Numerical Simulation of P3HT Based Organic Light Emitting Diode

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Abstract: Recently, organic light emitting diodes (OLEDs) have become quite popular in the field of microelectronics like optoelectronics application, modulated light source and internet connection etc. Owing to the advantages of solid-state, self-emission, full color capability and flexibility, OLED has been recognized as one of the most promising flat panel display technology. This paper presents the results of single polymer layer OLED (ITO/P3HT/Ca) 1D and 2D-numerical simulation and analysis using Silvaco TCAD tools, which is a physically-based simulator. The physically-based simulation of the electrical and optical characteristics, such as luminescence power, current density versus electric field, current versus voltage and I-V characteristics for different thicknesses and doping concentration of emitting layer is presented. The distribution of Langevin recombination inside the structure is also presented and discussed for better understanding of physical processes and operation principal of OLED.

Keywords: Organic light emitting diode, Atlas, Silvaco TCAD, Simulation, P3HT.

1. INTRODUCTION

In last decade enormous research has been done by various researchers all over the world in the field of organic devices, OLEDs are one of them. In particular, organic light emitting diodes (OLEDs) gradually over rule the inorganic diodes due to the following advantages. OLEDs are brighter, flexible, cheaper, lightweight, transparent, wide view angle and provide faster response than inorganic ones [1]. OLEDs has huge range of application which includes fabrication of thin and flexible displays for TV, GPS navigators, digital cameras, portable media players, car radios and night-vision devices among others. OLEDs have been widely used long ago in most Motorola and Samsung color mobile phones, as well as some LG, Nokia and Sony Ericsson models [1]. Moreover, OLEDs are quite attractive as optoelectronic applications for communication purposes. They are widely used as modulated light sources (fiber optic signal transmission, remote control devices, light phones).

In this paper, single layer polymer OLED is investigated and its electrical optical characteristics obtained through the Technology Computer Aided Design (TCAD) software ATLAS from Silvaco [2]. ATLAS is a physics-based, 2D and 3D device simulator that predicts the electrical behavior of specified semiconductor structures and provides insight into the internal physical mechanisms associated with device operation. It gives detailed knowledge about the components included in device during operation like

two-dimensional profile of carrier concentration, electric field and current density profiles etc. Simulation and modeling of OLEDs within the framework of TCAD can provide the necessary information about device characteristics, also it helps to look inside the structure and allow us to avoid the long and costly device optimization process by numerous experimental runs. Technology and device modeling with a help of Technology CAD are widely used in organic electronic components development and manufacturing and many scientists around the world are interested in the investigations in this sphere [3-30].

The rest of the paper is organized as following. Section II contain general information about OLEDs, their structure, materials, and operating principles, describes the process of OLED simulation including the building of device structure, choosing the physical models and getting the distribution of Langevin recombination. Section III presents the simulation results and electrical and optical characteristics. Section IV draws the conclusions from this work.

2. SIMULATION

A. Device Structure

The simplest OLED structure consists only one active polymer layer/emissive layer (EML) sandwiched between two charged electrodes, anode and cathode. The active layer is composed by conducting polymer, e.g. polythiophenes (Pts), poly p-phenylene vinylene (PPV), poly N vinylcarbazole (PVK), or polyaniline (PANI).

The top electrode of OLED (cathode) is a metallic mirror with high reflectivity made of calcium and bottom

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electrode (anode) is indium tin oxide (ITO), which is transparent. The active layer is made up of P3HT. The electrical circuit diagram and structural diagram of OLED is shown in Figure 1 and 2 respectively.

Figure 1: Electrical circuit diagram of OLED.

Figure 2: Structural diagram of OLED.

Poly(3-hexylthiophene) P3HT is a regioregular (Describing a polymer in which each repeat unit is derived from the same isomer of the monomer) semiconducting polymer. It is used in organic electronics primarily because of its regular end-to-end arrangement of side chain, which allows efficient π - π stacking of the conjugated backbones.

Figure 3: Molecular structure of P3HT.

B. Operating Principle

When a voltage is applied to the electrodes the charges start moving in the device under the influence of the electric field. Electrons are injected by the cathode into the lowest unoccupied molecular orbital

(LUMO) of the adjacent molecules and holes are injected by the anode into the highest occupied molecular orbital (HOMO). Electrons leave the cathode and holes migrate from the anode in opposite direction. A fraction of them recombines and thus leads to excitons formation, some of which decay radiatively to the ground state by spontaneous light emission. Therefore, the electrical power applied between the anode and cathode is transformed into light.

For modeling and simulation of OLED structure, a commercially available device simulator ATLAS was used which provides general capabilities for accurate simulation of organic devices. Here we firstly define a mesh of structure (a series of vertical and horizontal lines and the spacing between them) using Atlas syntax. A good mesh is important for accuracy and numerical efficiency of model. Once mesh is defined, we assigned a material for every part of device [5]. Finally, the location of electrodes and doping level in each region is specified. After this we specify material parameters like permittivity, bandgap, carrier concentration, density of state in order to obtain electrical and optical characteristics of OLED. Furthermore, the polymer mobility parameters including carrier's mobility, thermal activation energy at zero electric field for the Poole-Frenkel-like mobility model and the workfunction for electrodes were also specified. Table 1 contains list of various parameters used for simulation purpose of P3HT based OLED.

