke, 1987). The radiative decay of exciton is achieved due to singlet, Hence the name Fluorescence based OLED. In the OLED stack the device efficiency is achieved by varying the electron transport layer. In order to improve the extraction efficiency, various transport layers are used with different work functions as in (Do et al., 2003).

In order to various losses that exist in OLED, many experiments were conducted in the literature. In order increase the device performance the Photonic Crystals (PC) is placed upon glass substrate to realize low power consumption using Nano imprint lithography technique which showed better performance than conventional OLEDs (Lee et al., 2003).

The Silicon Nitride (SiN) Photonic Crystals (PC) are used to control light which is acting as a dielectric medium to extract maximum amount of photons which is trapped in high index guided structures. Various approaches have been reported in the literature to improve efficiency and extract modes outside the OLED.

However different experiments on Organic LEDs are carried out to address substrate losses using different structures of the Photonic crystals and using different substrates as reported in (Kim et al., 2004). The light extraction efficiency has been achieved by incorporating dielectric Nano particles placed at the substrate and scattering efficiency is calculated by using Mie theory as discussed in (Mann et. al., 2017).

The Anti reflective coatings can be used on the backside of the glass substrate to achieve enhancement in the luminescence and was fabricated by Magnesium Fluoride (Saxena et al., 2008) In the recent advancements the Moth eye Antireflective coatings were introduced to used it for display applications, such as solar cells (Tan et al., 2017).

The light out coupling efficiency is enhanced by using Bio inspiring concept of moth eye anti reflective coatings. This is used to suppress

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reflection and extract maximum modes outside the OLED compared to Conventional approaches of OLED. (Zhou et al., 2014).

This research work is being carried out aiming at increasing the light extraction efficiency of OLED. In this paper an OLED with moth eye Anti reflective coatings are used with glass as a substrate and by using point dipole source to increase the number of photons in the emissive layer. In this work, we are addressing substrate losses that exist when light is coupling out into the air. This is done by incorporating moth eye Anti reflective coatings between air medium and the substrate. Comparative study is carried out for different structures of OLED.

2 OLED STRUCTURE

2.1 Design of OLED

Figure 1, shows the structure of Organic Light Emitting Diode (OLED) which is modeled using Lumerical FDTD (Finite Difference Time Domain). The proposed structure uses glass substrate. The device structure consists of thin active organic layers integrated into injected electrons and holes. These transport and organic Layers which is about 200nm is placed between anode and cathode layer. In this structure, the Moth eye Anti reflective coatings are placed between air medium and the Glass substrate. This OLED designed is proposed in this paper to achieve maximum light out coupling from the fluorescence based green light emitting device. The green light is due to the organic layers present in the device which is aiming to emit light at green wavelength at 540nm.

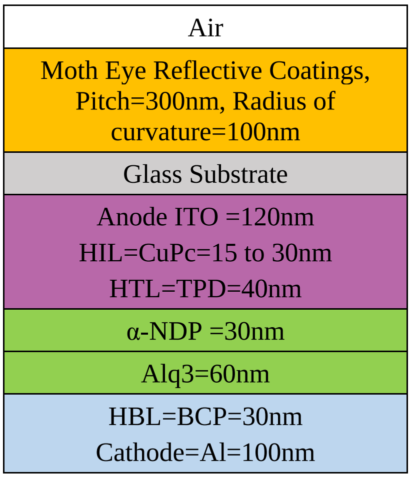

Figure 1: Fluorescence based OLED.

2.2 Modeling of Moth Eye Anti Reflective Coatings

The Moth eye Anti Reflective coatings very important in various display applications like LEDs, photo detectors and solar cells, where reflection loss is to be minimized. This structure is inspired by Bio mimic array and reduces the internal reflectance outside their operating wavelength(Cho et al., 2017).

The eye of a Moth insect has a periodic nanostructure in coating layer are tapered and air fraction decreases in the coating towards the substrate

We set x span and y span to be 0.5um for the simulation region, which includes only one unit cell. Since the structure exhibits both symmetry and periodicity.

