Rapid Calibration of Organic Layer Thickness by ETFOS software

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Abstract

By ETFOS software simulation to swiftly find out the shortcomings of the device structure and conserve the wastage of time cost in experiments, including the instruments deviations or human errors. Thereby we can calibrate the correct organic layer thickness by comparing the EL spectra with different NPB thicknesses.

1. Introduction

Since the publication by C.W.Tang et al in 1987 on production of multiple layers of OLED structure with organic molecules by vacuum metallization [1], researchers of various disciplines have been attracted to this area, and in recent years except for development of molecular structure, research on polymer structure and flexible substrate and organic solar cells have sprouted.

Many theses and data have proven that the ETFOS software jointly developed by the University of Zurich Computing Physics Center and US IBM has provided an engineering simulation software for design of OLED display products and other thin film devices such as microcavity LED, thin film solar cells and passive thin film optics. It has been proven by experiments that this software is capable of simplifying and accelerating [2,3] design of light emitting components for organic material structure now proliferating on the market.

This article discusses the frequently encountered issue of optimizing the film thickness in experiments and uses this software to rapid-calibrated deviations generated by instruments and human errors: for instance, using the material film thickness data the lab might not get the same results and consequently it is required to add more contrast groups to find out the optimum film thickness value and if this value is not actually measured it is highly possible that its film thickness value is different from what is recorded.

2. Experimental

Step 1. Set up Table Ⅰ simulated component film thickness and set other optics parameters in ETFOS where peak wavelength is the simulated value. Step 2. Add the measured light emitting optical spectrum with Spectra Scan PR650 into ETFOS and compare the experimental value with the simulated value. Step 3. Output the various simulated optical spectrum data to the file and import to the drawing formula to compare the spectrum and the difference in intensity. Step 4. Location is defined as a recombination zone and is generally set at 1 (that is HTL/ETL interface), and the smaller the value the more it moves toward ETL region.

3. Results and discussion

We suspect the thickness of organic films should be uncorrected which obtained from the quartz oscillator. According the simulation steps, from Fig. 1 and Table 1, we found that the wavelength peak value and the waveform are different in EL spectra (with peak value at 530nm) obtained by the simulated software film thickness value (assuming location=1) measured by the quartz oscillator in the lab and the actual EL spectra (with the peak value at 554nm), thereby proofing deviation in film thickness produced in the lab.

Table I Optimum thicknesses and parameters of anode for ITO and IZTO.

Device	A	B	*C	D	E	F(exp.) meas. by quartz
NPB (nm)	60	80	105	120	50	50
Alq_3 (nm)	80	80	80	80	80	80
location	0.68	0.68	0.68	0.68	1	-
Luminance:	33.4	33.1	30.3	28.6	31.8	-
Peak Intensity:	**0.54**	0.49	0.40	0.34	0.49	-
Peak Wavelength : (nm)	532	542	**554**	560	530	**554**

*C: The matching thickness of simulated value which the measured and simulated devices have the same waveforms and the wavelength both are at 554 nm. *The thicknesses of NPB/Alq3 from quartz oscillator monitor in lab are 50/80 nm, but the experimental device F's wavelength 554 nm can not fit to the wavelength of 530 nm of simulated device C.

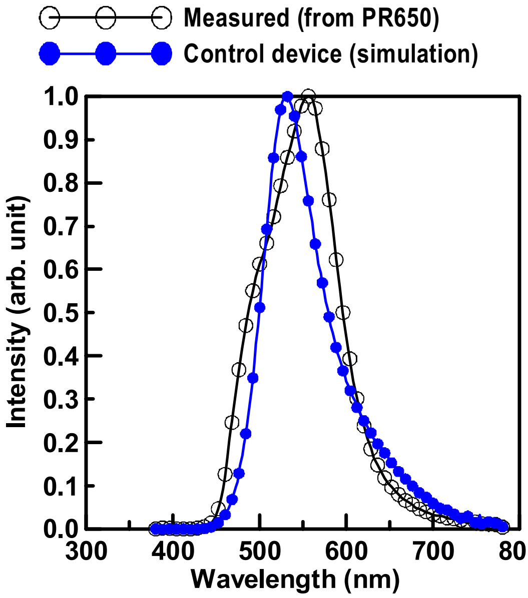

Fig. 1. Comparison of EL spectra between the measured 50-nm-thickness of NPB (measured by PR650 in lab) and the simulated 50-nm-thickness of NPB (set in ETFOS) of control device.

In ETFOS we get an almost fully matched EL spectra with the lab value (as shown in Fig. 2) by adjusting the NPB thickness at 105nm, the Location value at 0.68 while other material thickness remains unchanged as shown in Table 1.

