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Finite Element Study on the Micro-cavity Effect in OLED Devices

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***Abstract*—In this paper, we discuss on the optimal design scheme of the bilayer OLED (Organic Light Emitting Diodes) with micro-cavity structure. We carried out the optical simulation on the OLED device and calculated optimal scale of devices with taking the micro-cavity effect into account. Our emission model is based upon an ensemble of radiating dipole antennas. Consequently, we applied Maxwell's equation to this sequence, followed by the analysis on the electrical behaviors of OLED device using Poisson's equation. It contains carrier injection and transportation mechanism. In this process, we found out the thickness of each layer can affect the recombination rate at the emission layer. Therefore, we optimized the thickness of each layer to improve the efficiency of the device.**

***Index Terms*—Numerical analysis, OLED, microcavity**

I. INTRODUCTION

In OLED industry, improving external quantum efficiency (EQE) is crucial. There are many sort of method to maximize external quantum efficiency. From among these, we focused on micro-cavity effect which is resonance effect between reflect layer and semi-reflect layer.

In this work, we investigated OLED devices with numerical method. The OLED device structure is composed of an organic electro-luminescent layer stuck between two metal electrodes. We carried out a finite element method to solve mechanism in OLED devices such as charge injection, transport and recombination, exciton diffusion, transfer and decay. Thereby, we can understand that how electrical characteristics are affected by thickness of each layer. Also our model contains out-coupled luminescence which is numerically calculated as a function of whole path of the light pass through in the OLED device. In this way, we could simulate electrically optimized structure of OLED device with micro-cavity structure, too.

II. EXPERIMENTS AND DISCUSSION

1. Device Structure

We used S-TAD for the hole transport layer (HTL) and Alq3 for the electron transport layer (ETL). We inserted the emission layer (EML), which is composed of S-DPVBi, between HTL and ETL. The work function of the anode is assumed to be 5.2 eV while that of the cathode is 3.3 eV [1]. Electrons are injected into the ETL and transferred to the EML. Holes are injected into the HTL and transferred to the EML as well. When carriers arrive at the emission layer, they recombine and generate excitons in the emission layer. As these excitons diffuse and emit in the EML. The structure and mechanism are depicted in Fig. 1.

We chose five types of OLED devices. Device A is a reference device with 42.5 nm length of HTL, 15nm length of EML and 45 nm length of ETL. We varied the thickness of the HTL of Device A to 20 nm and 65 nm,

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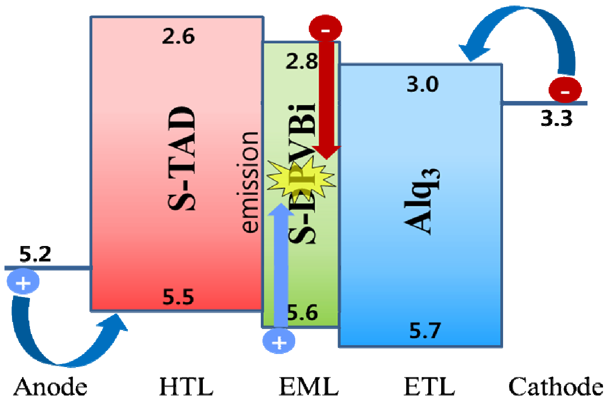


Fig. 1. Model structure and emission mechanism.

Table 1. Five types of OLED devices

	HTL(nm)	EML(nm)	ETL(nm)
Device A	42.5	15	45
Device B	20	15	45
Device C	65	15	45
Device D	42.5	15	20
Device E	42.5	15	65

which are designated as Device B and C, respectively. In addition, we also varied the thickness of the ETL of Device A to 20 nm and 65 nm, which are designated as Device D and Device E. Five types of devices are listed in Table 1.

2. Numerical Model

For investigating the behaviors of carriers in organic light emitting diodes (OLEDs), we conducted a numerical study using finite element method. Our model includes Poisson's equation for carrier injection and transportation in OLED devices. Poisson's equation is

$$\frac{\partial E(x)}{\partial x} = \frac{q}{\varepsilon\varepsilon_o}(p(x) - n(x)) \tag{1}$$

Traditional drift-diffusion equations explain charge transport mechanism in OLED [1]. The carrier densitiy in poisson's equation contains both trapped charge in interface of layers and flowing charge through whole device. The current density is composed of drift current caused by electric field and diffusion current which can occur because of carrier density. The continuity equations for carriers are written as follow [1].

