Numerical Analysis Using Finite Element Method On Phosphorescent Organic Light Emitting Diodes

Y. W. Hwang, H. G. Lee, and T. Y. Won*

Abstract—**In this paper, we report our numerical simulation on the electronic-optical properties of the phosphorescent organic light emitting diodes (PHOLEDs) devices. In order to calculate the electrical and optical characteristics such as the transport behavior of carriers, recombination kinetics, and emission property, we undertake the finite element method (FEM). Our model includes Poisson's equation, continuity equation to account for behavior of electrons and holes and the exciton continuity/ transfer equation. We demonstrate that the refractive indexes of each material affect the emission property and the barrier height of the interface influences the behavior of charges and the generation of exciton.**

Index Terms—**Numerical analysis, FEM, phosphorescent OLED**

I. INTRODUCTION

Organic light-emitting diodes (OLEDs) have many advantages such as high contrast, wide viewing angle, low driving voltage and fast response time. Recently, phosphorescent organic light emitting diodes (PHOLEDs) devices based on phosphorescent emission are being developed actively. PHOLEDs use a guest-host system in the emitting layer of the OLED device. It is known that energy transfer from host to guest occurs via excitons. Excitons are generated by the recombination of carriers in emitting layer, which attracted our attention on the charge balance in the host material comprising the PHOLEDs. In order to solve this problem, several kinds of material have been investigated by research groups. However, there is little research for theoretical study on kinetics of carriers in PHOLEDs. Consequently, we have undertaken the numerical study to analyze the recombination kinetics of carriers in emitting layer [1-3].

In OLED structure, optical energy is divided into several modes such as waveguide mode, substrate guided mode, out-coupled mode, evanescently-coupling mode, absorption-loss mode. We observe the calculated optical energy distribution for the variation of the refractive of index by modal analysis. Furthermore, we investigate the luminance for the variation of the thicknesses of ETL and HTL [4, 5].

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II. NUMERICAL MODEL

The electrical properties of multilayer OLEDs critically depend on the device structure, which includes the species of LUMO and HOMO, the work function of anode and cathode, and sequence of layers. In order to analyze each element, we need to employ a numerical model which allows us to optimize the OLED structure.

$$\frac{\partial E(x)}{\partial x} = \frac{e}{\varepsilon\varepsilon_0}(p(x) - n(x) + p_t - n_t + A_{Doping} - D_{Doping}) \quad (1)$$

Eq. (1) is the Poisson equation that yields the electric field distribution. $n(x)$ is the density of electrons (cm^{-3}), $p(x)$ is density of holes (cm^{-3}), and $E(x)$ is the electric

field (kV/cm). p_t,n_t are the trap terms. A_{doping}, D_{doping} are the doping term; however, we don't consider trap terms and doping term. ε is dielectric permittivity (F/cm), e the elementary charge (C).

$$\frac{\partial n(x)}{\partial t} = \frac{1}{e}\frac{\partial J_e(x)}{\partial x} - r(x)\cdot p(x)\cdot n(x) \tag{2}$$

Eq. (2) is continuity equation for electrons determines the time evolution of the system. $r(x)$ means recombination rate coefficient. $J_e(x)$ is the electron current (mA/cm^2).

$$\frac{\partial S_i(x)}{\partial t} = G_i R(x) + \overrightarrow{\nabla J_{S_i}}(x) - (k_{rad}(x) + k_{nonrad})\cdot S_i(x) - k_{annihilation}\cdot S_i(x)^2 + \sum_{j=1}^{n_{exc}}(k_{ji}\cdot S_j(x) - k_{ij}\cdot S_i(x)) \tag{3}$$

Eq. (3) is the rate equation for exciton (cm^{-3}), denoted by $S_i(x)$, contain generation, diffusion, radiative and non-radiative decay, annihilation, and exciton energy transfer term. The generation term G_i = 0.25 for singlet exciton while it would be G_i = 0.75 for triplet exciton. The exciton energy transfer term $k_{ij}\cdot S_i$ can be taken from the literature [6, 7].

$$R = \eta\cdot n\cdot p(\mu_n + \mu_p)\cdot\frac{q}{\varepsilon} \tag{4}$$

Eq. (4) is the recombination density that is dependent on the local charge mobility and the local charge density. The parameter η stay for the Langevin recombination efficiency [8].

