Performance Analysis of Layered and Blended Organic Light-Emitting Diodes

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Keywords : OLED, blended structure, oxidative degradation

Abstract

We make performance simulations of three different organic light-emitting diodes (OLEDs), one of which is based on a conventional layered structure and the others on a blended structure where an emitting layer (EML) is either uniformly or stepwise mixed with an electron transport layer (ETL), Tris-(8-hydroxyquinoline) aluminum (Alq_3).

1. Introduction

Because of their superior features such as high efficiency, wide viewing angle, fast response, and low cost, organic light-emitting diodes (OLEDs) have attracted much attention for applications in displays and lightings [1]. However, poor stability of OLEDs is still of practical concern. The formation of dark spots has been found to be one of factors degrading OLEDs, yet it can be suppressed by virtue of passivation and encapsulation. For OLEDs based on Tris-(8-hydroxyquinoline) aluminum (Alq_3) employed most commonly as an electron transport molecule, the injection of holes into Alq_3 is also known to degrade the device stability [2]; namely, cationic Alq_3 species are responsible for a reduction of device lifetime. Several schemes have been proposed to suppress such hole injection [2]. The hole transport layer (HTL) is doped or a buffer layer is inserted between an anode and the HTL in such a way that the hole transport is disturbed to some extent and thus steep hole pileup at the HTL/ETL interface becomes subdued. As an alternative, many studies of bilayer OLEDs with uniformly or stepwise mixed emitting layers of HTL and ETL (without the heterojunction interface) have also been made [3], [4]. In [5], an ETL is blended with a conjugate polymer to improve the injection of electrons of polymer LEDs. It has been speculated that the hole injection into the ETL is suppressed in those configurations due most likely to a shift of recombination zone by the blending effect. To demonstrate it in this paper, we carry out numerical simulations of those layered and blended OLEDs, which can provide or rather visualize clear device characteristics such as the hole injection into the ETL, spatial charge density distribution, electric field distribution, and exciton density distribution.

2. Model

With attempt to capture the underlying physics and complex behaviors of OLEDs in response to a variety of design parameters, we have implemented a 1D numerical model consisting of Poisson's equation, time-dependent drift-diffusion equations, and exciton rate equation [6]. The electric field distribution can be calculated at each time in each subsection discretized in space by solving Poisson's equation given as:

$$\frac{\partial E(x,t)}{\partial x} = \frac{q}{\varepsilon(x)}\left(p(x,t) - n(x,t) + p_t(x,t) - n_t(x,t) + p_g(x,t) - n_g(x,t)\right) \quad (1)$$

where the variable q denotes the electron charge, ε (F/m) the permittivity of the organic materials, E (Vcm^{-1}) the electric field, p (cm^{-3}) and n (cm^{-3}) the hole and electron densities, respectively, P_t(cm^{-3}) and n_t(cm^{-3}) the hole and electron densities trapped on the organic materials, respectively, P_g (cm^{-3}) and n_g (cm^{-3}) the hole and electron densities trapped on the guest dopant, respectively.

Those carrier densities are governed by the following drift-diffusion equations based on the Langevin recombination process;

$$\frac{\partial n(x,t)}{\partial t} = \frac{1}{q}\frac{\partial J_n(x,t)}{\partial x} - \frac{q}{\varepsilon(x)}\left\{\left(\mu_n(x,t)+\mu_p(x,t)\right)n(x,t)p(x,t)+\mu_n(x,t)n(x,t)p_g(x,t)\right\}$$

$$\frac{\partial p(x,t)}{\partial t} = -\frac{1}{q}\frac{\partial J_p(x,t)}{\partial x} - \frac{q}{\varepsilon(x)}\left\{\left(\mu_n(x,t)+\mu_p(x,t)\right)n(x,t)p(x,t)+\mu_p(x,t)n_g(x,t)p(x,t)\right\} \quad (2)$$

where

$$J_n(x,t) = q\mu_n(x,t)n(x,t)E(x,t) + kT\mu_n(x,t)\frac{\partial n(x,t)}{\partial x}$$

$$J_p(x,t) = q\mu_p(x,t)p(x,t)E(x,t) - kT\mu_p(x,t)\frac{\partial p(x,t)}{\partial x} \quad (3)$$

with the variable μ_n (cm^2/Vs) defined as the electron mobility, μ_p (cm^2/Vs) the hole mobility, k (J/K) the Boltzmann constant, and T (=300K) the temperature.