Drift-Diffusion equation:

$$J_n(x) = q\mu_n n(x)E(x) + D_n \frac{\partial n(x)}{\partial x} \tag{2}$$

$$J_p(x) = q\mu_p p(x)E(x) + D_p \frac{\partial p(x)}{\partial x} \tag{3}$$

Continuity equation:

$$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla J_n - R(n,p) - \frac{\partial n_t}{\partial t} \tag{4}$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q}\nabla J_p - R(n,p) - \frac{\partial p_t}{\partial t} \tag{5}$$

J_n is current density due to electron transfer and J_p is current density caused by hole movement. n_t and p_t is trapped carrier. R is recombination rate of electron and hole. The trapped carrier's continuity equation is

$$\frac{\partial n_t}{\partial t} = r_c n(N_t - n_t) - r_e n_t \tag{6}$$

$$\frac{\partial p_t}{\partial t} = r_c p(N_t - p_t) - r_e p_t \tag{7}$$

r_c, N_t, r_e are the capture rate, the trap density and the emission rate, respectively. In our numerical study, we included the generation, transport and decay of exciton. The exciton continuity equation represents exciton which is constantly radiated before decayied or transferring it's energy to other exciton [1].

$$\frac{\partial S_i(x,t)}{\partial t} = G_i R(x,t) + \nabla\overrightarrow{J_{S_i}}(x,t) - (k_{rad_i}(x,t) + k_{nonrad_i}) \times S_i(x,t) - k_{annihilation_i} \cdot S_i(x,t)^2 + \sum_{j=1}^{n_{exc}} (k_{ji} \cdot S_j(x,t) - k_{ij} \cdot S_i(x,t)) \tag{8}$$

G_i is a constant for generation efficiency, k_{radi} is radiative decay rate, is $k_{nonradi}$ non-radiative decay rate and kannihilationi is an annihilation rate.

We considered emission model as an ensemble of radiating dipole antennas. The dynamics of the oscillating dipole moment is described as the Eq. (9). ω

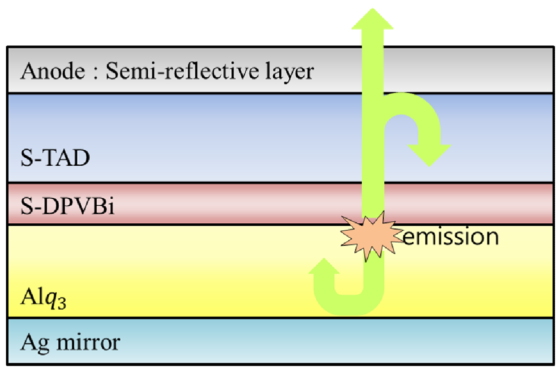


Fig. 2. Emission model structure.

is the oscillator frequency [1].

$$\frac{d^2}{dt^2}\vec{p}+b_0\frac{d\vec{p}}{dt}+\omega^2\vec{p}=\frac{e^2}{m}\overrightarrow{E_R}(\omega) \qquad (9)$$

Also, we performed optical analysis on tri-layer OLED which is inserted between reflective layer and semi-reflective layer. This structure is depicted in Fig. 2. In this structure, the light passes through each layer and experiences the reflection at the two reflecting layers. For certain width of the device, this structure can exhibit the resonance effect, which is called as microcavity-structure [2, 3]. When the resonance occurs in the microcavity structure, the resonance condition of the Eq. (10) is satisfied [3, 4].

$$\frac{2L}{\lambda_{\max}}+\frac{\Phi}{2\pi}=m \qquad \text{(m: integer)} \qquad (10)$$

$\lambda_{\max}$ is the peak wavelength of light, L is the optical path length, and Φ is the sum of the phase shift resulted from the reflection.