Table 1: Parameters Used in P3HT- Based OLED Simulation

Parameters	Values
Thickness	50nm
Electron affinity	3.5eV
Bandgap	1.7eV
Dielectric constant (ϵ)	3
Hole mobility (μ_h)	$1 \times 10^{-2} \text{ cm}^2/\text{Vs}$
Electron mobility (μ_n)	$1 \times 10^{-4} \text{ cm}^2/\text{Vs}$
Effective density of states in the conduction band (N_c)	$2 \times 10^{21} \text{ cm}^{-3}$
Effective density of states in the valance band (N_v)	$2 \times 10^{21} \text{ cm}^{-3}$
Acceptor concentration	$5.75 \times 10^{17} \text{ cm}^{-3}$
Activation energy at zero electric field for holes (deltaeap.pfmob)	$1.792 \times 10^{-2} \text{ eV}$
Hole Poole–Frenkel factor (betap.pfmob)	$7.758 \times 10^{-5} \text{ eV}(\text{cm/V})^{1/2}$

C. Physical Models

For OLEDs, several organic models like Poole-Frenkel-like mobility model, Langevin bimolecular recombination model and the singlet exciton model are used to describe the charge transport in the OLEDs. Poole-Frenkel-Like mobility model and Langevin recombination model are used to describe the transport and recombination mechanism of the polymer respectively, while the singlet exciton model is used to calculate the radiative rate for luminescence due to the Langevin recombination in the OLED.

The Poole-Frenkel mobility model describes the charge transport through the sub-bandgap density of state [6] and expressed by the following equations

$$\mu_n(E) = \mu_{n0} \exp\left(\frac{-\text{DELTAEN.PFMOB}}{kT_{\text{neff}}} + \left(\frac{\text{BETAN.PFMOB}}{kT_{\text{neff}}} - \text{GAMMAN.PFMOB}\right)\sqrt{|E|}\right) \quad (1)$$

$$\mu_p(E) = \mu_{p0} \exp\left(\frac{-\text{DELTAEP.PFMOB}}{kT_{\text{neff}}} + \left(\frac{\text{BETAP.PFMOB}}{kT_{\text{neff}}} - \text{GAMMAP.PFMOB}\right)\sqrt{|E|}\right) \quad (2)$$

where $\mu_n(E)$ and $\mu_p(E)$ are the Poole-Frenkel mobilities for electrons and holes respectively, μ_{n0} and μ_{p0} are the zero field mobilities for electrons and holes respectively, and E is the electric field. DELTAEN.PFMOB and DELTAEP.PFMOB are the activation energy at zero electric field for electrons and holes respectively. BETAN.PFMOB is the electron Poole-Frenkel factor, and BETAP.PFMOB is the hole Poole-Frenkel factor. Tneff and Tpeff are the effective temperature for electrons and holes respectively.

Due to the strong dependence on the electric field, the Poole-Frenkel mobility model can cause convergence problems. To increase the stability of the Poole-Frenkel mobility model, the following equations are used [5].

$$\mu_p(E) = \frac{1}{\frac{1}{\mu_p(E)} + \frac{1}{\mu_{p\text{lim}}(E)}} \quad (3)$$

$$\mu_n(E) = \frac{1}{\frac{1}{\mu_n(E)} + \frac{1}{\mu_{n\text{lim}}(E)}} \quad (4)$$

where $\mu_n(E)$ and $\mu_p(E)$ are mobilities for electrons and holes respectively, $\mu_{n\text{lim}}(E)$ and $\mu_{p\text{lim}}(E)$ are limiting mobility calculated from the thermal velocities.

The distribution of singlet excitons is used to infer the radiative rates for luminescence or phosphorescence in organic material LEDs. In Atlas, we can self-consistently solve the singlet exciton continuity equations along with the electron and hole drift diffusion equations. The singlet exciton continuity equation is given by [6]

$$\begin{aligned} \frac{dS(x, y, t)}{dt} = & [RST.EXCITON R_{Ln,p} + (F.GENSINGLET(x, y, z, t, n, p)) + \\ & \left(\frac{RST.TT.EXCITON}{1 + RST.TT.EXCITON} KTT.EXCITON T^2(x, y, t) \right) - \\ & (KISC.EXCITON S(x, y, t)) - (KST.EXCITON S(x, y, t) T(x, y, t) - (K_{dd} S(x, y, t)) \\ & - KSP.EXCITON S(x, y, t) (n(x, y, t) + p(x, y, t) - \\ & \left(\frac{KSS.EXCITON}{2} S^2(x, y, t) \right) - KNRS.EXCITON \\ & S(x, y, t) - \frac{PHEFF.EXCITON}{TAUS.EXCITON} S(x, y, t) + D_s \partial S(x, y, t) - \\ & Q(x, y) S(x, y, z) - R_{Dn,p} S(x, y, t) + G_{ph} \\ & QE.EXCITON] \end{aligned} \quad (5)$$

where,

$S(x, y, t)$, $T(x, y, t)$ = Spatial and temporal singlet exciton and triplet exciton density respectively.

