Modeling for Carrier Transportation in Organic Light-emitting Diode by Considering Effective Tail States

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***Abstract*—We developed the 1D Poisson and drift-diffusion Solver by considering the effective tail states and field-dependent mobility to simulate the organic materials, such as NPB or TAZ. With the obtained tail state distribution and the field dependent mobility model, we applied this result in modeling organic light emitting diodes.**

***Index Terms*—Organic, OLED, NPB, TAZ, simulation**

I. INTRODUCTION

For the typical inorganic Poisson and drift-diffusion solver, there are a few problems which make the modeling of organic material difficult. The first issue is that the semiconductor has a well-defined bandgap and density of state (DOS). However, although the organic material has the similar concept of highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), there are still many tail states, defect states distributed in the bandgap. Therefore, the Schottky contact emerged at the heterojunction interface of metal/organic materials is not a perfect barrier. Therefore, in modeling, we cannot treat the contact to be a perfect Schottky barrier junction and carriers do not flow in the traditional bandedge but in those tail states.

To improve this, we localized tail states to the Poisson and drift-diffusion solver, and to find the effective distribution of tail states. In this paper, we assume that the tail state distribution as Gaussian distribution and add this tail state into the traditional semiconductor model. The $N_{tail,DOS}\left(E\right)$ can be expressed

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

Where N_t is the total tail state density. E_t is the Gaussian peak position and σ is relative to the broadening factor of this Gaussian shape tail states.

Besides, we know that the process of carrier transportation in organic molecular is known as hopping process, which is different from the traditional diffusion process of typical inorganic semiconductor. According to the previous work, the effective mobility of hopping process is related to the temperature, the electric field and the local carrier density.

In Bassler's work, it shows the dependence of temperature. In addition, the hopping ability actually improves as the electric field increases because the electric field assist carriers to leave their original localized states. Therefore, to model the carrier transport, we also need to use the so-called Poole-Frenkel field dependent mobility.

In Miller-Abrahams model, we know that the local carrier density might affect the hopping rate from site to site. In high carrier density region, the carriers will occupy the states which the distance from site to site is more closer than the low carrier density region. It makes the carriers easier to hop inter states, which the mobility is higher.

To simplify the equation in numerical simulation, we got the expression of mobility

$$\mu = \mu_0 \exp\left[-\left(\frac{T_0}{T}\right)^2\right] \exp\left(\beta\sqrt{E}\right) \exp\left[u\left(2C\right)^{\nu}\right] \quad (2)$$

By fitting the characteristics of a single material measured by the experiment, we can analyze the properties of OLED such as the I-V curve, the IQE, etc.

II. RESULT AND DISCUSSION

To find the effective tail states of a single organic material, we fit the I-V curve for the data from experiment. By tuning the Gaussian distribution of tail states and the field-dependent mobility, we get the effective states. Then, using the same distribution and mobility to simulate the others with different thickness, the I-V curves are supposed to be identical with the experiment.

A. The Hole Transporting Layer (HTL)

For the hole transporting layer, the hole mobility dominates the process of carrier transport. Therefore, we added the effective Gaussian shape tail states around the HOMO to increase the hole injection at the interface of HTL and contact. One of material has been widely used for HTL of OLED which is called NPB. For NPB, the HOMO is 5.5 eV, and the LUMO is 2.5 eV [1]. The cathode (Al) work function is 4.0 eV, and the anode (ITO) is 5.1 eV. As shown in Fig. 1(a), with fitting the measured I-V characteristics of ITO/NPB/Al hole-only devices, we found that the density of Gaussian distribution of effective tail states N_t is $1 \times 10^{18}\text{cm}^{-3}$, the σ is around 0.05 eV, the peak value of distribution (E_t) is at the HOMO. Also, the zero-field mobility (μ_0) of the Poole-Frenkel field

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dependent mobility is $1 \times 10^{-4}\text{cm}^2/\text{Vs}$, the β is 0.03. Note that β is slightly larger in this fitting but this may be affected by the poor contact properties ITO and we will need to further verify this.

B. The Electron Transporting Layer (ETL)

For the electron transporting layer, the electron mobility dominates the process of carrier transport. We added the effective states around the LUMO to increase the electron injection at the interface of ETL and contact. TAZ is one of ETL which has been widely used in OLED. The HOMO and LUMO of TAZ are 6.3 eV and 2.7 eV, respectively [2]. The Al/LiF work function of cathode and anode is about 3.1 eV. As shown in Fig. 1(b), by fitting the I-V characteristics of Al/LiF/TAZ/LiF/Al electron-only devices, we found that the N_t of Gaussian distribution of effective tail states is $3 \times 10^{17}\text{cm}^{-3}$. The σ is 0.2 eV, and the peak value of distribution (Et) is 0.1 eV below the LUMO. In addition, the zero-field mobility of the Poole-Frenkel field dependent mobility is $5 \times 10^{-9}\text{cm}^2/\text{Vs}$ and β is 0.01.