The boundary condition chosen is as follows:

•x-min bc = x-max bc = antisymmetric

•y-min bc = y-max = symmetric

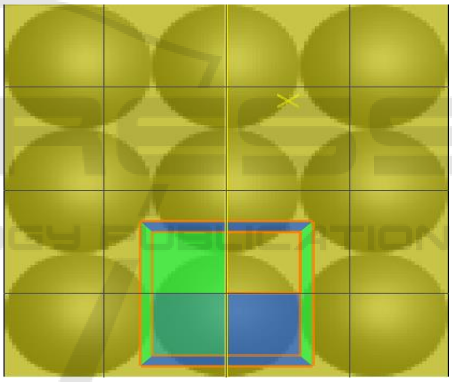

Figure 2: Modeling of Moth-eye anti reflective coatings (ARC) with pitch chosen to be 300nm and radius of curvature of 100nm.

In this simulation, the reflectance with respect to wavelength is measured and get insight of where Electromagnetic energy is absorbed and where photoelectrons are created. FDTD simulation method is used to model this Moth-eye gold nanostructure.

2.3 Modeling of OLED using Moth Eye Anti Reflective Coatings

The OLED device structure is modeled and simulated as shown in the Figure 3 using various materials as shown in Table 1. The modeling is done by using Lumerical FDTD (Finite Difference Time Domain). The device structure consists of thin active organic layers which are integrated with moth-eye anti reflective coatings using Silicon Nitride material and glass substrate.

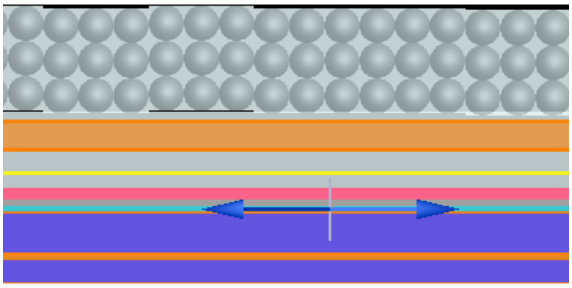

Figure 3: Modeling of OLED using Moth eye Reflectors (XY View).

The thickness of organic layers is about 200nm and is positioned between anode and cathode. The Moth-eye Anti reflective coatings are made of silicon Nitride material is of around 400 nm thickness. The total stacking height of OLED structure is of the order of 1500 nm.

The modelling is done for the proposed structure shown in Figure 1. The moth-eye Anti-reflectors coatings are used to reduce the internal reflectance on the surface of the substrate.

These coatings are used upon the surfaces to improve the out coupling efficiency of the devices. The Moth-eye Antireflective coatings nanostructures increase the efficiency of Organic Light Emitting Diode .This structure is inspired by Bio mimic array and operating at 540nm and reduces the internal reflectance outside their operating wavelength.

2.4 Modelling of OLED using Two Dimensional Hexagonal Photonic Crystals

Figure 4, shows the modelled Photonic Crystal (PC), used in OLED.

The photonic crystal is used for modeling for different OLED structures as discussed in

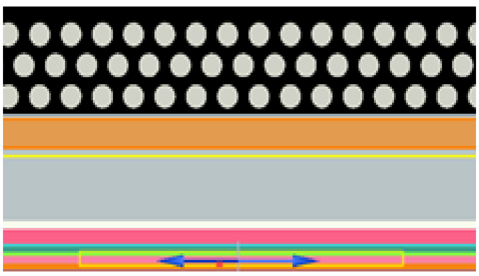

Figure 4: Modeling of OLED using Hexagonal Photonic Crystal (XY View).

literature work. The PC used in this work has lattice constant of 300nm and radius is of 100nm. The simulation is done using Photonic crystal made up of Silicon Nitride which has refractive index of 1.9.The Brillouin zone chosen is in the form of a hexagon. Hence it is called as Hexagonal Lattice Brillion Zone (Joannopoulos et al.,2008).