$RST.EXCITON$ = Fraction of singlets formed during Langevin recombination,

$RST.TT.EXCITON$ = Fraction of singlets formed during triplet-triplet annihilation,

RLn,p = Langevin recombination rate,

$n(x, y, t)$ and $p(x, y, t)$ = Electron concentration and hole concentration,

$TAUS.EXCITON$ $TAUT.EXCITON$ = Singlet radiative decay lifetime and Triplet radiative decay lifetime respectively.

$KISC.EXCITON$ = Intersystem crossing constant

$KST.EXCITON$ = Singlet-triplet constant

$KSP.EXCITON$ = Singlet-polaron constant

$KTT.EXCITON$ = Triplet-triplet constant

KNRS.EXCITON and KNRT.EXCITON = Singlet non-radiative decay constant and triplet non-radiative decay constant respectively.

kdd = Dipole-dipole exciton transfer rate (Forster)

$Q(x,y)$ = Metal quenching rate

PHEFF.EXCITON = Host photoluminescence quantum efficiency.

RDn,p = Exciton dissociation rate

Gph = Photoabsorption rate

QE.EXCITON = Proportion of absorbed photons that is responsible for generating singlets

The bimolecular recombination rate is described by Langevin recombination rate that is given by the following equation

$$R_{L,p} = r_L(x, y, t) (np - ni^2) \quad (6)$$

where ni is intrinsic carrier concentration, $r_L(x, y, t)$ is Langevin recombination rate coefficient.

The Langevin recombination rate coefficient expressed as [7]

$$R_L(x, y, t) = A_{LANGEVIN} \frac{q [\mu_n(E) + \mu_p(E)]}{\varepsilon_r \varepsilon_0} \quad (7)$$

where ε_r is relative permittivity, ε_0 is absolute permittivity, $A_{LANGEVIN}$ specifies the prefactor for the bimolecular Langevin recombination model. By default, the value of model parameter $A_{Langevin}$ is 1.

OLED structure and Langevin recombination using Silvaco TCAD tonyplot is shown in Figure 4 and 5 respectively.

Figure 4: Structure of OLED in Silvaco Atlas.

Figure 5: Langevin recombination rate.

Figure 6: Conduction band energy and valence band energy.

Conduction band energy and valence band energy is given in Figure 6. Figure 7 shows 1D-mode simulated singlet exciton density distribution.

Figure 7: 1D-mode simulated singlet exciton density distribution.

3. RESULTS AND DISCUSSION

I-V characteristic, luminescence power and current density versus electric field are obtained to estimate the performance of the OLED. The electrical characteristics of the device were obtained by changing the desired parameters (thickness and doping concentration) in the Silvaco TCAD Atlas file and the results of simulation are visualized in Tonyplot.

Figures 8, 9 and 10 represents I-V characteristics, luminescent power and electric field vs. current density of OLED for different thicknesses of emitting layer (P3HT) (60, 120, 180 and 240 nm) respectively.

Figure 8: I-V characteristics of OLED for different thickness of emitting layer (P3HT)

It is evident from the figure that the device "turns-on" at about 1.2 Volt and as the anode voltage increases, the potential luminescent power increases. It is also clear from the figure that the intensity of light decrease as the thickness of emitting layer (P3HT) increases thus it may concluded that it is better to make emitting layer thinner.

Figure 9: Luminescent power vs anode voltage for different thickness of P3HT

Figure 10: Electric field vs. current density for different thickness of P3HT

Similarly, Figures 11, 12 and 13 represents I-V characteristics, luminescent power and electric field vs. current density of OLED for different doping concentration of P3HT respectively.

Figure 11: I-V Characteristics for different doping concentration.

Figure 12: Luminescent power vs anode voltage for different doping concentration of P3HT.

Figure 13: Electric field vs. anode current for different doping concentration.

CONCLUSION

In this paper, the structure, materials and operation principle of OLED with P3HT as the emitting layer is presented. 1D and 2D simulation of OLED were conducted using Silvaco TCAD software to investigate the device and predict its electrical and optical characteristics. The process of simulation is based on solving the differential equations describing the transport and recombination mechanism of the polymers and calculating the radiative rate for luminescence due to Langevin recombination in the OLED. Using TCAD tools we have obtained luminescence power characteristics, current density versus electric field, current density versus voltage and I-V characteristics for different thicknesses and doping concentration of emitting layer (P3HT). Simulations with varying P3HT thickness showed that the decreasing thickness results in improvement of device characteristics.

The performed simulation allowed us to look and analyze physical processes inside the structure for better understanding the operation principles of OLED. Furthermore, the model helps us to optimize the diode design and to avoid time-consuming and costing experiments on real devices, thus streamlining the design process.

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