Device Simulation and Performance Enhancement of OLED Using Higher Recombination Rate

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Abstract: - Currently, researchers are interested in the field of organic light-emitting diodes (OLEDs). OLEDs are used in a variety of applications, such as displays, for lighting, digital cameras, MP3 players, mobile phones, PDAs, and some notebook displays. One of the most important applications of OLEDs is the flat panel display due to its self-illumination and full color capabilities flexibility. This article describes the comparison of single-layer and multi-layer organic light-emitting diodes in one- and two-dimensional numerical simulation and analysis, using the Silvaco TCAD tool, a physics-based simulator. Electrical and Optical Properties, such as Luminous Power and Applied Bias This paper presents voltages, current and voltage, current density and electric field, and IV characteristics under dark conditions for different thicknesses and doping concentrations of the organic light-emitting layer.

Index Terms - Organic Light emitting diode (OLEDs), Multilayer, ATLAS, Silvaco TCAD.

I. INTRODUCTION

In the past two decades, OLED has been the most attractive research topic in the world [1]. The display of organic light emitting diodes (OLEDs) has many advantages over conventional display devices, such as high brightness, fast response time and high luminous efficiency, light weight, and most importantly low power consumption [2, 3]. An organic light emitting diode (OLED) is an electronic device consisting of one or more semiconducting organic layers interposed between two thin film conductive electrodes, one of which must be transparent. Carbon-based molecules are used in OLEDs that illuminate light as it passes through the organic layer. An OLED is an energy conversion device that converts electricity into light based on an electroluminescence phenomenon. Electroluminescence is a method of illuminating an organic material through which an electric current passes. The OLED consists of one or more semiconducting organic thin films interposed between two electrodes, one of which must be transparent. A typical OLED is shown in Figure 1. Indium tin oxide (ITO) is a high work function metal used as a cathode and is often used as a transparent anode. The device is fabricated by depositing an organic film in chronological order and then depositing a thin metal cathode defined by a shadow mask onto a transparent substrate, such as glass or flexible plastic. When an external bias is applied to the device into the organic semiconductor layer, holes and electrons are injected from the anode and the cathode, respectively. The holes and electrons in the organic layer move and recombine to form excitons. Finally, the excitons fail to illuminate and illuminate through the substrate state."Heterogeneous structure" has become the standard practice of OLED design. Electrons and holes injected from the cathode and the anode, respectively, are collected at the hetero junction. The probability of electron-hole recombination at this organic/organic interface will increase, which results in a relatively high efficiency. This breakthrough has also attracted many chemists and engineers to focus on the further development of high-performance OLEDs. In the past two decades, efforts have been made to maximize device efficiency through the design of [4, 5] and the synthesis of new materials and device engineering [6, 8]. By using a highly efficient emitter in photoluminescence (PL), the internal quantum efficiency of the OLED is greatly increased. This work is also recognized as another milestone in the development of OLEDs.

In electrode design, Mg was used as a cathode in early device designs. However, Mg is very sensitive to moisture and oxygen and is therefore prone to oxidation, resulting in a very short life. Tohoku Pioneer uses Li compounds (such as Li 2 O) as an electron injection layer to achieve another breakthrough in OLEDs, so that a more stable metal Al acts as a cathode. Currently, LiF / Al double-layer cathodes are the most commonly used cathodes for injecting electrons into devices. Indium tin oxide (ITO) is a commonly used anode due to its high electrical conductivity and transparency. In fact, almost all device designs and optimizations are based on ITO. Prior to making the device to study, the effects of the three-dimensional layer were introduced into the OLED structure, and these structures were analyzed using a Software Silvaco Atlas 2-D digital device simulator. The simulator helps understand the physical structure of the device in a good way. User-defined materials can also be used in this simulator. In the Atlas simulation process, we first define the dimensions, structure, and mesh. Second, the physical model of the device is defined. Third, the parameters of the organic material are extracted after applying the operating bias conditions. [11][12]. Both optical (photoluminescence) and electrical (electroluminescence) excitation can be formed by exciton state. In the electrical excitation, if singles and triplets are formed with equal probability, 25% of the excitons would be singlets and 75% would be triplets.