This modelling is done using lumerical FDTD for the design shown in Figure 1 using materials shown in Table 1. This is simulated using Photonic crystals to make the comparative study with the OLED structure with Moth eye Anti reflective coatings placed on the surface of the glass substrate.

3 OLED MATERIALS

The various materials used in OLED structure are shown in the Table 1.

The work function for various materials used in OLED are carefully chosen depending on the energy levels at metal organic interface abiding by Mott Schottky limit (Novotny et al., 2006).

Table 1: Materials used in the OLED Structure.

Materials	**Work Function**	**Refra-ctive index (n)**
Anode –ITO- Indium Tin Oxide	4.7eV	1.806
Cathode- Al- Aluminium	4.1eV	1.031
Hole Blocking Layer (HBL)-BCP-(2, 9 Dimethyl-4, 7-diphenyl-1, 10 phenanthroline	3.2eV	1.686
Hole Injection layer(HIL)-CuPC-(Copper (II) phthalocyanine)	3.1eV	0.47
Hole Transport layer(HTL)-TPD-(N, N'-Bis (3-methylphenyl)-N, N'-diphenylbenzidine)	2.6eV	1.67
Alq_3-Tris(8-hydroxyquinoline)aluminum	HOMO-5.62eV LUMO-2.85eV	1.68
α-NDP- N,N`- diphenyl-benzidine	2.5eV	1.82
Photonic crystals–SiN-Silicon Nitride-(Lattice Constant =350nm) Moth Eye Anti Reflective coatings (pitch=300nm, radius=100nm)	----	1.9
Glass Substrate	----	1.53

The thickness variations and Organic Layers with the HOMO (Highest Occupied Molecular Orbital) and LUMO (Lowest Unoccupied Molecular Orbital) levels of organic molecules are given. The most commonly used HIL is CuPC (Copper (II) phthalocyanine) is used to improve the carrier injection efficiency. The HTL used here is TPD (N, N'-Bis (3-methylphenyl)-N, N'-diphenylbenzidine).

The hole transport layer and hole injection layer placed above organic layers. The hole injection layer is used to improve the carrier injection efficiency, and serves two purposes, first, it provides a path for smooth travel of injected holes up to emitting layer. Second, it functions like electron blocker to confine electrons within an emitting layer.

4 METHODOLOGY

The Finite Difference Time Domain (FDTD) method is most widely used method to solve Maxwell's equations and simulate Nano-photonic devices(Gedney,2011). FDTD method is used to investigate and analyze the light propagation. Light of UV, Visible and IR regions propagating through different layers with complex geometries can be analyzed and simulated with the help of FDTD (Taflove,1995). Thus it is possible to analyze the propagation of Electromagnetic wave inside the structure(Sullivan,2013).

Since the OLED device configuration is limited for single wavelength at 540nm, the optical thickness of Moth eye is given by(Cho BJ et al.,2017),

$$\mathbf{n_2 * d = \lambda/4} \tag{1}$$

Where, d= geometrical thickness of the film,λ= peak wavelength of light emitted by OLED,n_2=refractive index of the coating material..

Therefore, $\mathbf{d = \lambda/4 * n_2}$

Where, d= geometrical Thickness of the film, λ= peak wavelength of light emitted by OLED.
Under these conditions destructive interference occur and cancel each other and light is coupled out. For a single homogeneous layer with refractive index n, will suppress reflectance between substrate**(n_s)** and air **(n_a)** for normal incident of light and optical thickness **λ/4,** If, $\mathbf{n=(n_s\, n_a)^{0.5}}$ is fulfilled.

The Far field analysis accounts for the reflection and refraction that would occur at the Far-field substrate air interface. The fraction of source power transmitted into far field is derived.

