Optical Simulation of Top-emitting Organic Light Emitting Diodes

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ABSTRACT

An optical model based on classical electrodyanmics has beeb exploited to simulate the optical effects for the top-emitting organic light emitting diodes. The optical performance of the devices can be obtained through calculation of the power density in each planar thin film. The far field emission profile and spectrum are derived base on this model. Predicated optical performance is compared with experiments

Keywords: Top-emitting organic light emitting diode, optical modeling, microcavity

INTRODUCTION

Top-emitting organic light emitting diodes (TOLEDs) have attracted increasing interests because they are compatible with the CMOS technology and desirable for an active-matrix OLED display with high aperture ratio. Unlike the conventional bottom emitting diode, TOLED is fabricated on opaque substrate with a high reflective electrode. The light generated is extracted out after traveling through the other electrode that is semitransparent.

For the bottom emitting structure, the outcoupling efficiency is calculated to be $1/2n^2$ if ignoring the absorbing losses and waveguiding effects, where n is the refractive index of the emitting media. And the far field emission profile is assumed to show Lambertian behavior. These calculations are based on the simple geometrical optics assumption due to the bulk glass substrates. The geometrical optics assumptions, however, are obviously invalid for the top emitting structure because the dimension of the devices is close to the light wavelength. Meanwhile, highly reflective electrodes lead to a strong cavity effect in the optical performance of TOLEDs. Therefore, a rigorous theoretical model is required to study emission characteristics of the TOLEDs and design structure with high efficiency. In this paper, we exploit a theoretical model based on Green function and plane wave expansion to study the spontaneous emission modification inside the TOLEDs. Far field emission profile and emission spectra at the different angles of the typical TOLEDs structure are simulated. Theoretical results are compared with the experiments to test the accuracy of the model. The optimal capping layer thickness is investigated theoretically with this model as well.

THEORY

Figure 1(a) shows a typical structure of TOLEDs. The spontaneous emission of excitons formed by injected electron/hole pairs recombination is treated in terms of an oscillating electrical dipole in the stratified structure. Alternative TOLEDs employ inverted structure, i.e. high reflective cathode and semi-transparent anode. But the representations of dipole radiation in optical environment are the same, as shown in figure 1(b), that emitting medium is sandwiched between to reflective mirrors which form an optical cavity. The radiation from a dipole over a flat layer was first studied by Sommerfeld.[1] Lukosz and coworkers[2,3] extended the case and developed a model to calculate the dipole radiation in n-layer thin film structure. The core of this model is the plane wave expansion of the wave fields generated by the electrical dipoles and the

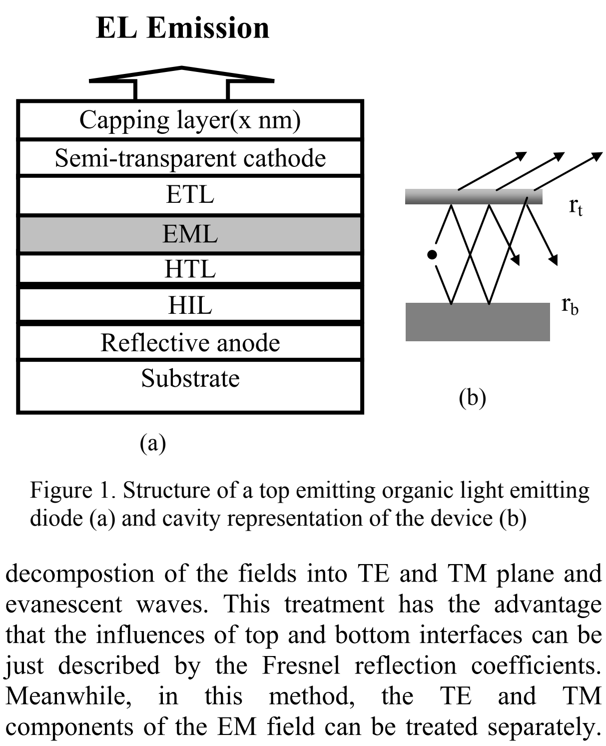

Figure 1. Structure of a top emitting organic light emitting diode (a) and cavity representation of the device (b)

decompostion of the fields into TE and TM plane and evanescent waves. This treatment has the advantage that the influences of top and bottom interfaces can be just described by the Fresnel reflection coefficients. Meanwhile, in this method, the TE and TM components of the EM field can be treated separately. By solving the boundary-value problems, we can obtain the s- and p-polarized plane and evanescent waves in each layer from which the electric and magnetic strength can be calculated. After that, it will become easy to calculate total power radiated by the dipole, radiative power distributions in each layer, far field radiation pattern and emission spectra viewed outside.