IV. Simulation Results

1. Steady State Analysis

Fig. 3(a) shows the distribution of the charge density for Devices A, B, and C. Electrons and holes are accumulated mainly at the interface of each layer. Particularly, most carriers are concentrated at the boundary between the emission layer (EML) and the electron transfer layer (ETL). These aspects are similar to

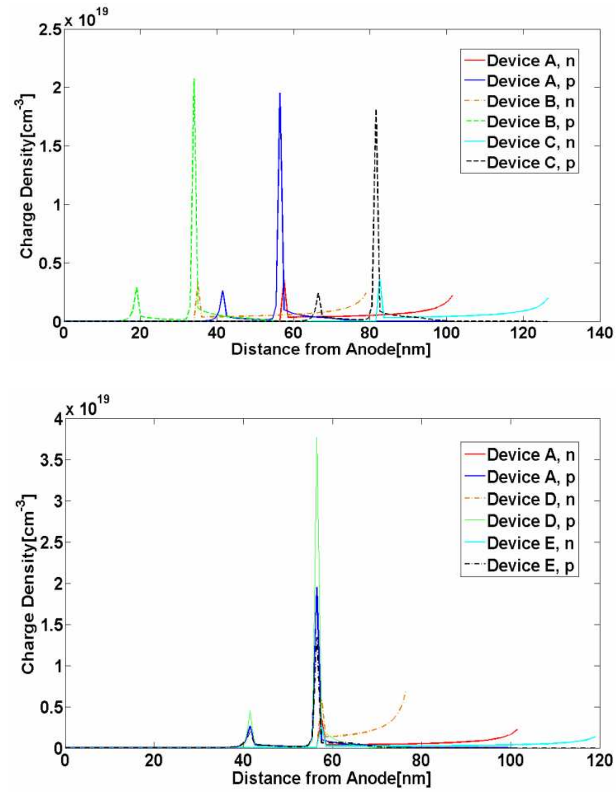


Fig. 3. (a) Charge density of Device A, Device B and Device C as a function of distance from anode, (b) Charge density of Device A, Device D and Device E as a function of distance from anode.

experimental results represented in reference [4]. We can recognize that the charge density slightly decreases as the HTL gets thicker. Consequently, we can see that the amount of the carriers is the most in Device B, as shown in Fig. 3(a).

Fig. 3(b) represents the distribution of the charge density for Devices A, D, and E. In this case, the aspect of result is similar to those shown in Fig. 3(a). As the ETL becomes thicker, the charge density diminishes. The degree of the reduction is more significant than the case shown in Fig. 3(a), which seems to be due to the fact the electron mobility is smaller than the hole mobility in this device [4, 5]. Because the thicknesses of the HTL in Devices A, D, and E are the same, the location where carriers are accumulated is identical.

Fig. 4 shows recombination rate of our entire models, Device A to E. Basically, because existence of both hole and electron is necessary to recombination, it can occur at the position where accumulated electrons are overlaped with accumulated holes. The quantity of

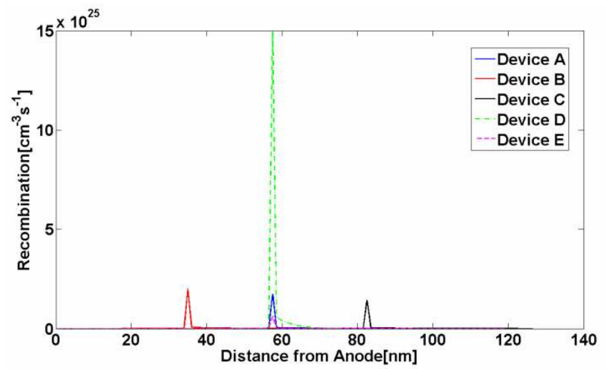


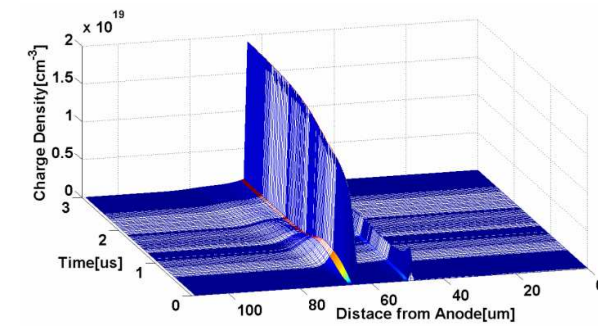
Fig. 4. Recombination rate of each device.

carriers are related to recombination rate. Accordingly, the amount of the recombination rate is the most in the Device D.

