Electromagnetic Modeling of Organic Light-Emitting Devices

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Abstract—Based on the rigorous electromagnetic wave theory, a numerical model for simulating the radiation characteristics of organic light-emitting devices (OLEDs) is developed. In particular, a novel method for overcoming the numerical difficulty in taking the thick glass substrate into account is proposed. The numerical results confirm the importance of the effects of the thick glass substrate. The algorithms based on the numerical model are then used for evaluating the dependencies of OLED radiation characteristics on various parameters, including the thickness of different device layers and the cathode metal variety. In the study of the effect of emission layer (EML) thickness, it is found that the radiation spectral peak red shifts with increasing EML thickness. This trend is consistent with the experimental result.

Index Terms—Organic light-emitting device (OLED), simulation.

I. INTRODUCTION

ORGANIC light-emitting devices (OLEDs) have attracted much attention because of their advantages such as low-power consumption, high brightness, high contrast, and low cost [1], [2]. Conventional OLEDs are fabricated on glass substrates of several hundred micrometers in thickness. In a typical device, an indium–tin–oxide (ITO) anode, several organic layers, and a metal cathode are deposited on the glass substrate. The thickness of each layer is in the range of several tens of nanometers. Electroluminescence (EL) is generated from the organic layers and coupled out of the device from the ITO side. Because the total thickness of the organic layers is comparable to the wavelength, the reflections at various interfaces lead to significant interference effects. By varying the thickness of the organic layers, the external quantum efficiency, output spectrum, and viewing angle are significantly changed [3], [4]. To understand the optical characteristics of an OLED, a simulation of the EL wave propagation in such a device is very important [5]. Although the scattering and transmission matrix formulations can be used to successfully simulate the

Fig. 1. Schematic illustration of a typical OLED structure.

light propagation properties of organic photovoltaic devices [6], [7], they cannot be directly applied to OLEDs because an OLED uses a thick glass substrate, which results in computational difficulty. In addition, although in the top-emission OLED configuration, the simulation results could be easily obtained without considering the thick glass substrate [8], [9], the effect of the thick glass substrate needs to be considered in a bottom-emission OLED. Electromagnetic wave propagation in stratified media has long been an important classical problem [10], [11]; however, it is still a difficult task to rigorously evaluate the radiation in a bottom-emission device. Recently, radiation from a dipole embedded in a dielectric slab was analytically treated [12]. In this treatment, both radiated and guided powers were investigated.

In this research, we develop a rigorous and efficient numerical method to simulate the radiation characteristics of an OLED. In particular, we intend to overcome the numerical difficulty due to the thick glass layer. To reach this goal, we first neglect the air region, and assume a semi-infinitely thick glass layer. In this situation, the wave field distribution in the glass layer can be computed using the saddle-point method [13]. Then, the air region is taken into account in the practical device design. An incident wave is multiply reflected and transmitted into the air region to give the output radiation. The obtained field distribution in the glass layer with the last assumption is used for the whole device simulation. Because the development of our numerical algorithms is based on the general electromagnetic theory, the proposed method is, in principle, applicable to an OLED consisting of any number of layers. For a dipole source operating at a single frequency, strong interference of the coherent fields reflected from interfaces between layers results in a rapidly oscillatory radiation pattern. However, in

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TABLE I
OLED PARAMETERS USED FOR SIMULATION

Parameter	Symbol	Value	Unit
Refractive index of the air region	n_1	1	
Refractive index of the glass layer	n_2	1.48	
Refractive index of the ITO (indium-tin oxide) layer	n_3	1.8	
Refractive index of the HTL (hole-transport layer)	n_4	1.7	
Refractive index of the EML (emission layer)	n_5	1.8	
Refractive index of the ETL (electron-transport layer)	n_6	1.7	
Refractive index of the metal cathode	n_{Metal}	$\sqrt{\epsilon_{Metal}}$	
Position of dipole sources	z_0	0.23	μm
Lower boundary of the ETL	z_6	0	μm
Lower boundary of the EML	z_5	0.2	μm
Lower boundary of the HTL	z_4	0.23	μm
Lower boundary of the ITO layer	z_3	0.39	μm
Lower boundary of the glass layer	z_2	0.475	μm
Lower boundary of the air region	z_1	850.475	μm

reality, light emission from a dipole source should have a finite bandwidth. Hence, the interference effect will be smoothened. In our calculations, the resultant radiation field is obtained by coherently averaging the fields over a spectral range. In this paper, the theoretical formulations are given in Section II. The numerical results and related discussions are presented in Section III. Finally, conclusions are drawn in Section IV.