A point dipole power source is used to generate charge carriers. The power radiated by an electric dipole in homogenous material is calculated (Novonty et al., 2006)

$$P = \frac{\mu_0}{4\Pi} n \,|\, \overrightarrow{p_0}^{\,2} \,|\, \frac{\omega^4}{3c} \tag{2}$$

Where, ρ_0 (Cm)=dipole moment and μ_0 = magnetic permeability, c =speed of light.
When the light emerges out of substrate, it would undergo refraction, reflection at the interface of substrate and air. This is analyzed by Far Field analysis.
The mathematical formulation for the electric field at far field is as shown below:

The Substrate air interface relation is derived by Fresnel's law(Chutinan et al., 2005),

$$\frac{1}{2}\sqrt{\frac{\varepsilon_0}{\mu_0}} n_2 \,|\, E_2 \,|^2 .d\theta_2 d\Psi_2 \sin\theta_2 = \frac{1}{2}\sqrt{\frac{\varepsilon_0}{\mu_0}} n_1 (T_{s.} \,|\, E_s \,|^2 + T_s . \,|\, E_p \,|^2) d\theta_1 d\psi_1 \sin\theta_1 \tag{3}$$

Where, ε_0 = Absolute permittivity, μ_0 = Absolute Permeability, n_1 =Refractive index of air, n_2 = Refractive index of Substrate, T_s and T_P are calculated as below using Fresnel equations,

$$|\, E_2 \,|^2 = (T_s . \,|\, E_s \,|^2 + T_s . \,|\, E_p \,|^2) \, {d\theta_1}\big/{d\theta_2} \tag{4}$$

Where, T_s and T_P are Fresnel transmission power coefficients in far field, E_s and E_P are Fresnel Electric field coefficients in far field. E_2 = Electric field beyond the far field interface. The Finite difference Time Domain (FDTD) method is used for solving Maxwell's equations in complex geometries.

5 RESULTS

5.1 Far Field Intensity of OLED

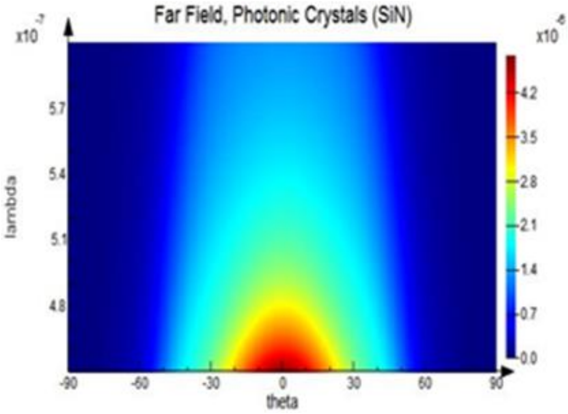

Figure 5(a): Far field Intensity of OLED with Photonic crystals using SiN Material.

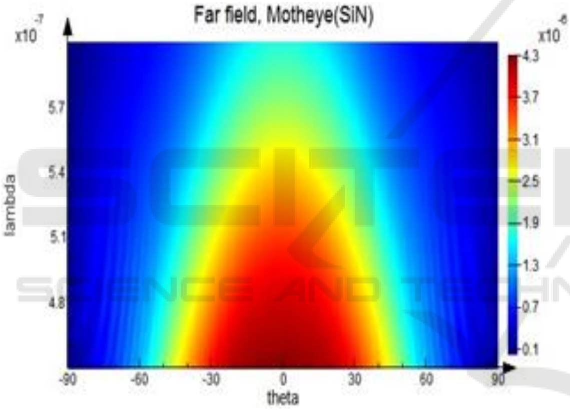

Figure 5(b): Far field Intensity of OLED with Moth eye Anti Reflective surface with SiN Material.

Figure 5, shows the maximum Light extraction efficiency from the modeled OLED structure that escapes into air. θ is the angle at which light emerges out of OLED. This angle is with respect to the normal to the interface surface. Figure 5(a) indicate the light emerges out in the range of -30^0 to + 30^0, when Photonic crystal is placed upon the substrate. That is range of light emergence is spread out for near 80^0.

However the intensity of light is subtended. In comparison Figure 5(b) shows that light emerges out with wider range of -50^0 to +50^0. Also the light emitted is much more bright when moth eye ARC is placed upon the substrate.