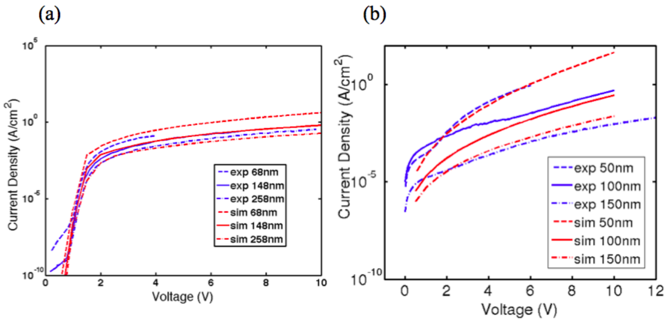

Fig. 1. (a) I-V characteristics of experiment [3] and simulation with different NPB thickness (b) I-V characteristics of experiment [3] and simulation with different TAZ thickness

C. The modeling of proposed OLED structures

Furthermore, we simulate a multi-layer OLED as shown in the inset of Fig. 2 [4]. The structure is composed of 4 layers. NPB is the hole injection layer (HIL), mCP is the hole transporting layer (HTL), ID-1 is the emitting layer (EML), TAZ is the electron transporting layer (ETL). Here, the simulation parameters of the NPB and TAZ are the same as previous sections. Due to the thickness of mCP layer is not quite large, the field-dependence is not included in the mCP and we set a fixed hole mobility as $5 \times 10^{-4}\text{cm}^2/\text{Vs}$ for mCP (HTL). The emitting layer is made from the ID-1 and the 12% of FIrpic. The HOMO and LUMO of this emitting layer are 6.2 eV and 2.6 eV, respectively. In addition, we added two sets of effective tail states for electron and hole. For the electrons in ID-1, we set the N_t of Gaussian distribution of effective tail states is $5 \times 10^{18}\text{cm}^{-3}$, the full width at half maximum is 0.15eV, the peak value of distribution(Et) is 0.5 eV below the LUMO. For the holes in ID-1, we set the density of Gaussian distribution of effective tail states N_t is $5 \times 10^{18}\text{cm}^{-3}$, the σ is around 0.15 eV, the peak value of distribution (Et) is 0.4 eV above the HOMO. The energy difference is 2.7 eV, which corresponds the emission wavelength of the OLED structure reported by experiments. Due to the lack of experiment, we assume the zero-field mobility μ_0 of electron to be $3 \times 10^{-7}\text{cm}^2/\text{Vs}$, and β to be 0.0016. The μ_0 and β of hole are $3 \times 10^{-7}\text{cm}^2/\text{Vs}$ and β 0.0016, respectively. Fig. 2 shows the I-V characteristic of experiment and simulation, the blue one is the data of experiment, the green one is our simulation result. The driving voltage of simulation and experiment are about 6.9 eV and 7.1 eV at 2 mA/cm^2, respectively.

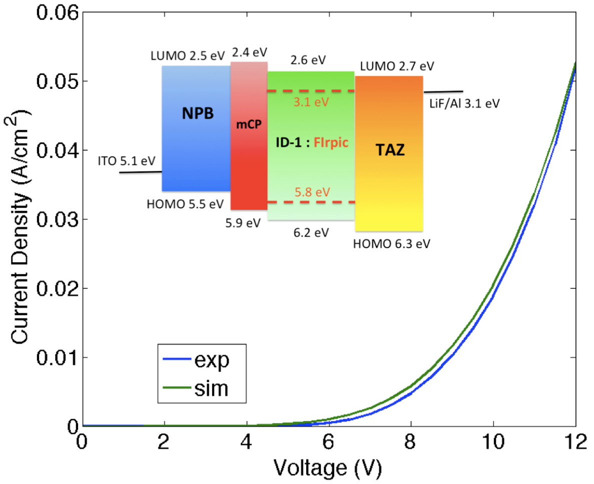

Fig. 2. Band diagram and I-V characteristic of ITO/NPB/mCP/ID-1:FIrpic/TAZ/LiF/Al device

III. CONCLUSION

In this paper, we have developed our 1D Poisson and drift-diffusion solver by considering the tail states of organic material and field-dependent mobility. We modeled the I-V characteristics of single layer organic materials such as NPB and TAZ to calibrate the basic material parameters. Then we applied this parameters in predicting the I-V characteristic of a proposed OLED device and get a reasonable fitting. Further experimental examination will be needed in the future work to make parameters setting more accurate.

IV. ACKNOWLEDGMENTS

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