II. THEORETICAL FORMULATIONS

Consider an OLED with a seven-layer structure, as schematically shown in Fig. 1. The device parameters are listed in Table I. Although our theoretical model is applicable to any multilayer structure, the following derivations are based on a seven-layer device. We first solve the governing equation for the electric Hertzian vector potential $\vec{\Pi}$, which is due to a vertical or horizontal dipole embedded in the emission layer (EML) and near the upper boundary of the layer. Then, with the $e^{j\omega t}$ time-harmonic dependence, the electric and magnetic fields can be evaluated through the following expressions [13]:

$$\begin{aligned}\vec{E} &= \nabla (\nabla \cdot \vec{\Pi}) + k_0^2 n^2 \vec{\Pi} \\ \vec{H} &= j\omega \epsilon_0 n^2 \nabla \times \vec{\Pi}.\end{aligned}\quad (1)$$

Here, n is the complex refractive index ($n = n_i$ in the i th layer) and $k_0 = \omega \sqrt{\mu_0 \epsilon_0} = 2\pi/\lambda$ is the wave number or propagation constant in vacuum.

The equation governing $\vec{\Pi}$ can be derived as

$$(\nabla^2 + k_0^2 n_5^2) \vec{\Pi}(\vec{r}) = \frac{-\vec{p} \delta(\vec{r} - \vec{r}')}{\epsilon_0 n_5^2} \quad (2)$$

in the fifth EML, and

$$(\nabla^2 + k_0^2 n_i^2) \vec{\Pi}(\vec{r}) = 0 \quad (3)$$

in the i th nonemission layer. Here, $\vec{p}$ denotes a dipole moment located at $\vec{r}'$. We employ the property of axial symmetry and take the Fourier–Bessel transform to obtain an integral expression for the Hertzian vector potential in each layer. The boundary conditions include the continuity of the tangential electric and magnetic fields across each boundary. Using the boundary conditions at each interface, we can determine the unknown coefficients in the integral expression of $\vec{\Pi}$. With this procedure, all the field components can be evaluated through (1).

To be specific, we first consider a vertical dipole source with its moment $\vec{p} = \hat{z}p$ located at $\rho = 0$ and $z = z_0$ in the fifth EML. After some mathematical manipulations, the Hertzian vector potential $\vec{\Pi}_i$ in the i th region can be derived as

$$\vec{\Pi}_1(\rho, z) = \hat{z} \frac{jp}{4\pi\epsilon_0 n_5^2} \int_0^\infty T_{1b}(\alpha) J_0(\alpha\rho) e^{-j\tau_1(z-z_1)} \alpha d\alpha \quad (4)$$

in the air region

$$\begin{aligned}\vec{\Pi}_i(\rho, z) = \hat{z} \frac{jp}{4\pi\epsilon_0 n_5^2} \int_0^\infty & \left[T_{ia}(\alpha) e^{j\tau_i(z-z_i)} \right. \\ & \left. + T_{ib}(\alpha) e^{-j\tau_i(z-z_i)} \right] J_0(\alpha\rho) \alpha d\alpha \quad (5)\end{aligned}$$

in the i th ($i = 2, 3, 4, 6$) layer

$$\vec{\Pi}_5(\rho, z) = \hat{z} \frac{j p}{4\pi\epsilon_0 n_5^2} \int_0^\infty \left[T_{5a}(\alpha) e^{j\tau_5(z-z_5)} + T_{5b}(\alpha) e^{-j\tau_5(z-z_5)} - \frac{1}{\tau_5} e^{-j\tau_5|z-z_0|} \right] J_0(\alpha\rho) \alpha d\alpha \quad (6)$$

in the fifth EML, and

$$\vec{\Pi}_7(\rho, z) = \hat{z} \frac{j p}{4\pi\epsilon_0 n_5^2} \int_0^\infty T_{7a}(\alpha) J_0(\alpha\rho) e^{j\tau_7(z-z_6)} \alpha d\alpha \quad (7)$$

in the metal layer. Here, J_0 is the first-kind Bessel function of zeroth order, $T_{ia}(\alpha)$ and $T_{ib}(\alpha)$ are the expansion coefficients to be determined, $\tau_i = (k_0^2 n_i^2 - \alpha^2)^{1/2}$, and z_i is the z -coordinate of the lower boundary in the i th layer. Note that only the outgoing waves exist in the air and the cathode regions.