This indicates that by introducing Moth eye antireflection coatings on the substrate of OLED, the emission of light is spread over greater range of angle and also intensity of light is greater at 540nm.

This is because the Moth eye has a periodic nanostructure in coating layer are tapered and air fraction decreases in the coating towards the substrate, whereas the Photonic crystals has planar coating layer.

5.2 Angular Distribution of OLED at 540nm

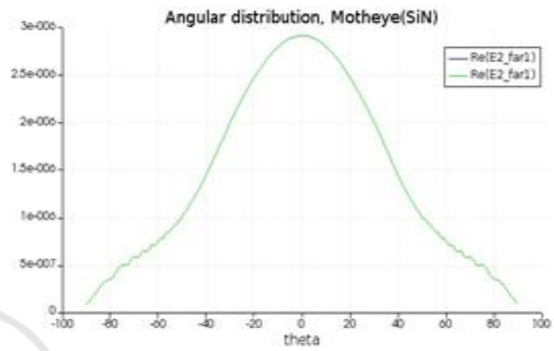

Figure 6(a). Angular Distribution of OLED with Moth eye Anti Reflective surface with SiN Material.

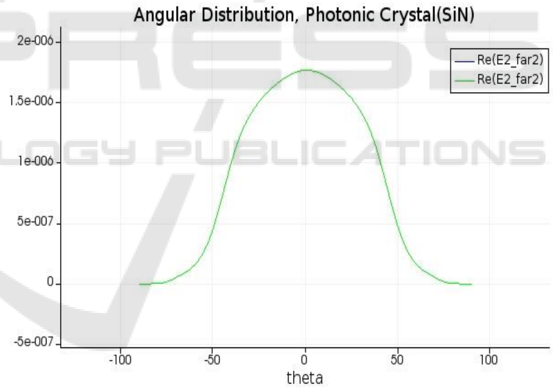

Figure 6(b). Angular Distribution of OLED with Photonic crystals with SiN Material.

The Angular distribution outputs are shown for OLED structures with moth eye and photonic crystals in figs 6(a) and 6(b).

The output is obtained for the modelling strucutre shown in figure 3, and the simulation is done using FDTD method.

It is observed that, the far field intensity for OLED with moth eye structure is 3 µV/m and that of OLED with PC is 1.8µV/m. Both the OLED structures are simulated for Silicon Nitride material.

Hence there is an significant improvement in the far field intensity in extracting light out coupling efficiency from an OLED.

However the presence of Moth-eye structure has channelized more light through the same angle of emission which otherwise would have been lost due to TIR within OLED and reducing internal reflection.

5.3 Simulation Outputs for OLED Structure without Moth Eye ARC

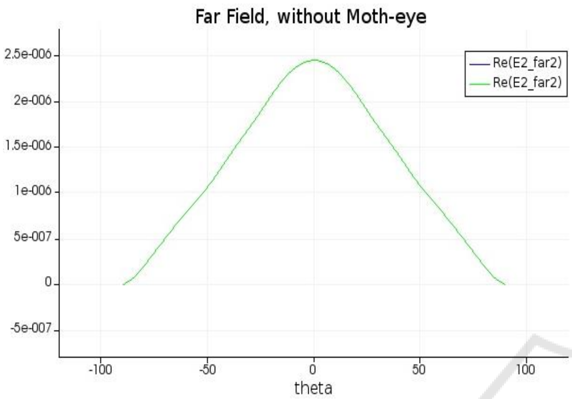

Figure 7(a). Angular Distribution for OLED without Moth eye ARC.

