Modeling of Random Dopant Effects of Organic Light Emitting Diode with Two Dimensional Simulation

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***Abstract*—In this paper, We not only developed Poisson and drift-diffusion solver with effective tail states and field-dependent mobility, but set up a 2D random model to treat the doping effect on the organic materials. Understanding these models helps us in modeling OLED.**

***Keywords*—2D model, doping, BImBP, FIrpic, OLED**

I. Introduction

Organic light emitting diodes (OLED) have been gradually entering the display markets in recent years. Therefore, it is important to develop a useful tool assisting in the device design of the organic materials. Unlike semiconductors, however, the bandgap and density of states (DOS) of organic materials are not well-defined due to the amorphous and disordered molecules in organic materials. Apart from this, the process of carrier transportation, known as hopping process, is different from traditional diffusion process of typical inorganic semiconductor. We hence modify the traditional Poisson and drift-diffusion equations. And in this paper, the structure we use is shown in Fig. 1.

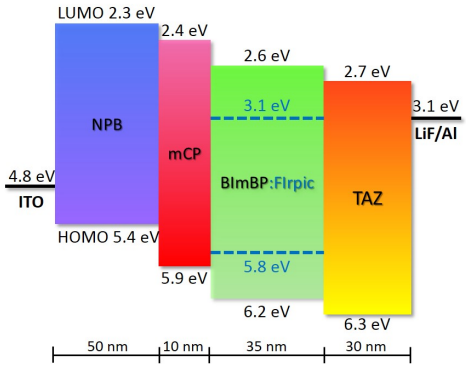

Fig. 1: Structure of OLED. NPB, mCP, BImBP, and TAZ are used as the hole injection layer (HIL), hole transporting layer (HTL), emitting layer (EML), and electron transporting layer (ETL), respectively.

II. Methodology

Earlier studies [1] have shown that according to the absorption spectrum of organic materials, there are some Gaussian-like DOS near the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO).So we set the distribution of DOS by the equation (1)

$$N_{tail,dos}\left(E\right) = N_t \frac{1}{\sigma\sqrt{2\pi}} exp\left[-\frac{\left(E-E_t\right)^2}{2\sigma^2}\right], \qquad (1)$$

where N_t is the total tail state density, E_t is the Gaussian peak position, and σ is the broadening factor of this Gaussian shape state.

Then, we use the Poole-Frenkel field dependent mobility (2) to model the carrier transport since the ability of hopping improves as the electric field increases [2].

$$\mu = \mu_0 \times exp\left(\beta\sqrt{E}\right), \qquad (2)$$

where μ is the mobility, μ_0 is the mobility in zero field, β is the factor of the field dependence, and E is the localized electric field.

Finally, we consider the trapping effect of lower concentration doped [3]. In the lower concentration, the behavior of carrier transporting in guest states is like that the carriers have been trapped in these lower density states. So we develop 2D model, and decide where the dopant is in the host material by random seeding method. Fig. 2 shows the distribution of Firpic with 12% dopant density.

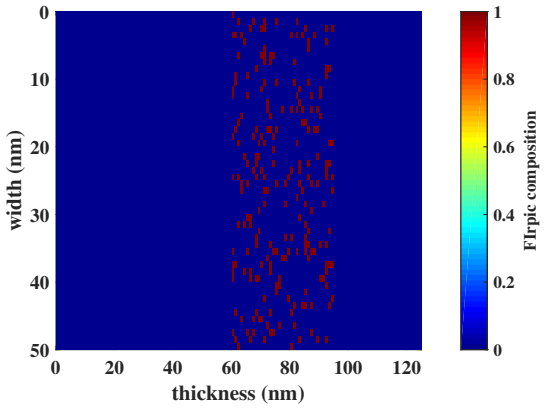

Fig. 2: The random distribution of 12% FIrpic .