By using the boundary conditions for the continuities of the tangential electric and magnetic fields across all the boundaries between different layers, we can derive the algebraic equations for the expansion coefficients $T_{ia}(\alpha)$ and $T_{ib}(\alpha)$. After solving these equations, the Hertzian vector potential and hence the electric and magnetic fields in all regions can then be calculated accordingly.

Now, we consider the radiation characteristics from a horizontal dipole with the dipole moment $\vec{p} = \hat{x}p$ located at $\rho = 0$ and $z = z_0$ in the EML. We again employ the Hertzian vector potential $\vec{\Pi} = (\hat{x}\Pi_x + \hat{z}\Pi_z)$, which satisfies the Helmholtz (2) and (3). Note that both the x - and z -components of the Hertzian vector potential are needed for all the electromagnetic fields to satisfy Maxwell's equations and the boundary conditions [13].

Using the derivation procedures similar to the case of a vertical dipole, we can derive the representation of $\vec{\Pi}_i(\rho, \phi, z)$ in the i th region as

$$\vec{\Pi}_1(\rho, \phi, z) = \hat{x} \frac{j p}{4\pi\epsilon_0 n_5^2} \int_0^\infty U_{1b}(\alpha) J_0(\alpha\rho) e^{-j\tau_1(z-z_1)} \alpha d\alpha + \hat{z} \frac{j p \cos \phi}{4\pi\epsilon_0 n_5^2} \int_0^\infty A_{1b}(\alpha) J_1(\alpha\rho) e^{-j\tau_1(z-z_1)} \alpha^2 d\alpha \quad (8)$$

in the air region

$$\begin{aligned} \vec{\Pi}_i(\rho, \phi, z) &= \hat{x} \frac{j p}{4\pi\epsilon_0 n_5^2} \int_0^\infty \left[U_{ia}(\alpha) e^{j\tau_i(z-z_i)} + U_{ib}(\alpha) e^{-j\tau_i(z-z_i)} \right] \\ &\quad \times J_0(\alpha\rho) \alpha d\alpha + \hat{z} \frac{j p \cos \phi}{4\pi\epsilon_0 n_5^2} \\ &\quad \times \int_0^\infty \left[A_{ia}(\alpha) e^{j\tau_i(z-z_i)} + A_{ib}(\alpha) e^{-j\tau_i(z-z_i)} \right] J_1(\alpha\rho) \alpha^2 d\alpha \end{aligned} \quad (9)$$

in the i th ($i = 2, 3, 4, 6$) layer

$$\begin{aligned} \vec{\Pi}_5(\rho, \phi, z) &= \hat{x} \frac{j p}{4\pi\epsilon_0 n_5^2} \int_0^\infty \left[U_{5a}(\alpha) e^{j\tau_5(z-z_5)} + U_{5b}(\alpha) e^{-j\tau_5(z-z_5)} \right. \\ &\quad \left. - \frac{1}{\tau_5} e^{-j\tau_5|z-z_0|} \right] J_0(\alpha\rho) \alpha d\alpha + \hat{z} \frac{j p \cos \phi}{4\pi\epsilon_0 n_5^2} \\ &\quad \times \int_0^\infty \left[A_{5a}(\alpha) e^{j\tau_5(z-z_5)} + A_{5b}(\alpha) e^{-j\tau_5(z-z_5)} \right] J_1(\alpha\rho) \alpha^2 d\alpha \end{aligned} \quad (10)$$

in the fifth EML, and

$$\begin{aligned} \vec{\Pi}_7(\rho, \phi, z) &= \hat{x} \frac{j p}{4\pi\epsilon_0 n_5^2} \int_0^\infty U_{7a}(\alpha) J_0(\alpha\rho) e^{j\tau_7(z-z_6)} \alpha d\alpha \\ &\quad + \hat{z} \frac{j p \cos \phi}{4\pi\epsilon_0 n_5^2} \int_0^\infty A_{7a}(\alpha) J_1(\alpha\rho) e^{j\tau_7(z-z_6)} \alpha^2 d\alpha \end{aligned} \quad (11)$$

in the metal layer. Here, the dependence of the azimuth angle ϕ is explicitly presented. The expansion coefficients $U_{ia}(\alpha)$, $U_{ib}(\alpha)$, $A_{ia}(\alpha)$, and $A_{ib}(\alpha)$ can be obtained by solving the simultaneous algebraic equations derived from the boundary conditions.