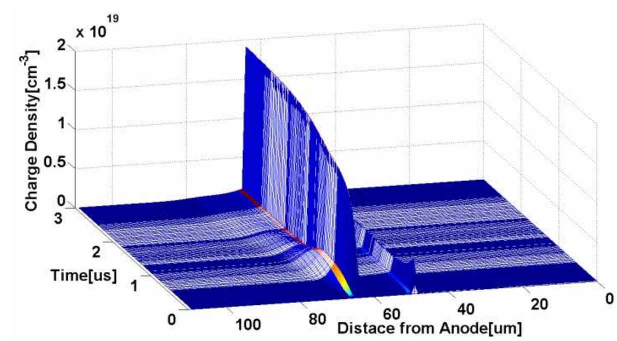
2. Transient Analysis

Figs. 5(a) and (b) are Transient profiles of hole density and electron density, respectively. When we consider this figure, we can confirm the thing that hole mobility is faster than electron mobility. In the beginning after turn on, hole density pass through the interface between emission layer and electron transfer layer. Because hole density is transfered farther distances while same time, it is first evidence of the fact that hole mobility is faster than electron mobility in this device.

In the Fig. 5(b), some elecrons are accumulated elecron transfer layer, whereas there is almost no hole density in hole transfer layer except interface. It is also evidence of the fact that hole mobility is faster than electron mobility in this device. We can confirm the transient response and the carrier mobility of materials in the reference [5].



(a)



(b)

Fig. 5. (a) Transient profile of hole density, (b) Transient profile of electron density.

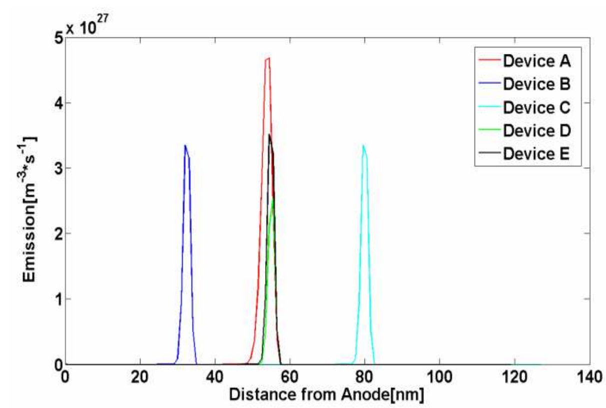


Fig. 6. Emission profiles of Device A to E.

3. Optical Analysis

In steady state analysis, we checked the fact that the thinner width of each layers, the more recombination occur. However, the thinner width of each layers is not always a great help to external quantum efficiency. Since we must consider the microcavity effect refered in numerical model section. It is represented in Fig. 6. Althogh Device B and Device D have an thinner thickness than Device A, and they have much more recombination rate, they are emitted less brightly. These results are minutely described by experimental data concerning thickness dependance of OLED is represented in reference [6]. If we want to get the most efficient OLED device, it is necessary to satisfy Eq. (10) for OLED device. Fig. 7 is simulation results of luminance with various thickness of hole transfer layer and electron transfer layer. The maximum value is the top of first peak. As we see previously, change of ETL has an more striking effect on recombination rate than those of

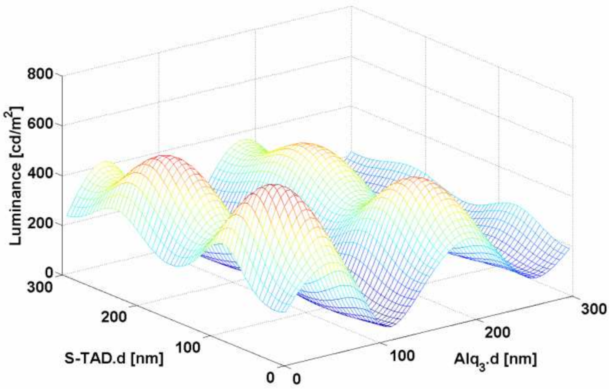


Fig. 7. Emission profiles of Device A to E.

HTL. This is inferred after comparing second peak value of both sides.

V. CONCLUSIONS

We report our numerical study on the OLED structure based on Alq_3, S-TAD and S-DPVBi. In this work, we found that the thickness of each layer can impact an appreciable effect on the external quantum efficiency. The recombination rate is affected by the thickness of each layer comprising the OLED structure and the amount of emission is determined by the whole thickness of the OLED structure due to micro-cavity effect which is observed in between the total reflection layer and the half reflection layer [7]. Our numerical solver enables us to optimize the OLED structure and thereby improve the external quantum efficiency. In Fig. 7, the optimized thicknesses of this device are 40nm of ETL and 60nm of HTL. We demonstrate that luminance of device improves as 7.3% compared with those of Device A.

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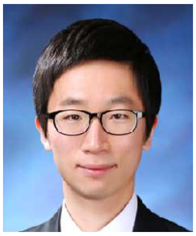

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