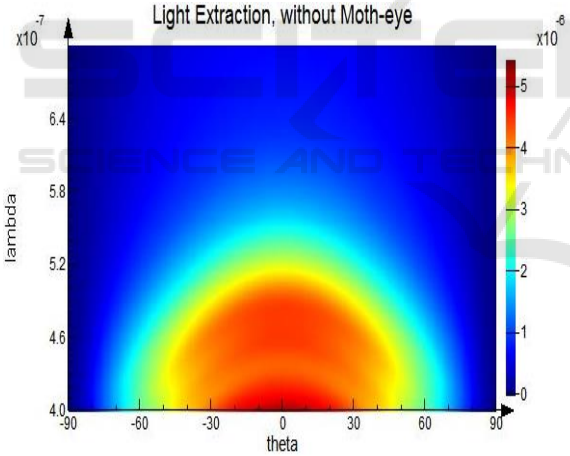

Figure 7(b). Far field Intensity for OLED without Moth eye ARC.

The simulation was carried out for the OLED structure without using Moth eye Structure on the surface of the glass substrate. This OLED structure has no Nano structure placed on the surface of the glass substrate. The far field intensity is observed to be 2.5µV/m as shown in the Figure 7(a) and 7(b). Hence we observe that, by placing Moth eye ARC better light coupling is achieved.

5.4 Moth Eye Anti Reflective Coatings Transmission and Reflectance Curves

The Moth eye Anti Reflective coatings are used to increase the transmission and to suppress the reflection that occur while light is out coupling from the glass substrate and outside OLED.

Figure 8 shows the amount of light transmitted from the substrate. This simulation output is obtained for the modelling of moth eye structure as shown in Figure 2.

In fact such a light source can be monolithically integrated with Lab-on-a-Chip sensor systems. Fabrication of such an OLED structures can find future applications used as a integrated light source for optical Lab-on-a-Chip based bio-sensors.

Hence, there is a improved light extraction efficiency for the structure with Moth eye ARC on the substrate compared to the OLED structure with Photonic crystals

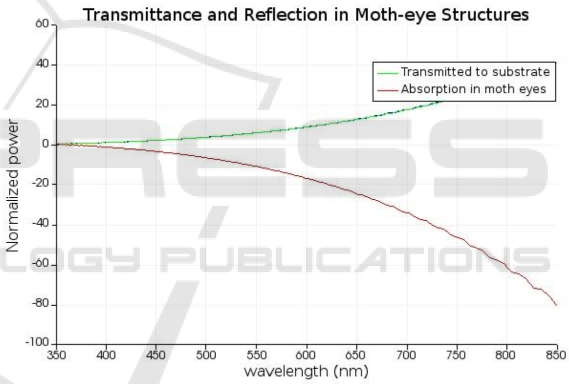

Figure 8. Transmittance and Reflectance curves.

Figure 8 shows amount of light absorbed by the moth eye ARC i.e., anything that transmits light is all absorbed in the substrate. The moth eye ARC are used because of its periodic nanostructure and are tapered.

The optimized output for different OLED structures with different materials are simulated and the far field intensity values for the same is tabulated at a wavelength of 540nm as shown in Table 2.

Table 2: Optimized output obtained for different OLED structures and different materials.

Parameters	**Materials**	**Far field intensity achieved**
OLED with Moth eye Anti Reflective coatings	Gold(Au)	3.5 µV/m
	Silicon Nitride(SiN)	2.9 µV/m
	Al_2O_3	3.2 µV/m
OLED with Photonic crystals placed on substrate	Gold(Au)	1.3 µV/m
	Silicon Nitride(SiN)	1.75 µV/m
	Al_2O_3	1.33 µV/m
OLED structure without any Nano structure	-----	2.5 µV/m

6 CONCLUSIONS

In this work, two dimensional Finite Difference Time Domain (FDTD) modeling of Fluorescence based OLED using glass substrate has been presented. An enhanced far field intensity of 3.5µ Vm^{-1} has been achieved for a wavelength of 540 nm by placing Moth eye Anti reflective coatings between the substrate and the air medium. The moth eye Antireflective coatings are placed on the surface of the substrate of OLED will enable maximum light out coupling efficiency compared to Conventional OLED structure. This Anti reflective coatings reduces reflection and increases transmission of light.

In this work, Different OLED structures have been designed with different materials. It is found that OLED with Moth eye Anti Reflective coatings with gold nano particles has increased far field intensity compared to other materials.

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