$$\frac{d^2}{dt^2}\vec{p} + b_0\frac{d\vec{p}}{dt} + \omega^2\vec{p} = \frac{e^2}{m}\vec{E}_R(\omega) \tag{5}$$

The optical characteristics of multilayer OLEDs are affected by the refractive index and thickness of each layer. We use the dynamics of the oscillating dipole moment described by Eq. (5). ω is the oscillator frequency, m the effective mass of the dipole, $E_R(\omega)$ the interface-reflected field.

$$F = \int_0^\infty f(u)du \tag{6}$$

Eq. (6) denotes optical feed-back. $f(u)$ means the radiation at a given position. Dipole power dissipation is deconvoluted by integration limits. The integration limits are given by following : $u \in [0,\ 1/n_e]$ for out-coupled intensity, $u \in [1/n_e,\ n_t/n_e]$ for substrate-guided intensity, $u \in [0,\ n_t/n_e]$ for absorption-loss intensity, $u \in [n_t/n_e,\ 1]$ for guided-mode intensity, $u \in [1,\ \infty]$ for evanescently-coupling intensity. n_t is the refractive index of the top layer. n_e is the refractive index of the emission layer.

$$L(\theta) = 683\frac{lm}{W}\cdot\int\bar{y}(\lambda)E_\theta(\lambda)d\lambda \tag{7}$$

Eq. (7) describes the luminance for the brightness of the source. $E_\theta(\lambda)$ denotes spectral emission, $\bar{y}(\lambda)$ is the photopic luminosity function.

We employ the multilayer structure that consists of Poly(3,4)-ethylendioxy thiophene -polystyrenesulfonate (PEDOT:PSS) as a hole injection layer(HIL); Bis[(1-naphthyl)-N-phenyl]benzidine (α-NPD) as a hole transport layer(HTL); 4,4'-N,N'-dicarbazole-biphenyl (CBP) doped with Ir(ppy)$_3$ as an emission layer(EML); a 2-(4-Biphenylyl)-5-(4-tert-butylphenyl-1,3,4-oxadiazole) (Bu-PBD) as an electron transport layer(ETL). The characteristic values of organic materials in this work are taken from literature. Tabel 1 is the characteristic value of organic materials. Fig. 1 is a schematic diagram illustrating the multilayer structure for PHOLEDs under this work [7-9].

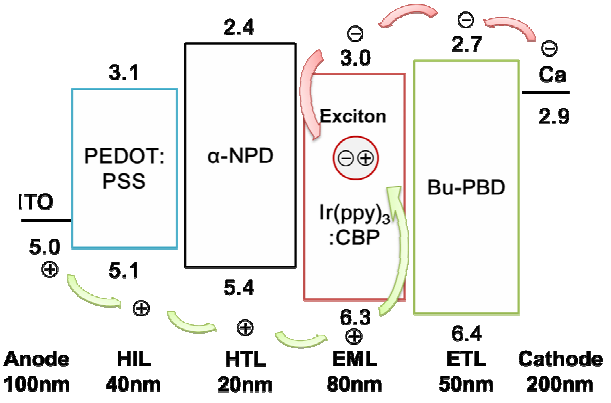

Fig. 1. Schematic diagram illustrating the multilayer structure under this study.

Table 1. The characteristic value of organic materials

Materials	E_e (kV/cm)	μ_e (cm^2/Vs)	E_h (kV/cm)	μ_h (cm^2/Vs)
a-NPD	152	10^{-9}	152	2.9×10^{-4}
Ir(ppy)3 : CBP (8wt%)	87	1.2×10^{-8}	158	2.3×10^{-8}
Bu-PBD	354	3.7×10^{-6}	354	1×10^{-9}

III. Simulation Results

Referring to Figs. 2(a) and (b), we can see how the density of carriers change as time continues. We choose cutting-off the time as 10 μs to show the moment that the electron penetrate into CBP layer. Fig. 2(a) shows the hole density and Fig. 2(b) shows the electron density in transient-state (10 μs). It is shown that hole density increase monotonously at the HTL/EML interface in Fig. 2(a). In Fig. 2(b), we can observe the behavior of electrons. Electrons are accumulated at the Cathode/ETL interface and penetrate through ETL from 0 μs to 2 μs. After that, the accumulated electrons at the ETL/EML interface penetrate through EML and gradually move toward EML/HTL interface. We think that the slow movement of electrons is affected by lower electron mobility in EML. It is known that the mobility of the $Ir(ppy)_3$-doped CBP films was nearly four orders of magnitude lower than that for a non-doped CBP film. By looking at the behavior of electrons and holes, we can expect that the recombination take place at the EML/HTL interface. As shown in Fig. 3, the recombination mainly takes place at the EML/HTL interface after 8 μs. If longer time is given, the amount of recombination increases exponentially [7].