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TABLE I: Simulation parameters settings for OLED

Material	$N_{te}\ (cm^{-3})$	$E_{te}(eV)$	$\sigma_e(eV)$	$N_{th}\ (cm^{-3})$	$E_{th}(eV)$	$\sigma_h(eV)$	$\mu_{0e}\left(\frac{cm^2}{Vs}\right)$	$\beta_e\left(\frac{cm^{0.5}}{V^{0.5}}\right)$	$\mu_{0h}\left(\frac{cm^2}{Vs}\right)$	$\beta_h\left(\frac{cm^{0.5}}{V^{0.5}}\right)$
NPB	1×10^{21}	2.3	0.15	1×10^{21}	5.4	0.13	1×10^{-7}	0.005	2×10^{-4}	0.0015
mCP	1×10^{21}	2.4	0.15	1×10^{21}	5.9	0.15	4×10^{-5}	0.00426	1.2×10^{-4}	0.00254
BImBP	1×10^{17}	2.6	0.111	1×10^{17}	6.2	0.111	1.9×10^{-9}	0.005	2×10^{-4}	0.0015
TAZ	1×10^{21}	2.7	0.07	1×10^{21}	6.3	0.08	8.57×10^{-6}	0.003	1.4×10^{-8}	0.0035

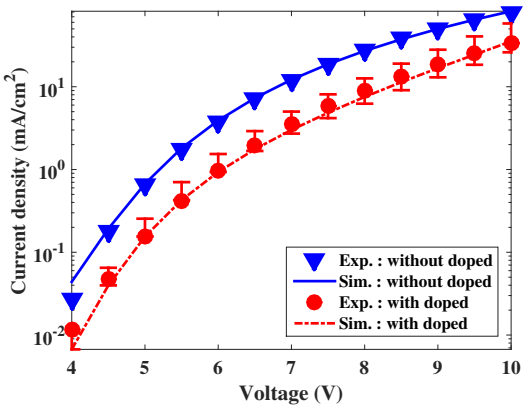

Fig. 3: The J-V curve of experiment and simulation with and without 12% FIrpic doped.

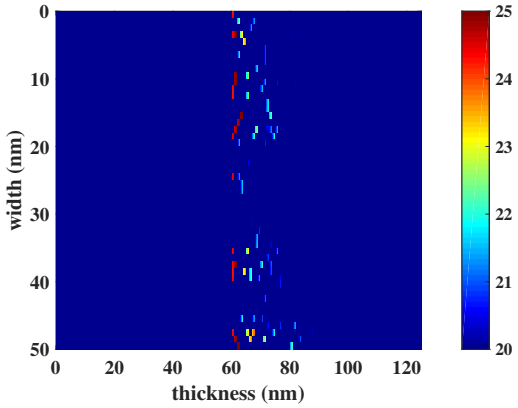

Fig. 5: The distribution of emitting area at 9 V.

III. Results And Discussion

Fig. 3 shows the J-V curve of experimental and simulated results. First, without any doped, we simulate the structure as mentioned in Fig. 1 and the parameters settings are shown in Table I. First, using these parameters without any doping can get blue solid curve. We set the random distribution doping and both N_t of electron and hole are $1\times10^{18}\text{cm}^{-3}$, E_t are at LUMO and HOMO, and σ are 0.2 eV in FIrpic. Refer to [4], μ_{0e} is 1×10^{-9} cm^2/Vs, β_e is 0.0075 $\text{cm}^{0.5}/\text{V}^{0.5}$, μ_{0h} is 2×10^{-9} cm^2/Vs, and β_h is 0.0065 $\text{cm}^{0.5}/\text{V}^{0.5}$ in FIrpic. Then we can get the red dashed curve. So we have pretty good simulated results. Fig. 4 is the distribution of LUMO in 2D area. And as expected, light emitting region is mainly at the interface between mCP and BImBP (see Fig. 5).

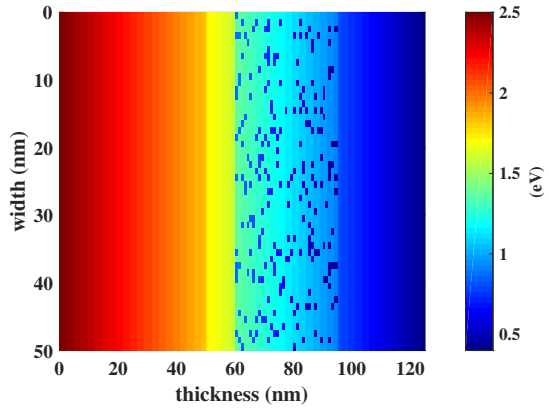

Fig. 4: The distribution of LUMO at 0 V.

IV. Conclusion

In this paper, We have developed 2D organic material model, not only considering Gaussian-like DOS, field-dependent mobility, but random distribution of doping in order to solve the problems of trapping and detrapping. Furthermore, we need more experimental data to make sure the setting parameters is more accurate.

V. Acknowledgments

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