In computing the radiation fields in the air region, we employ the method of saddle point for integrating with respect to α . However, because the thickness of the glass layer is usually much larger than the wavelength (by several hundred times), we cannot separate the slowly varying and the fast-varying terms in the expressions of $T_{ia}(\alpha)$, $T_{ib}(\alpha)$, $U_{ia}(\alpha)$, $U_{ib}(\alpha)$, $A_{ia}(\alpha)$, and $A_{ib}(\alpha)$ in using the saddle-point method. To overcome this difficulty, we first assume that the glass layer is semi-infinitely thick. With the new six-layer structure, we employ the saddle-point method to determine the mathematical expression for the radiation field $E_{\text{glass}}(\rho, z)$ at the original interface between the air region and the glass layer. Based on this idea, the following formula for the saddle-point method can be readily used:

$$\int_{-\infty}^{\infty} f(\alpha) e^{-j\alpha\rho - j\tau_2(z-z_2)} d\alpha \approx f(k_0 n_2 \sin \theta_{\text{glass}}) \sqrt{\frac{2\pi}{k_0 n_2 R_2}} \cdot k_0 n_2 \cos \theta_{\text{glass}} \cdot e^{-jk_0 n_2 R_2 + j\frac{\pi}{4}} \quad (12)$$

Here, $R_2 = (\rho^2 + (z - z_2)^2)^{1/2}$, θ_{glass} is the zenithal angle, and (ρ, z) represents an observation point on the original interface between the air region and the glass layer.

After obtaining the aforementioned results, we put the air region back to the device structure. Now, the $E_{\text{glass}}(\rho, z)$ field becomes an incident field onto the glass/air interface. It will propagate in the glass layer subject to multiple reflections and transmissions, as schematically shown in Fig. 2(a) and (b) for the parallel and perpendicular polarization components, respectively.

Fig. 2. (a) Parallelly and (b) perpendicularly polarized wave multiply reflected and transmitted in the glass layer.

Employing the electromagnetic theory with matrix multiplication enables us to evaluate the effective impedance η_{eff} of the multilayer structure at a location below the glass layer. Let us first use the Fresnel formulas to evaluate the reflection coefficient Γ_2 from the glass layer to the rest multilayer structure and the reflection coefficient Γ_1 and transmission coefficient T_1 from the glass layer to the air region. We can then determine the effective transmission coefficient T_{eff} for $E_{\text{glass}}(\rho, z)$ to transmit into the air region in the form

$$T_{\text{eff}} = \frac{T_1}{1 - \Gamma_1 \Gamma_2 e^{-2jk_0 n_{\text{glass}} d_{\text{glass}} \sec(\theta_{\text{glass}})}}. \quad (13)$$

Here, n_{glass} and d_{glass} are the refractive index and the thickness of the glass layer, respectively. Note that the two polarization components (parallel and perpendicular) with different reflection (Γ_2, Γ_1) and transmission (T_1) coefficients should be treated separately.

In fact, the radiated field in the glass layer $E_{\text{glass}}(\rho, z)$ is not a plane wave but a spreading beam wave. Using the principle of energy conservation and Snell's law [14], we can derive the spreading factor as

$$S = \left[\frac{\cos \theta_{\text{glass}}}{\cos \theta_{\text{air}}} \right]^2 \frac{\sqrt{\cos \theta_{\text{air}}}}{\sqrt[4]{1 - \left(\frac{n_{\text{air}}}{n_{\text{glass}}} \sin \theta_{\text{air}} \right)^2}}. \quad (14)$$

Here, θ_{glass} is the incident angle, and θ_{air} is the refractive angle from the glass layer to the air region. Therefore, the radiation field for each polarization due to a vertical or horizontal dipole source embedded in the EML can finally be expressed in the following form:

$$E_{\text{air}} = E_{\text{glass}} \cdot T_{\text{eff}} \cdot S. \quad (15)$$

A light wave cannot be emitted by an electric dipole of an infinitely long coherent time (i.e., of an infinitesimal bandwidth). In our calculations, we assume that a dipole source emits a spectrum of finite spectral width ($\lambda_0 - \Delta\lambda, \lambda_0 + \Delta\lambda$). The spectral width is determined by the material property of an OLED. Here, we coherently average the radiated fields over the spectral range ($2\Delta\lambda$) of 0.5 nm.