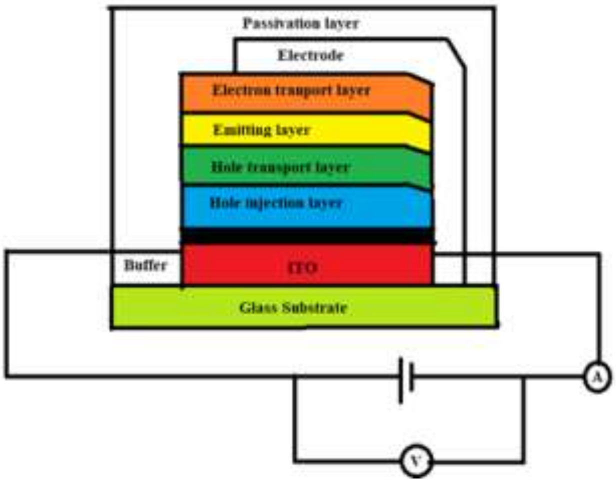

Fig 1: Multilayer OLED device structure

The following is a physical and mathematical description

$$\mu_n(E) = \mu_{n0}\exp\left(\frac{-DELTAEN.PFMOB}{KTneff} + \left(\frac{BETAN.PFMOB}{KTneff} - GAMMA, PFMOB\right)\sqrt{|E|}\right) \qquad \text{Eq 2.1}$$

$$\mu_p(E) = \mu_{\rho 0}\exp\left(\frac{-DELTAEP.PFMOB}{KTneff} + \left(\frac{BETAP.PFMOP}{KTneff} - GAMMP.PFMOB\right)\sqrt{|E|}\right)$$

where,
DELTAEN.PFMOB, DELTAEP.PFMOB = Activation energy at zero electric field for electrons and holes respectively.
µn0 (E) = Field dependent mobility
µn0= Zero field mobility
E = Electric field
BETAN.PFMOB, BETAP.PFMOB = Electron and hole Poole-Frenkel factor respectively.
To forecast the results of OLEDs under proper boundary conditions, The Langevin recombination rate coefficient is given by

$$R_L(x,y,t) = A \text{ LANGEVIN } \frac{q[\mu_n(E) + \mu_p(E)]}{\epsilon_r \epsilon_o}$$

where,
R = rate of recombination
e= the charge of electron which is 1.6 × 10-19,
μ_e = Mobility of electron,
μ_h =Mobility of hole,
ε= Permittivity of material,
ε_o= Permittivity of air which is 8.85×10^{-12} F/cm.

If the logical parameter KOSTER is specified on the MODEL statement, the Langevin rate is given by:

$$R_L(x,y,t) = A \text{ LANGEVIN } \frac{q_{min}(\mu_n \mu_\rho)}{\epsilon_r \epsilon_o}$$

The Langevin recombination rate is given by:

$$R_L\, n,p = r_L(x,y,t)(np - ni^2)$$

The fundamental equations consist of Poisson's equation, the continuity equations and the transport equations as follows
Poisson's Equation shows relation between variations in the electrostatic potential and local charge density of electrons and holes.
It is mathematically described by the following relation [7].

$$\nabla.(\varepsilon\nabla\psi) = -\rho$$

$$\nabla.(\varepsilon\nabla\psi) = -q\,(p-n+N_d^+-N_a^-)$$

Where,ψ= electrostatic potential
ρ = local space charge density
ε= local permittivity of the semiconductor (F/cm)
N_d^+ = ionized donor density(cm^{-3})
p= hole density (cm^{-3})
n = electron density (cm^{-3}) and

N_a^-= ionized acceptor density(cm^{-3}).

The reference potential is still considered to be the intrinsic Fermi potential for ATLAS simulation.
To account for the trapped charge, Poisson's equations are modified by adding an additional term Q_T, representing trapped charge:

$$\nabla.(\varepsilon\nabla\psi) = -q\,(p-n+N_d^+-N_a^-) - Q_T$$

Where $Q_T= q\,(N_{tD}^+ + N_{tA}^-)$.Here N_{tD}^+ and N_{tA}^- =ionizeddensity of donor like traps and ionized density ofaccepter like traps respectively For electrons and holes, the continuity equation sure defined as follows[7].

$$\frac{dn}{dt} = \frac{1}{q}\,\nabla.J_n + G_n - R_n \qquad \text{Eq 2.2}$$

$$\frac{dn}{dt} = \frac{1}{q}\,\nabla.J_p + G_p - R_p \qquad \text{Eq 2.3}$$

Where, n and p = The electron and hole concentrations
Jn and Jp= The electron and hole current densities
Gn(Rn) and Gp(Rp)=The generation(recombination) rates for the electrons and holes respectively
q =The fundamental electronic charge.