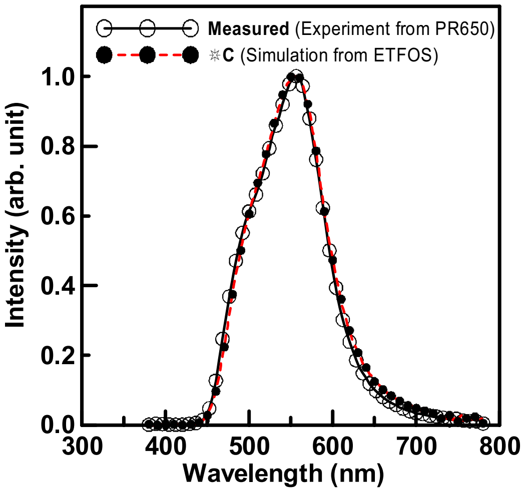

Fig. 2. Matching EL spectra of simulated value (Device *C) and experimental value (measured).

This result shows that the NPB thickness value (50nm) in the lab (measured by the quartz oscillator) is actually 105nm (simulated result), in other words, we have to calibrate 2.1 times the thickness ratio (lab thickness value × 2.1 = simulated value) to get the real thickness. In the course of adjusting the matching, take NPB thickness respectively at 80nm and 120nm as shown in Fig. 3, showing we cannot get the matched EL spectra, and find out that when NPB thickness increases the intensity lowers and the peak value moves toward the yellow light and caused changes to the waveform, thereby to get the optimum luminance and the correct light emitting EL spectra, the NPB thickness is required to adjust downward to increase the intensity.

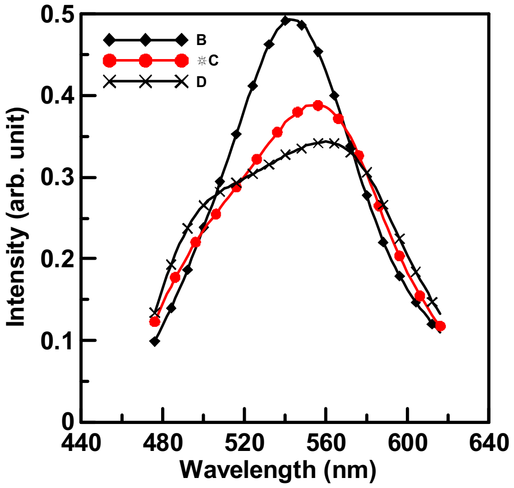

Fig. 3. EL spectra of the matched value (Device *C) as the reference value to adjust the different NPB thicknesses.

In Fig. 4, through batch simulation by ETFOS, the optimum value (Location=0.68) can be obtained with the thickness of NPB and Alq3 being 60 nm and 80 nm, respectively. In the simulated result, the optimum thickness of NPB is 60 nm for ITO anode. The L-V characteristic in thickness of 60 nm was superior than that of 80 nm for Alq3 layer in OLEDs. Because the distortion of organic layer occurs only in NPB layer, but the Alq3 layer is correct, from quartz oscillator in lab.

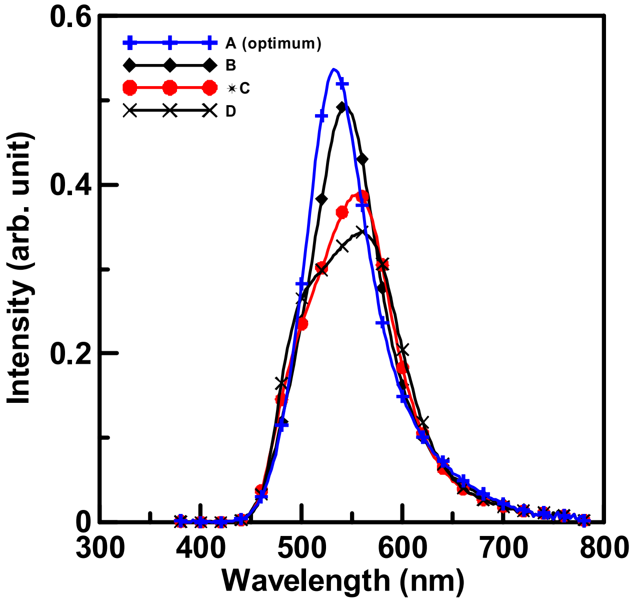

Fig. 4. EL spectra of different thicknesses of NPB. Device A has the optimum film thickness with NPB/Alq3 (60/80 nm).

4. Summary

By ETFOS software simulation to swiftly find out the shortcomings of the component structure and conserve the wastage of time cost in actual experiments and also the experimental deviation caused by the experimental apparatuses or human errors through simulation. Thereby we can calibrate the correct organic film thickness value. If we can utilize the simulated forecast results by this software before doing experiments, then we'll improve its effectiveness in production of the organic light emitting component with complicated production procedures.

5. References

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