Upon recombination, hole-electron pairs generate excitons on the host and guest materials. In addition, energy transfer from the host to the guest takes place, a phenomenon known as Förster energy transfer. Those excitons diffuse and decay radiatively but nonradiatively at the electrodes. If the concentration of the guest dopant is too high (more than 2 wt% for a fluorescent dopant), there arises a self-quenching among excitons, also referred to as singlet-singlet annihilation. All of those behaviors of excitons are described in the following exciton rate equations [6];

$$\frac{\partial S_h(x,t)}{\partial t} = G_h(x,t) - T_{h-g}(x)S_h(x,t) + D_h\frac{d^2S_h(x,t)}{dx^2} - \frac{S_h(x,t)}{\tau_h} - \frac{1}{2}\xi_{ss\_h}(x)S_h^{\,2}(x,t) - Q(x)\frac{S_h(x,t)}{\tau_q}$$

$$\frac{\partial S_g(x,t)}{\partial t} = G_g(x,t) + T_{h-g}(x)S_h(x,t) + D_g\frac{d^2S_g(x,t)}{dx^2} - \frac{S_g(x,t)}{\tau_g} - \frac{1}{2}\xi_{ss\_g}(x)S_g^{\,2}(x,t) - Q(x)\frac{S_g(x,t)}{\tau_q} \quad (4)$$

where S_h (cm^{-3}) and S_g (cm^{-3}) indicate the singlet exciton density on the host and on the guest, respectively, $T_{h\text{-}g}$ (1/s) the rate of Förster energy transfer from the host to the guest, τ_h and τ_g the exciton lifetimes, and τ_q the reduced lifetime by the exciton quenching at the electrodes. D_h (D_g) denotes the diffusion constant expressed as $D_h = l_h^{\,2}/\tau_h$ ($D_g = l_g^{\,2}/\tau_g$) with l (cm) defined as the diffusion length. ξ_{ss_h} and ξ_{ss_g} are the singlet-singlet annihilation constants of the host and the guest, respectively. More details as to the model and the definition of variables can be found in [7].

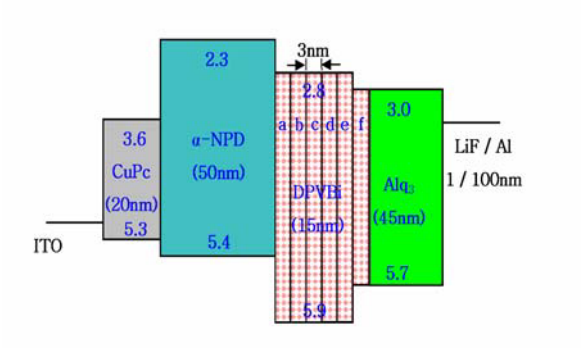


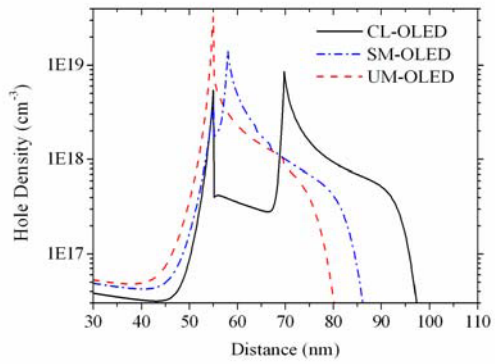
Fig. 1. Schematic view of the conventional layered structure (CL-OLED) and its energy level diagram.

3. Results and discussion

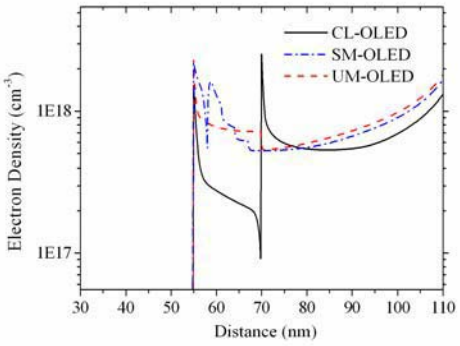
With the numerical model, we make a numerical investigation of the layered and blended (uniformly or stepwise mixed) OLEDs (Fig. 1). For the uniformly mixed OLED (UM-OLED), the EML is uniformly mixed with the ETL; namely, DPVBi : Alq_3 = 50% : 50% from (a) through (e). For the stepwise mixed OLED (SM-OLED), the composition of the EML is gradually varied; i.e., (a) DPVBi : Alq_3 = 100% : 0%, (b) DPVBi : Alq_3 = 75% : 25%, (c) DPVBi : Alq_3 = 50% : 50%, (d) DPVBi : Alq_3 = 25% : 75%, and (e) DPVBi : Alq_3 = 0% : 100%. For simplicity, we extract the carrier mobilities of UM-OLED by taking an average of or the ones of SM-OLED by gradually changing the mobilities of EML and ETL in proportion to the composition. Shown in Figs. 2 (a) and (b) are the simulation results of the hole and electron density distributions calculated at 10V. Keeping in mind that the EML (DPVBi) has very low carrier (both hole and electron) mobilities and the ETL (Alq_3) has relatively high electron mobility, the electron distribution is expected to be much affected in the blended structure. In the CL-OLED, a large number of electrons are piled up at the EML/ETL interface due to the energy level offset and mobility discontinuity. Since a smaller number of electrons are transported to the HTL/EML interface, a larger number of holes reach the EML/ETL interface, which causes more penetration of holes into the ETL layer. However, such a steep accumulation at the EML/ETL interface is considerably depressed in the UM-OLED and thus more electrons are transported to the