All values are obtained with normalization to the total power radiated by the same source created in infinite medium. In our calculation, we consider a TOLED using Alq3 as emitting medium.

POWER DENSITY SPECTRUM

According to the model the power generated $\overline{P}$ by a dipole source can be expressed as an integral over the magnitude of the inplane wavevector $k_{//}$ that varies from zero to infinite,

$$\overline{P} = \overline{P}_{TE} + \overline{P}_{TM} = \int_0^\infty [K_{TE}(k_{//}) + K_{TM}(k_{//})]dk_{//} \quad (1)$$

where K_{TE} and K_{TM} are defined as the power density based on $k_{//}$ space for TE- and TM wave, respectively. We show in figure 2 the $k_{//}$-space power spectrum for the case of a dipole oriented randomly in the optical cavity. Wavevector k_0 corresponds to the peak wavelength of Alq_3 emission in vacuum, k_{alq} to that in Alq_3 layer. The fraction of the generated power can be specified in terms of the wavenumber $k_{//}$. With the presence of the optical cavity, the power is dissipated through different channels. Dissipated power with inplane wavenumber that satisfy 0≤k//≤kalq corresponds to light that may propagate in the organic layer. Of this dissipated power, that fraction with k// in the range 0≤k//≤k0 corresponds to the extracted modes of the OLED structures capable of producing useful far field radiation. The fraction with k// in the range between k0 and kalq correspond to the guided modes in the organic layers. There is a sharp feature with k// a litter larger than kalq, which corresponds to surface plasmon (SP) modes. The surface plasmons result from the coupling between the free electrons at the metal electrode surface and the dipole radiation. The surface plasmon mode are bound to the interface between the metal and dialectical layer. Since the wavenumbers of the SP modes are greater than k0, they cannot propagate into the air. The surface plasmon emission, although often termed "nonradiative" since it is not directly observable, is actually radiative in character and can be coupled out into air by using a Bragg scattering.[4]. In the regime with larger $k_{//}$ there is a small peak which correspond to the junction modes due to the two reflective mirrors. The power spectrum in Fig 2 also indicates the surface plasmons only exist in TM waves, and no TE surface plasmon modes can exist at the interface between metal and dielectric. Considering the radiation from a vertical aligned dipole, all power generated dissipates in forms of TM modes. On the other hand, an in-plane aligned dipole will generated both TE and TM wave modes. Therefore, one effective method to improve the efficiency of the organic light emitting devices is to align the molecule to make the radiating dipoles oriented in the plane of substrate.

In the case of plane waves propagating through multilayers, an emitting angle θ in the outside can be associated with $k_{//}$ and wavevector k0 in the air,

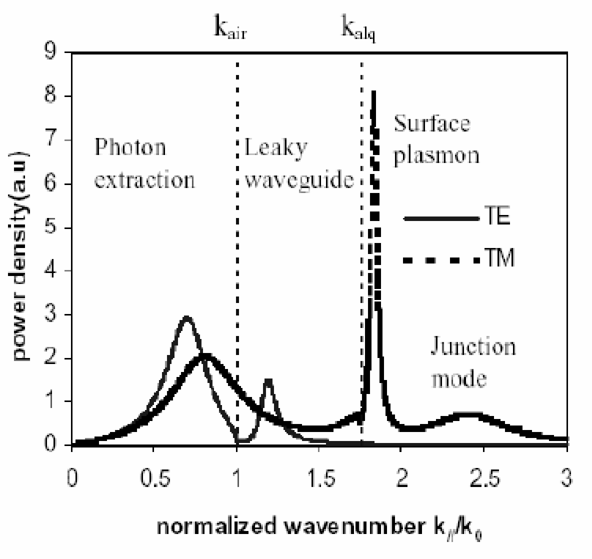

Figure 2. Power density spectrum for the Alq3 based top-emitting OLED.

according to the formula of $k_0 \sin\theta = k_{//}$. The power density in k//- space can then be transformed to a power density in real spatial space. The intensity angular distribution is related to the power density K by

$$I(\theta) = \frac{K(k_0 \sin\theta) k \cos\theta}{2\pi \sin\theta} \quad (2)$$

The intensity calculated in the equation (2) is for a single dipole source. We treat the total emission as an ensembles of various dipole sources with different oscillating frequencies and strength. The dipole oscillator strength is wavelength-dependent and is assumed to be proportional to the measured photoluminescence (PL) of the emitting material. Therefore, Eq 2 is modified as

$$I(\theta, \lambda) = \frac{K(k_0 \sin\theta) k \cos\theta}{2\pi \sin\theta} I_0(\lambda) \quad (3)$$

giving the emission intensity detected at different viewing angle and wavelength, where $I_0(\lambda)$ is the normalized PL spectrum.