Fig. 4 is a plot in case when the energy level of cathode has been changed. Keeping the energy level of the other layers unaltered, we varied the energy level of cathode from 2.7 eV to 3.1 eV. The recombination density reaches its peak when the work function of cathode is 2.9 eV. After a sufficient period of time, the vertical scales of Fig. 4 increase exponentially and reach those of Fig. 5. This result can be understood as an effect of the charge balance. Fig. 5 shows optical energy distribution for the variation of refractive index of substrate from 1.4 to 2. As the refractive index of substrate is increased, substrate-guided intensity is increased while guided-mode intensity is reduced.

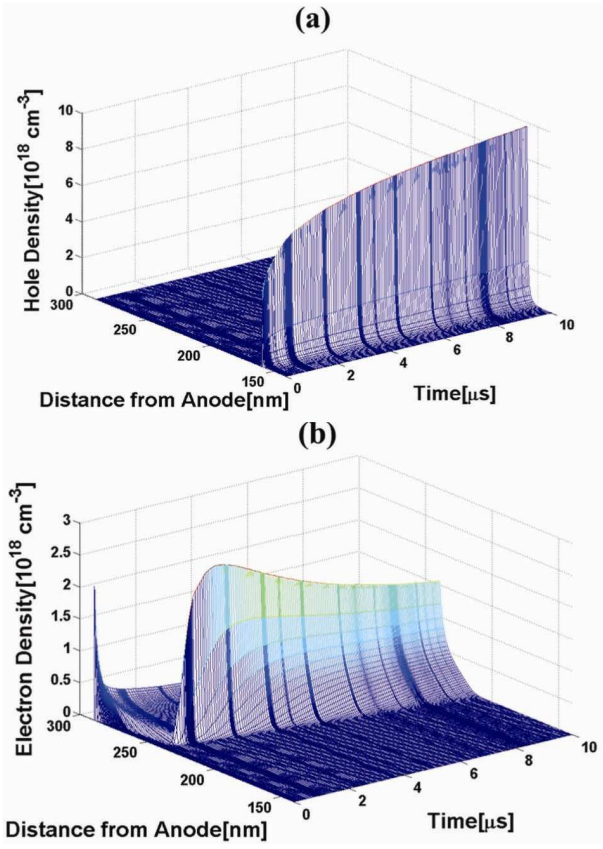

Fig. 2. (a) Calculated hole density profile in OLED after turn-on[10 μs], (b) Calculated electron density profile in OLED after turn-on[10 μs].

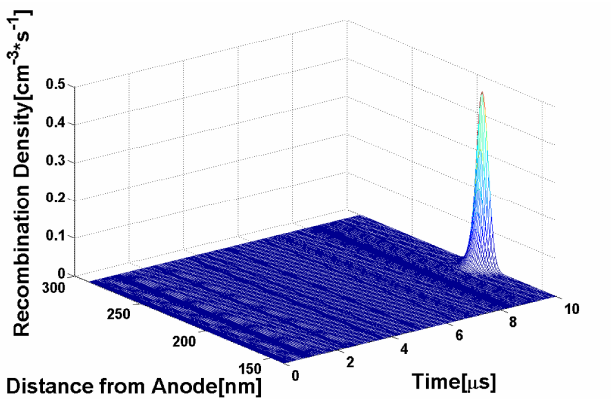

Fig. 3. Calculated recombination density profile in OLED after turn-on[10 μs].

According to reference [4], it is difficult to make use of waveguide mode for the purpose of the enhancement of out-coupling efficiency because of light absorption in organic layers. However, substrate mode can use to take the light out of the device structure. As a result, we speculate that the refractive index of 1.8 will improve the out-coupling efficiency of devices through several

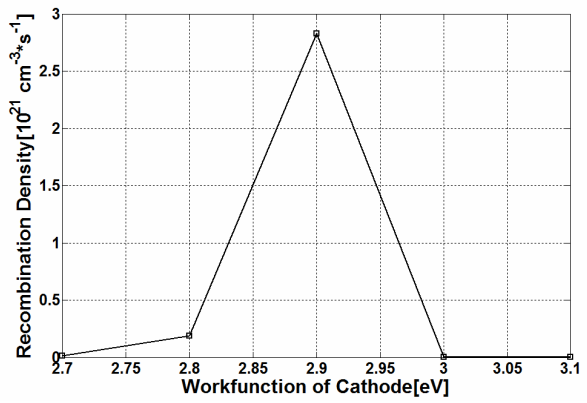

Fig. 4. Calculated recombination density profile for different work function of cathode.