The drift-diffusion model is described as follows [7].

$$J_n = qnu_nE_n + qD_n\,\nabla_n$$

$$J_p = qnu_pE_p + qD_p\,\nabla_p$$

Where, µn and µp = the electron and hole mobility's
Dnand Dp=the electron and hole diffusion constants
En and Ep = the local electric fields for electrons and hole respectively
∇nand ∇p=the three dimensional spatial gradient of n and p.

The area of the device is 10^8 µm^2. Indium tin oxide (ITO) is used as anode for hole injection due to its high work function and transparency. The cathode used here is of LiF/Al as electron injection. The two-layer device contained of a stack of 1-Naphdata and Alq_3 each, whereas the three-layer device consisted of a stack of 1-Naphdata, α-NPD, and Alq3. The organic layers were inserted between ITO and LiF/Al electrodes.

TABLE I. Simulation Parameters

Parameters Used	**Value**		
	1Naphdata	**α-NPD**	**Alq3**
Thickness of active layers (µm)	0.06	0.02	0.02
Band gap of active material(ev)	5.5	3.1	2.8
Electron affinity (ev)	2.3	2.4	3
Relative Permittivity	3.5	3.5	3.5
Hole mobility (cm^2/vs)	1.1e^{-4*2}	2.13 e-^{05*2}	5.52e-^{06*2}
Electron mobility (cm^2/vs)	8.83e^{-5*2}	5.15 e-^{6*2}	3.68e-^{7*2}
N_C300 (cm^{-3})	2e^{19}	2e^{19}	2e^{19}
N_D300 (cm^{-3})	2e^{19}	2e^{19}	2e^{19}

II. SIMULATION AND RESULTS

Efficiency can be increased by adding EML (emitter layer). After manufacturing a single layer, the two-layer and three-layer OLED L-V characteristics of device structure 3 are superior to those of device 2. Due to the higher recombination rate, the three-layer structure has Low anode current but high luminescence power [10]. Higher recombination rate because the organic/organic interface reduces the energy barrier height and enhances carrier injection. The current depends on voltage and temperature. The current density should also follow The number of layers increases and increases. The rate of recombination depends on the mobility of the holes, electrons and the dielectric constant of the materials used. The recombination of carriers is the most important phenomenon in OLEDs because the light emission is completely dependent on it. By adding more layers of high dielectric constant, the recombination rate can be increased. The probability of recombination due to electrons and holes increases the likelihood of exciton formation. Therefore, the number of photons increases and the emission of light increases.

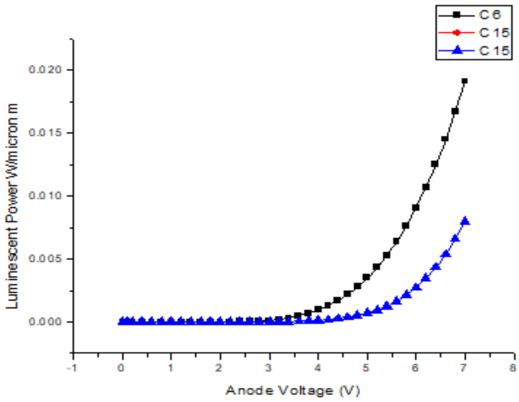

Fig 2: L-V characteristics of Device structures

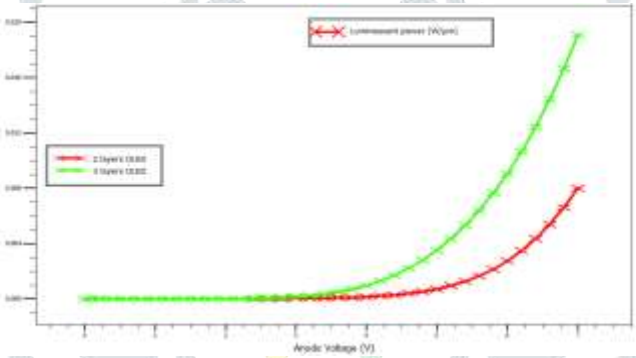

Fig 3: Comparative Analysis of Power Output of Device structures

In a two-layer OLED, an organic layer is interposed between the hole transport layer and the electron transport layer. ETL is added to the metal cathode and is responsible for transporting electrons from the cathode to the emissive layer (EML). The ETL used here is Alq3. The hole transport layer (HTL) used herein is 1-naphdata. The purpose of this layer is to transport holes from the luminescent layer to the anode. This must be the analog structure of the p-type semiconductor device 2 as shown.

