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Theoretical model for the external quantum efficiency of organic light-emitting diodes and its experimental validation

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ABSTRACT

An optical energy loss mechanism including the surface plasmon polariton (SPP) loss, wave guide (WG) mode and substrate mode in organic light-emitting diodes (OLEDs) is introduced based on CPS theory. The theoretical calculations of both the out-coupling efficiency (OCE) and the external quantum efficiency (EQE) of OLEDs are proposed. MATLAB tools are applied to simulate the optical model and provide the results of the two efficiencies. It is demonstrated that, the OCE and the EQE in a green phosphorescence OLED with optimized device structure can reach up to 20% and 27%, respectively (intrinsic quantum efficiency $q = 90\%$ assumed). The simulation results based on the theoretical model are further validated experimentally.

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1. Introduction

Organic light-emitting diodes (OLEDs) are regarded as the next generation of display and solid-state lighting techniques owing to their broad viewing-angle, fast response, low driving voltage, flexibility and so on [1–4]. Currently, they have been applied in mobile phones and other digital electronic products. Further developments towards the active full color displays, silicon–based micro-displays (OLED on Silicon, OLEDoS) [5], transparent and flexible display (FOLED) [6], and large area OLED lighting panels [7] are in progress. Luminous efficiency is one of the key performance factors in OLEDs. In phosphorescence OLEDs [8], the internal quantum efficiency (IQE) can reach to 100% theoretically. The external quantum efficiency (EQE) mainly depends on the out-coupling efficiency (OCE) which is generally less than 20% [9]. Therefore, the improvement of the OCE is very important for obtaining high-efficiency OLEDs. In the past decades, many light out-coupling techniques have been developed and some studies on the optical energy loss mechanism in OLEDs have been reported [10–22]. Most reports applied the experimental measures to improve the out-coupling efficiency but did not provide the optical loss model theoretically. Some of them mentioned the model was mentioned in some reports but no simulations were provided. Especially, few clear simulation algorithms on the optical energy loss mechanism are presented. Therefore, theoretical understanding on the optical energy loss mechanism in OLEDs is necessary to further increase the OCE and the EQE. In this work, we investigate the energy loss mechanism in OLEDs in detail using MATLAB tools for the simulation based on the CPS theory. The theoretical model, the simulation algorithms and the experimental validation were carried out simultaneously in this work.

2. CPS model

2.1. Theoretical model

According to classic electrodynamics and electromagnetic field theory, the exciton formation in OLEDs can be treated as a bound harmonically oscillating dipole (hereinafter referred to as dipole). When the exciton is very close to the metal surface, the radiation of the exciton will be affected by the metal. Due to the loss property of metal (its dielectric function is a complex number), the

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exciton will lose its energy, even be quenched. As is known, the near-field radiation of an exciton is very different from its far-field radiation. In far-field radiation, the spherical wave from the dipole can be simplified as a planar wave; however, in near-field mode, the radiation of the dipole must be calculated precisely. In order to consider the near-field effect, R. R. Chance, A. Prock and R. Silbey (CPS) investigated the interaction between fluorescent molecules and the nearby metal surface, and came up with the following model [23]

$$\frac{d^2p}{dt^2} + \omega_0^2 p = \frac{e^2}{m} E_r - b_0 \frac{dp}{dt} \tag{1}$$

where m is the mass of the dipole; e is the elementary charge. The first term denotes acceleration, in which p is the electric dipole moment of the dipole. The second term is of the elastic restoring force, in which ω_0 is its inherent oscillation frequency. The third term is of the driving force caused by reflected electric field, and E_r is the reflected radiation field acted on the dipole itself; the fourth term deals with damping, relating to the anti-force of the electromagnetic radiation. b_0 is the radiation damping rate of the dipole in free space.

In principle, the dipole radiation damping rate can be figured out in the presence of a reflecting metal surface by solving the above differential equation. The reflected electric field at the dipole position should be firstly determined. The total reflected electric field is the superposition of waves of all directions reflected by the metal surface. Sommerfeld model [24] solved the problem and got the solution in integral form via a tedious deduction based on classic electrodynamics. The nature behind is that the near-field radiation is different from the far-field radiation. The far-field radiation is approximated into the plane wave and the reflected light will not exert an impact on the dipole oscillation. Its incidence angle is limited in the range of 0–90°. The approximate spherical wave of near-field radiation can be expanded into a Fourier series sum of plane waves with a coefficient of zero-order Bessel function J_0 (ur).

Fig. 1 shows the parameters in far-field incidence. The equivalent incidence angle of near-field radiation is more than 90° in Fig. 1. In near-field radiation, considering the completeness in mathematics, the in-plane wave-vector values of the incident light k_{1x} (x direction) vary from 0 to ∞. This means that the component in the z direction, k_{1z} ($=\sqrt{k_1^2 - k_{1x}^2}$) is an imaginary number although the eigen wave-vector of incident light k_1 ($=2\pi/\lambda_1$) is a constant. From the viewpoint of optics, this concept refers to the evanescent wave. When interaction occurs, energy transfer/loss will arise if the reflecting material is a lossy medium (such as metal, whose dielectric constant is a complex number). As shown in Fig. 1, the normalized in-plane wave-vector ($u = k_{1x}/k_1$) corresponds to $\sin\theta$ of the incident angle in the case of far-field incidence. Its value also ranges from 0 to ∞ in the case of near-field incidence.