To simulate a real device, we consider the radiation from a set of randomly oriented dipole sources embedded in the EML. The number of dipoles used is 10^5 . For each dipole oriented in the direction (θ_r, ϕ_r) , it is decomposed into a vertical component and a horizontal component, from which the radiation can be individually calculated. Here, the random variable θ_r is uniformly distributed between 0 and π , and the random variable ϕ_r is uniformly distributed between 0 and 2π . We generate random samples of dipole orientation and calculate the incoherent summation of their radiation contributions to give the output of the considered OLED.

III. NUMERICAL RESULTS AND DISCUSSIONS

In this section, we demonstrate and discuss the numerical results based on the formulations in the previous section. Most simulation parameters are listed in Table I, unless specified otherwise. In Fig. 3(a) and (b), we show the radiation spectrum by varying the thickness of the glass layer from 0.5 to 850 μm . Here, the assumed photoluminescence (PL) spectrum of the EML layer is plotted as the dot-dashed curve. Note that the spectrum is taken in the zenithal direction, i.e., $\theta = 0$ (the same condition is used hereafter). When the glass layer is thin, as shown in Fig. 3(a), the oscillation behavior becomes more prominent as the glass layer thickness increases. To interpret this trend, we can use a simple model for estimating the free spectral range $\Delta\nu$ of the Fabry-Pérot interference fringe as

$$\Delta\nu = \frac{c}{2nd \cdot \cos \theta_i}. \quad (16)$$

Here, c is the speed of light, n is the average refractive index of device materials, d is the thickness of the effective microcavity, and θ_i is the incident angle. The free spectral ranges (in terms of wavelength) for the cases of glass thickness at 0.5, 1, and 3 μm are about 156, 78, and 26 nm (centered at 478 nm), respectively, resulting from the microcavity formed by the electron transport layer (ETL)/cathode interface and the glass/air interface. In the case of 0.5- μm glass layer thickness, the free spectral range is broader than the PL spectrum such that no Fabry-Pérot modulation can be observed. In the case of 1- μm glass layer thickness, the free spectral range is reduced to 78 nm. Hence, Fabry-Pérot modulation is shown at the spectral tails. Following this trend, strong modulation is shown in the case of 3- μm glass layer thickness, as confirmed by the corresponding curve in Fig. 3(a). On the other hand, when the glass layer is thick, i.e., up to several hundred micrometers, the free spectral range is reduced to the range of tenths of a nanometer such that the Fabry-Pérot oscillation is beyond the noticeable spectral resolution. Therefore, the three curves in Fig. 3(b) are essentially smooth. The comparison between

Fig. 3. Simulation results of the EL spectra at $\theta = 0$ with various (a) thin and (b) thick glass layer thicknesses. The assumed PL spectrum of the EML layer is plotted as the dot-dashed curve.

Fig. 3(a) and (b) indicates the importance of our simulation model. With our accurate algorithm, one can clearly see the oscillating spectrum by using a numerical model of thin glass layer. The oscillating spectrum is not observed in a real device. It is noted that the output intensity decreases with increasing glass thickness. With a thicker glass layer, the waveguiding effect becomes stronger such that the external quantum efficiency is decreased.

Fig. 4(a) and (b) shows the viewing angle dependence of radiation intensity with different glass layer thicknesses at $\lambda = 470$ nm. In Fig. 4(a), the Fabry-Pérot modulation becomes stronger as the glass thickness increases from 0.5 to 3 μm . This trend is consistent with the results in Fig. 3(a). In addition, the same trend in Fig. 3(b) can be observed in Fig. 4(b). Meanwhile, the radiation intensity variation trend is the same as that described later in the text. In addition, due to the weaker waveguiding effect in a device of thinner glass layer, its viewing angle is larger.