EXPERIMENT AND SIMULATION RESULTS

In the present report, the fabrication and characterization of top-emitting OLEDs with composite anodes constructed of aluminum (Al, 150 nm)/platinum (Pt, 2 nm)/praseodymium oxide (Pr_2O_3, 1 nm) are described. The use of thin films of Pt and Pr_2O_3 [5] was motivated by their reported ability to enhance hole injection. Al was used as both a reflecting mirror and a low-resistance current-carrying interconnect. The functional organic layers were copper (II) phthalocyanine (CuPc, 20 nm) as an anode buffer layer,

N,N'-diphenyl-N,N' bis(3-methylphenyl-1,1'-biphenyl-4,4'-diamine (TPD, 40 nm) as a hole-transport layer and tris-8-hydroxyquinoline aluminum (Alq_3, 50 nm) as an electron-transport and emitting layer. Transparent cathodes were constructed of lithium fluoride (1 nm)/Al(12 nm)/ITO(60 nm).
The calculation of power density was based on a considerable body of data taking the optical properties of the materials into account. The optical properties of each layer including both organic layers and metal electrodes were obtained with spectroscopic ellipsometer. And the Fresnel reflection and transmission coefficients of the two mirrors of the optical cavity were calculated using transfer-matrix methods.

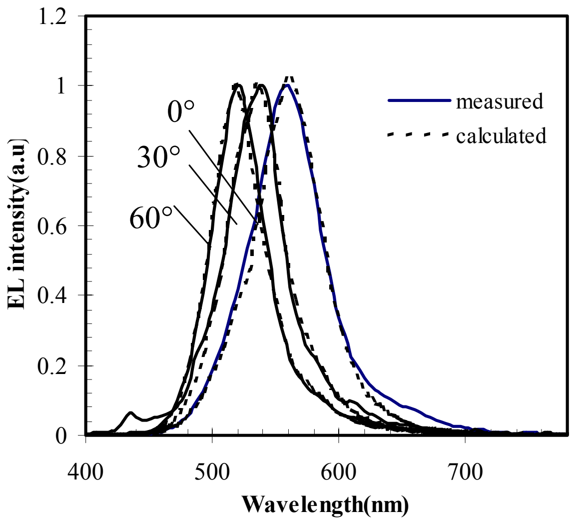

Figure 3. Experimental and simulated normalized EL spectra observed at different angles from normal.

Figure 3 shows the normalized electroluminescence (EL) spectra measured under different viewing angles. The simulated results agree with the experimental very well. This spectrum shift with viewing angles is caused due to the strong microcavity effects. The power density K in Eq. 1 is inversely proportional to the Airy factor $A = \left|1 - r_b r_t \exp(i2kzd)\right|^2$, where r_b (r_t) is the Fresnel coefficient for the reflection at the bottom (top) boundary, d is the organic layer thickness and $k_z=2n_{alq}\pi \cos\theta/\lambda$. Both reflections and kz vary with angles, which leads to minimal A at different resonant wavelength, giving a rise to the spectrum peak shift with angles. This spectrum change is undesirable for display application. According current model, proper choose of the metal electrodes and organic layer thickness can minimize the color shift.
Figure 4 shows the EL intensity angular distribution of the device. As the theoretical calculation predicts, the emission profile was far different from Lambertian-cosine distribution. The peak intensity occurred at large viewing angle, unlike the conventional bottom-emitting device with strongest emssion observed at normal direction. We compared the output emission of top-

