Simulation for double ultra-thin separately doped red organic light-emitting diode

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1. Introduction

Organic light emitting diode (OLED) has attracted considerable interest of researchers since it was successfully developed in 1987 [1]. Doping is one of the common techniques for producing tricolor light. But the transfer of energy from host to guest in the doping system is insufficient, and high doping concentration would lead to quenching effect. Thus it has been difficult to fabricate ideal OLEDs that offer both full saturation (pure color) and high luminance efficiency. The experiments in this study employ ultra-thin separately doped OLED structure to achieve low turn-on voltage, high luminance efficiency and high electroluminescence [2]. In the simulation part of this study, the photoluminescence (PL) spectrum intensity of each emitting layer (Alq3 and DCJT) and full width at half maximum (FWHM) of its Gaussian distribution are changed to obtain the electroluminescence (EL) spectrum of ultra-thin separately doped device, which is then compared to the experimental data.

2. Experiment

This study employed ultra-thin separately doped structure as published previously [2]. The device structure is ITO(230nm)/NPB(40nm)/DCJT-dopedAlq3(5nm)/Alq3 (5nm)/DCJT-dopedAlq3(5nm)/Alq3(45nm)/LiF(0.5nm)/Al (60nm). The emitting layer Alq3 was doped with DCJT by means of ultra-thin double-layer separate doping to produce red light. The energy band diagram of the OLED is shown in Fig. 1. In the experiment, three concentrations of DCJT dopant, 1, 2.7, and 3.5 % wt, were used. After the organic layers were deposited, the substrate was moved to metal evaporation chamber to deposit electron injection layer LiF and cathode Al. After the device was fabricated, Keithley 2400 and SpectraScan PR650 were used to measure the EL spectra and light-current-voltage (L-I-V) characteristics.

The Emissive Thin Film Optics Simulator (ETFOS) developed by Zurich University of Applied Sciences - Center for Computational Physics and IBM was used for simulation. To run the simulation: 1. set the film thickness and optical parameters (e.g. n, k values) for each layer; 2. define the emitting layer, dipole location (D.L.) of emission area (in Table 1, D.L.=1 means the emission area was at the NPB-DCJT doped Alq3 interface; D.L.=0 means the emission area was at the Alq3-LiF interface) and PL spectra of emitting materials Alq3 and DCJT; 3. adjust the FWHM of

PL Gaussian distribution (by the percentage of FWHM to the full width of Alq3 spectrum) and intensity values of PL spectrum of emitting materials (Alq3 and DCJT). Table 1 shows the simulation parameters of each emitting layer. Finally the simulated EL spectra of devices were obtained and compared with the measurements obtained in the experiment.

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#	Parameters for simulation	DCJT doped AlQ3 layer -1	Undoped AlQ3 layer	DCJT doped AlQ3 layer -2
Device A	DCJT concen.	1 %	0	1 %
	D.L. (a.u.)	1	0.84	0.79
	I (a.u.)	1	0.75	1
	FWHM (a.u.)	1	0.5	1
	λ_{p} (nm)	610	530	610
Device B	DCJT concen.	2.7 %	0	2.7 %
	D.L. (a.u.)	1	0.84	0.79
	I (a.u.)	1	0.25	1
	FWHM (a.u.)	1	0.5	1
	λ_{p} (nm)	620	530	620
Device C	DCJT concen.	3.5 %	0	3.5 %
	D.L. (a.u.)	1	0.84	0.79
	I (a.u.)	1	0.1	1
	FWHM (a.u.)	1	0.5	1
	λ_{p} (nm)	636	530	636

Table 1 Parameter values of emitting layer in simulation process

D.L. : Dipole Location relative to full Alq3 layer ; D.L.=1 at NPB/DCJT-doped Alq3 interface ; D.L.=0 at Alq3/LiF interface ; FWHM : FWHM of each spectrum ; I : Intensity of spectrum ; λ_p : peak wavelength of DCJT-doped Alq3 or undoped Alq3; a.u. : arbitary unit.



Fig.1 Energy band diagram of OLED for experiment and simulation.

3. Results and Discussion

Fig. 2 shows the EL spectra of ultra-thin double layer separately doped structures with various DCJT (red dopant) concentrations measured in the experimental process. The spectrum emitted by host emitting layer Alq3 remained distinct (at the left shoulder in Fig. 2) when the doping concentration was only 1 %wt and did not diminish until the doping concentration was increased to 3.5 % wt. It is found by modulating the intensity value (I in Table 1) of host emitting layer (Alq3) in the simulation process that as the dopant concentration used in the experiment became higher, the intensity value I of undoped Alq3 spectrum must be adjusted to a smaller one in order to simulate the weak EL spectrum at the left shoulder in Fig. 3, so the simulated waveforms would approximate the experimental data. At the doping concentration of 1, 2.7 and 3.5 % wt, the intensity value I was adjusted by 0.75, 0.25, and 0.1, respectively, and the simulation results obtained in Fig.3 matched the experimental results in Fig. 2 very well. Experimental data show that purer red light was obtained when the concentration of red dopant was higher, but the luminance weakened. It was due to the concentration quenching effect [3]. Conversely, lower red dopant concentration resulted in stronger red light emission, but the device emitted orange instead of intense red color. This is because DCJT at lower concentration cannot absorb massive excitons' energy from Alq3. As a result, the red light from DCJT would be mixed with green light emitted by Alq3 [3]. A number of papers have alluded to similar phenomenon [4-6]. To coincide the simulation results with the experimental data, it is deduced that the PL spectrum of DCJT (red dye) exhibits red shift as doping concentration increases.

4. Conclusion

It is found in the simulation process that as the DCJT doping concentration used in the experiment becomes higher, the PL intensity of Alq3 in simulation must be smaller, and as the doping concentration gets lower, the PL intensity of Alq3 must be greater in order to approximate the simulation results to experimental data. The simulation results show that higher red dopant concentrations produce purer red light, but the light intensity diminishes. Conversely lower red dopant concentrations result in brighter red light, but the device emits orange instead of pure red color.

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Fig. 2 Experimental spectra of OLED with various doping concentrations



Fig. 3 Simulated spectra of OLED for different doping concentrations by using parameters listed in Table 1.