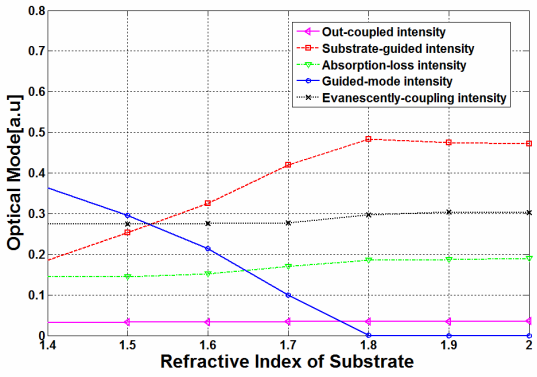

Fig. 5. Optical energy distribution as a function of the refractive index of substrate.

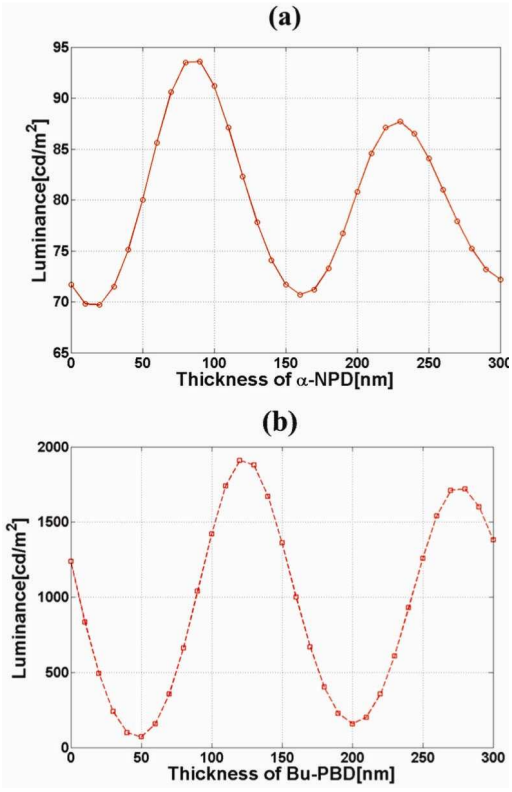

Fig. 6. (a) Luminance as a function of thickness of α-NPD, (b) Luminance as a function of thickness of Bu-PBD.

methods such as micro lens and light scattering medium.

Figs. 6(a) and (b) are plots of the luminance property when the thicknesses of ETL and HTL have been changed, respectively. As shown in Fig. 6(a), Bu-PBD is fixed on 50 nm, α-NPD has been changed from 0 to 300 nm. We can observe the luminance of device is maximum value when α-NPD is at 90 nm. Likewise, keeping the thickness of α-NPD fixed on 20 nm, we varied the Bu-PBD from 0 to 300 nm in Fig. 6(b). The device has maximum luminance when Bu-PBD is at 120 nm. This phenomenon is due to micro-cavity effect. The microcavity effect is formed by reflecting faces on the two sides of devices and governed by Eq. (6). φ is the emission intensity, L_{cav} the length of cavity, λ the wavelength in vacuum, $\overline{n}$ the refractive index in cavity [10].

$$\phi = 2\pi \frac{\overline{n} L_{cav}}{\lambda} \tag{8}$$

IV. CONCLUSIONS

We report our theoretical study on the electrical and optical properties in multilayer phosphorescent organic light emitting diode (PHOLEDs) device structure. The physical model covers the Poisson equation accounting for the behavior of charge carrier and the exciton model including generation, diffusion, and energy transfer. And optical model covers the dipole moment equation and microcavity effect. We could observe the moment of carrier in OLED devices. Furthermore, we could demonstrate that thickness of each layer and refractive index of substrate has a strong effect on the optical properties.

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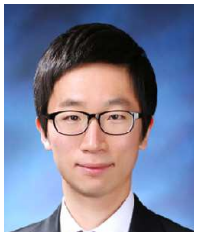

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