In the following paragraphs, we will use the built numerical model for investigating the radiation characteristics of an OLED by varying various parameters. First, in Fig. 5, we show the radiation spectra for several cathode materials. The complex dielectric constants of those metals were obtained from [15]. In Fig. 5, one can see that the spectral peak position varies among different cathode metals. It is interesting to note that the output spectra in the cases of Au, Al, and perfect electric conductor

Fig. 4. Viewing angle dependence of the radiation pattern at $\lambda = 470$ nm with various (a) thin and (b) thick glass layer thicknesses.

Fig. 5. Simulation results of normalized EL spectra at $\theta = 0$ with various cathode metals.

(PEC) as the cathode materials are almost identical. In addition, their peak intensities are about the same and are higher than those of Ag and Ni as cathode materials. The spectral peaks are located at 470, 475, and 480 nm when the cathode materials are Ni, Au, and Ag, respectively. The results shown in Fig. 5 imply that a careful selection of cathode material may help in increasing the output intensity and controlling the radiation spectrum.

Fig. 6(a) shows the normalized spectra of four devices with different EML thicknesses of 20, 30, 40, and 60 nm. It clearly shows the red-shift trend with increasing the EML thickness. For comparison, a series of OLEDs was fabricated. We used ITO-coated glass substrates of low sheet resistivity (10 Ω/sq) and small surface roughness (standard deviation < 1 nm). The size of the active region was 1×1 cm^2 . In those devices, we used N,N'-diphenyl-N,N'-bis(1-naphthyl)-1,1'-biphenyl-4,4'-diamine (NPB) as the hole transport layer (HTL) material, 4,4'-bis[2-(4-(N,N-diphenylamino)phenyl)vinyl]biphenyl (DPAVB) as the blue dopant of the EML, (9,10-bis(29-naphthyl)73 anthracene) (ADN) as the host of the EML, and tris-(8-hydroxyquinoline) aluminum (Alq3) as the ETL

Fig. 6. (a) Simulation and (b) experimental results of the normalized EL spectra at $\theta = 0$ with various EML thicknesses.

material. The doping concentration of DPAVB_i in ADN was 2% in mole ratio. The thicknesses of the HTL and ETL were kept at 160 and 200 nm, respectively. The thickness of the EML was varied at 20, 30, 40, and 60 nm. LiF of 1.2 nm in thickness was used between the ETL and the aluminum cathode for a more efficient electron injection. The thickness of the aluminum cathode was 100 nm. After organic and metal deposition, the devices were encapsulated in the glove box with the O₂ and H₂O concentrations below 1 ppm. Devices were characterized with an SR-2 photometer for the brightness measurement. The resulting spectra are shown in Fig. 6(b). The red-shift trend with increasing layer thickness shows a similar behavior to the simulation results, as shown in Fig. 6(a).

Fig. 7 shows the spectral variation with HTL thickness. The spectral peak position blue shifts from 483 to 471 nm when the HTL thickness increases from 80 to 130 nm. However, it red shifts from 471 to 483 nm when the thickness is further increased from 130 to 200 nm. Typically, when the thickness of a thin film (such as ITO, HTL, and EML) changes, the light intensity of a particular wavelength oscillates because of the interference effect [16], [17]. The blue-shift and then the red-shift trends in Fig. 7 can be attributed to the interference oscillation. Fig. 8 shows the optical intensity variations at $\lambda = 500$ nm versus the ITO, HTL, EML, and ETL thickness. The calibrated periods of the oscillatory behaviors are about 140, 145, 140, and 144 nm in varying the ITO, HTL, EML, and ETL thicknesses, respectively. These periods roughly correspond to one-half of the wavelength in the OLED materials. We

Fig. 7. Simulation results of the EL spectra at $\theta = 0$ with various HTL thicknesses.

Fig. 8. Intensities at $\lambda = 500$ nm and $\theta = 0$ as functions of the ITO, HTL, EML, and ETL thicknesses.

also note that the optical intensity oscillations in changing the EML and ETL thicknesses are stronger than those of changing the HTL and ITO thicknesses. In an OLED, the strongest single-face reflection occurs at the interface between the ETL and cathode layer. Therefore, the variation of the ETL thickness generates strong intensity oscillation. In addition, varying the EML or ETL thickness is equivalent to changing the optical path between the dipole source and the ETL/cathode interface. Such a change may strongly affect the radiation output intensity, as shown in Fig. 8.