2.2. IQE & power dissipation spectrum (PDS)

From the deduction of CPS theory, the actual internal quantum efficiency (AIQE, q') with existence of mirror of a single wavelength dipole radiation can be expressed as

$$\mathrm{AIQE}(d,s,\lambda) = q'(d,s,\lambda) = \frac{qF(d,s,\lambda)}{(1-q) + qF(d,s,\lambda)} \tag{2}$$

where q is the intrinsic quantum efficiency of the dipole in dielectric without metal mirrors, $(1-q)$ refers to the non-radiation part and $F(d,s,\lambda) = \int_0^\infty I(u)du$ is an introduced additional factor to the radiation efficiency of the dipole due to the reflected electric field exerted on itself by the metal mirror. $I(u)$ is the PDS which has different forms for the two types of dipole orientations.

$$\begin{aligned} I_\perp(u) &= \mathrm{Im}\left\{\frac{3}{2}\frac{u^3}{l_1}\frac{(1-r_{1,2}^p e^{-\beta_{1,2}})(1-r_{1,3}^p e^{-\beta_{1,3}})}{[1-r_{1,2}^p r_{1,3}^p e^{-(\beta_{1,2}+\beta_{1,3})}]}\right\} \\ I_\parallel(u) &= \mathrm{Im}\left\{\frac{3}{4}\frac{u}{l_1}\left\{\frac{(1+r_{1,2}^s e^{-\beta_{1,2}})(1+r_{1,3}^s e^{-\beta_{1,3}})}{[1-r_{1,2}^s r_{1,3}^s e^{-(\beta_{1,2}+\beta_{1,3})}]} + (1-u^2)\frac{(1+r_{1,2}^p e^{-\beta_{1,2}})(1+r_{1,3}^p e^{-\beta_{1,3}})}{[1-r_{1,2}^p r_{1,3}^p e^{-(\beta_{1,2}+\beta_{1,3})}]}\right\}\right\} \\ \beta_{1,2} &= 2l_1k_1d = \frac{4\pi}{\lambda_1}l_1d,\ \beta_{1,3} = 2l_1k_1s = \frac{4\pi}{\lambda_1}l_1s, \end{aligned} \tag{3}$$

$$\begin{aligned} l_1 &= -i\sqrt{1-u^2} = -i\sqrt{1-\frac{k_{1x}^2}{k_1^2}} \\ &= -i\frac{k_{1z}}{k_1}, (near-field) \\ &= -i\cos\theta, (far-field) \end{aligned}$$

$$\begin{aligned} l_2 &= -i\sqrt{\frac{\varepsilon_2}{\varepsilon_1} - u^2} = -i\sqrt{\frac{k_2^2}{k_1^2} - \frac{k_{1x}^2}{k_1^2}} = -i\sqrt{\frac{k_2^2}{k_1^2} - \frac{k_{2x}^2}{k_1^2}} \\ &= -i\frac{k_{2z}}{k_1},\ (near-field) \\ &= -i\sin\theta ctg\theta', (far-field) \end{aligned}$$

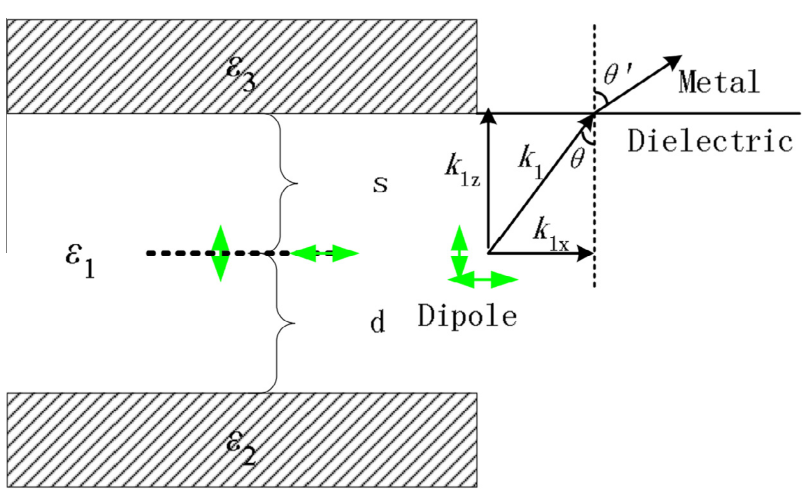

Fig. 1. Parameters in far-field incidence (two kinds of dipoles, the distances to electrode are s and d, the three dielectric constants are ε_1, ε_2, ε_3).

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