HTL/EML interface. It is at the HTL/EML interface that dominant electron-hole recombination arises in the UM-OLED. As such, fewer holes reach the EML/ETL interface and consequently penetration of holes into the ETL is much suppressed. Other than the other device structures, a significant number of carriers are populated inside the EML (not at the interfaces) in the SM-OLED. Therefore, penetration of holes into the ETL in SM-OLED is less serious than that in the CL-OLED but severer than that in UM-OLED. In general, holes penetrating into the Alq_3 layer lead to oxidative degradation of Alq_3 molecules, which is detrimental to the longevity of OLEDs. Thus, the UM-OLED is expected to have the longest lifetime, followed by the SM-OLED and then the CL-OLED, a result also observed experimentally [4].

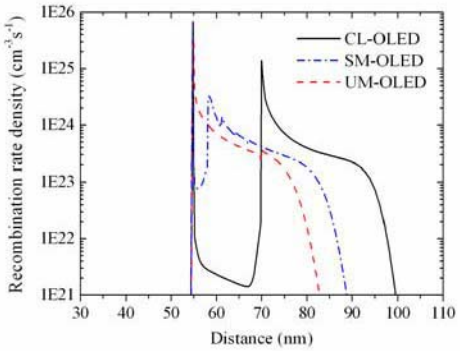
Shown in Fig. 2(c) is the simulation result of recombination rate density of those three devices. It is clearly seen that recombination occurs dominantly at the organic/organic interfaces in the CL-OLED; namely, no significant recombination takes place inside the EML. Unlike it, substantial recombination arises inside the EML in the blended structures due mainly to the delocalization of carriers from the organic/organic interfaces. Meanwhile, the strongest recombination occurs at the HTL/EML interface in those devices and thus the peak of exciton density is observed at the same interface as evident in Fig. 2(d). Presented in Fig. 2(e) is the electric field distribution inside those devices calculated under the bias voltage of 10V. One can find that further penetration of holes into the ETL shifts the electric field peak position from the EML/ETL interface toward the cathode. Accordingly, the electric field peak of the CL-OLED is positioned more closely to the cathode. The enhanced electric field in the Alq_3 layer will result in an improvement of the electron injection efficiency due to the fact that the mobility is proportional to the electric field.



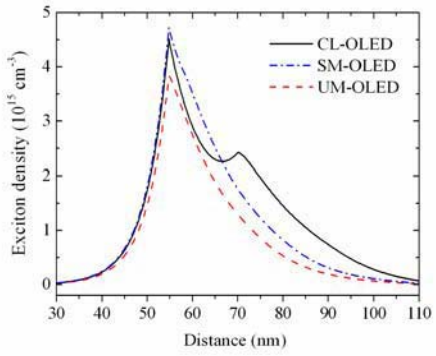
(a)



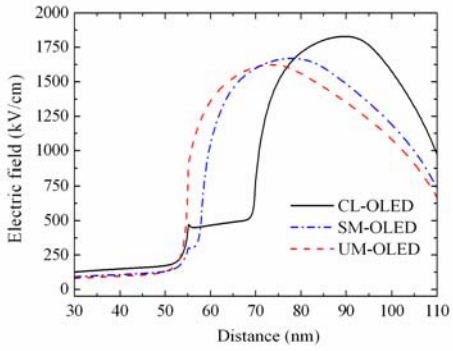
(b)



(c)



(d)



(e)

Fig. 2. Simulation results of (a) hole density, (b) electron density, (c) recombination rate density, (d) exciton density, and (e) electric field distributions at 10V for different device structures.

4. Summary

We have clearly shown by way of simulation that the blended configuration where the EML is uniformly or stepwise mixed with the ETL suppresses penetration of positive charges into the ETL (Alq_3) or rather oxidative degradation of Alq_3 molecules through the delocalization of electron-hole recombination, the longevity of OLEDs by which is expected to be enhanced.

5. References

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