Note that the real parts of the refractive indexes of the organic layers NPB and Alq₃ are around 1.7 to 1.8 [16], [18]. In our simulations, the real parts of the refractive indexes of these dielectric materials were set to be constants within the whole visible range, as shown in Table I. Actually, the real part of the refractive index of an organic material is dispersive and follows the Cauchy model. Such dispersion behaviors can also be considered in our simulations. Fig. 9 shows the EL spectra at $\theta = 0$ with various HTL thicknesses at 80, 130, 160, and 200 nm. The parameters used for calculations are the same as those in Fig. 7, except that the refractive indexes of NPB (for HTL) and Alq₃ (for ETL) become dispersive now.¹ One can see that the EL peaks are located at 483, 479, 479, and 483 nm for the four HTL thicknesses, respectively. Such an

¹From the Cauchy model, the refractive index of NPB is $n = 1.7118 + 0.03366/\lambda^2$ (λ in microns), and that of Alq₃ is $n = 1.6434 + 0.02533/\lambda^2$ (λ in microns) from measurements.

Fig. 9. Simulation results of the EL spectra at $\theta = 0$ with various HTL thicknesses when the dispersion behaviors are considered.

oscillatory behavior, which is due to the optical interference effect, is similar to that in Fig. 7. The slight variation in the EL peak position results from the change of optical length through the dispersion. Therefore, the dispersion does not significantly affect the output characteristics of an OLED. Hence, in our simulations, the real parts of the refractive indexes of the organic layers are set to be constants for simplifying the calculations.

Within the visible range, the imaginary parts of the refractive indexes of NPB, ADN, and DPAVB can be neglected due to their large band gaps [19]. The onset of the $\pi - \pi^*$ absorption band of Alq3 is located around 450 nm. Its absorption increases with photon energy and reaches a peak at 390 nm. However, because the primary emission spectra of OLEDs lie at longer wavelengths, as shown in Fig. 6, the absorption behavior of Alq3 should not significantly affect our simulation results. In addition, because the glass substrate is transparent and ITO is semitransparent, the absorption/gain dispersion behaviors of the used materials were neglected in our simulations. The negligence may explain the discrepancy between the simulation [Fig. 6(a)] and experimental [Fig. 6(b)] results at the short-wavelength tail. Nevertheless, the dispersive behaviors of those cathode metals [15] are important and were really taken into account in our simulations.

Other than the radiation into the free space, part of the dipole power is either trapped by the guided modes of the layered medium or absorbed by the device materials. Calculations of these powers for a dipole embedded in a dielectric slab have been carried out by Brueck [12]. However, the geometry of our problem is more complicated. In our device, we consider seven layers such that the boundary conditions at six interfaces must be matched. Analytical solutions seem impossible in our geometry. In the spectral domain of the Fourier–Bessel transform, only the numerical results of various expansion coefficients can be obtained in solving a matrix equation. Therefore, we could not take the advantage of evaluating the residues of poles in the spectral representation such that the guided power can be calculated. However, because we are interested in the radiation behaviors in the outmost air region, the use of the saddle-point approximation is a good choice. Because the feasible field computation in the air region represents one of the advantages of our numerical model, we can calculate

the total radiated power in the air region and divide it by the total radiated power of a dipole in the free space to estimate the external quantum efficiency. It is found that the external quantum efficiency is around 17% for a vertical dipole when the optimal layer thickness is used in our simulation. Although it is difficult to estimate the external quantum efficiency of a horizontal dipole, it is believed to be higher when compared with that of a vertical dipole. Therefore, if 10^5 random dipoles are averaged, the external quantum efficiency can be increased to about 25% under the optimized condition. This estimation is consistent with the value of a conventional OLED device [20].

IV. CONCLUSION

Based on the rigorous electromagnetic wave theory, we have developed a numerical model for simulating the radiation characteristics of OLEDs. In particular, we proposed a new method for overcoming the numerical difficulty of including the effects of thick glass substrate in simulating the radiation properties of an OLED. The numerical results confirmed the importance of the effects of the thick glass substrate. The algorithms based on the numerical model were then used for evaluating the dependencies of OLED radiation characteristics on various parameters, including the thickness of different device layers and the metal type used for the cathode. With regard to the effect of EML thickness, it was found that the radiation spectral peak red shifted with increasing EML thickness. This trend is consistent with the experimental result.

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