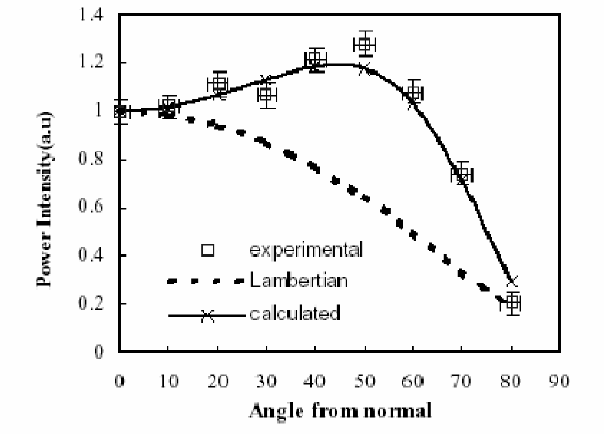

Figure 4. Angular distribution of the EL intensity of Alq3 based Top-emitting OLED and theoretical simulation

emitting device and bottom-emitting one. Although in normal direction the top-emitting devices emitted lower intensity light, the total integrated power of the top-emitting devices was about 30% higher.
To let the light emit out, the top metal electrode cannot be thick. However, too thin film will lead to high resistance. A transparent conductive or semi-conductive capping layer were applied on the thin metal film to solve the problem.[6,7] Meanwhile, this capping layer was found to be able to tune the optical transmittance of the top layers, modifying the output emission. Figure 5 depicts the simulation results of the total output power and the tranmittance of the top layers , LiF(1nm)/Al (10 nm/ITO(x nm) , as a function of the ITO capping layer thickness. The calculation indicates both total emission power and tranmittance of top layers have an oscillatory dependence on the ITO thickness. The first maxima in total power and

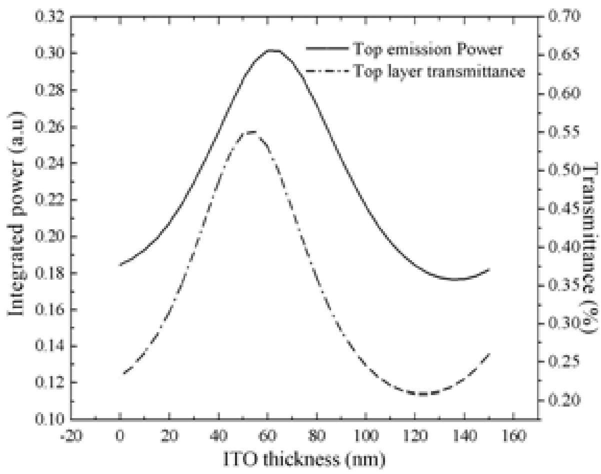

Figure 5 Calculated total emitting power and transmission of the top mirror vs the capping ITO thickness

transmittance of top layers are obtained at 60 nm and 55 nm ITO respectively. A 1.7X improvement in the total emission can be achieved with a ~ 60nm ITO capping layer compared with that without the capping layer. As indicated, the variation of total power with respect to the ITO thickness is similar with that of the transmisstance. With increase of the tranmittance of the top layers, more emission will be extracted out. However, it should be noted that the total top emission power is also affected by the organic layer thickness and bottom reflective electrode. The thickness and optical dispersions of these materials need to be taken into account while choosing the capping layer thickness to maximize the output emission.

SUMMARY

In summary, we have exploited a rigorous classical model to describe optical performance of top-emitting OLEDs. To understand how light propagates in device layered media, the power spectrum on the inplane wavenumber space were calculated. The model is shown to predict accurately the experimental data which suggest that strong microcavity effects have a great impact on the device performance. In addition, we have also demonstrated results that tuning the top capping layer thickness can strongly affect device extraction efficiency. Although this model has been related to top-emitting OLEDs, the formalism can be equally applied to bottom emitting OLEDs.

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REFERENCES

1. A. Sommerfeld. Ann. Phys. Leipz., 28, 665 (1909)
2. W. Lukosz, Phys. Rev. B., 22, 3030 (1980
3. W. Lukosz, J. Opt. Soc. Am. 71, 744 (1981)
4. Dawn K.Gifford and Dennis G. Hall, Appl. Phys. Lett. 81, 4315 (2002)
5. Chengfeng Qiu, Huajun Peng, Haiying Chen, Zhilang Xie, Man Wong and Hoi-Sing Kwok, SID'03 Digest, p974-p978, 2003
6. L. S. Hung, C. W. Tang, M. G. Mason, P. Raychaudhuri, and J. Madathil, Appl. Phys. Lett., 78, 544 (2001)
7. H. Riel, S. Karg, T. Beierlein, B. Ruhstaller, and W. Reiβ, Appl. Phys. Lett. 82, 466 (2003)