TABLE II. PARAMETERS FOR BILAYER OLED

Usage	**Material**	**Thickness(µm)**
Cathode	LiF/Al	0.02
Hole Transport Layer	1-naphdata	0.06
Electron Transport Layer	Alq_3	0.02
Anode	ITO	0.02

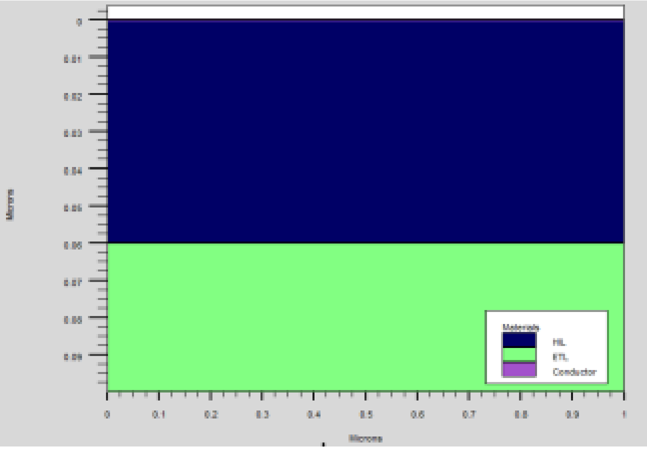

Fig. 4: Simulated structure of Device 2 (Bilayer OLED).

There are many layers in a multilayer OLED, but only one additional luminescent layer is introduced here, as shown in FIG. The EML layer used here is Alq3. An M1L layer is introduced in the middle of the OLED layer. In this layer, electron-hole pairs are recombined to produce photons [13]. By introducing various fluorescent and phosphorescent small molecules, the band gap energy between the HOMO and LUMO levels can be controlled [14].

$$E_g = h\nu Eq$$

Where, Eg = band gap energy
h =the Plank's constant and
ν = the frequency by adjusting Eg
The simulated structure of Device 3 is shown in Fig 4.

TABLE III. PARAMETERS FOR MULTILAYER OLED

Usage	Material	Thickness(μm)
Cathode	LiF/Al	0.02
Hole Transport Layer	1-naphdata	0.06
Emissive Layer	α-NPD	0.02
Electron Transport Layer	Alq_3	0.02
Anode	ITO	0.02

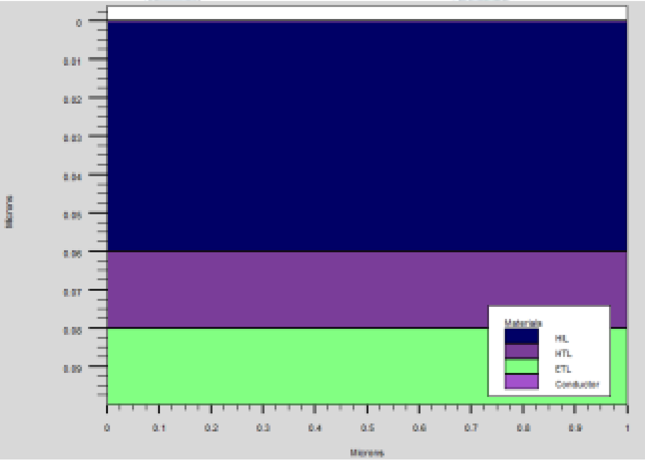

Fig. 5. Simulated structure of Device 3 (Multilayer OLED)

To improve the efficiency of OLEDs the Langevin recombination model is used to predict the results under proper boundary conditions. This model visualizes the conduction due to field enhanced thermal excitation. Increase in biasing voltage improved the recombination rate.

III. CONCLUSION

In this research paper on the addition of organic layers, the luminous efficiency is improved. The device structure 3i.e multilayer OLED produces the highest luminous efficiency, while device structure 2 produces the highest current density. The luminous efficiency and current density of the two-layer and multi-layer OLEDs were extracted and compared. It has been observed that the optimum efficiency of the OLED is demonstrated by the addition of an organic layer.

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