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Optimization of Organic Light Emitting Devices

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Abstract*— A program in MATLAB has been developed for calculating various parameters e.g., Efficient use of excitation energy by proper use of dopants (by studying exciton density profile as a function of time), locating correct position of emission zone (location of charge accumulation layer) and thus enabling maximum recombination in single layer and multilayer devices. The extracted features of organic material are used as input vectors for the standard equations, results in increasing the efficiency of OLED. The test results helps in the analysis of identify the fault and help us to use the device more accurately and has a better emission rate compared to the previous time analysis.

***Index Terms* — OLED, Exciton, Optimization, Organic Material, MATLAB, Device Simulation, Electronic and Optical Model.**

I. INTRODUCTION

In recent years, OLED devices have received considerable attention due to their inherent advantages such as high speed and high driving capability, high brightness, high efficiency, a wide viewing angle and fast response time**.**Due to such unique properties it is used in applications such as displays for mobile phones and portable digital media players, car radios and digital cameras and recently in tablets and TVs and many others. Disadvantages**:** Highly susceptible to degradation by oxygen and water molecules. So its main disadvantage is the smaller lifetime.

The basic OLED comprises an anode and a cathode deposited in a substrate, and sandwiched between these is a layer of organic material. The organic material is electrically conductive because of what is termed the delocalization of pi electrons caused by conjugation over all or part of the molecule. An exciton forms when a photon is absorbed by a semiconductor. This excites an electron from the valence band into the conduction band. In turn, this leaves behind localized positively-charged holes. Thus an exciton is a bound state of an electron and hole which are attracted to each other by the electrostatic Coulomb force.

These organic materials can range from insulators to conductors and are therefore classed as semiconductors. There are two definitions required, highest unoccupied molecular orbital, HUMO, and the lowest unoccupied molecular orbital, LUMO of organic semiconductors. These are analogous to the valence and conduction bands of inorganic semiconductors.

The OLED display consists of a number of layers. A typical stack may include:

- Anode
- Emissive layer
- Conductive layer
- Cathode

To achieve high quantum efficiency in phosphorescent OLEDs, charges and excitons must be confined to the emission region of a device. Therefore, the hole transport material and electron transport material should have shallow lowest-unoccupied-molecular-orbital (LUMO) and deep highest-occupied-molecular-orbital (HOMO) energy levels, respectively. In Polymer/polymer interfaces have an obvious advantage of conducting polymers compared to inorganic semiconductors is that polymers are soluble and can be spin-cast as thin films from solution. Instead of building up thin multi-layers in ultrahigh vacuum, one can make a blend of two or more polymers, spin-cast them as a film in air and have the interfaces already built into wasted that single layer. As one of the main problems with polymer LEDs is that charge carriers (holes in particular) may go through the device without recombining and recreating a photon. That creates wasted current and hence power. The recombination probability can be enhanced by inserting electron (or hole) blocking layers but that increases the thickness of the devices and therefore the driving voltage.

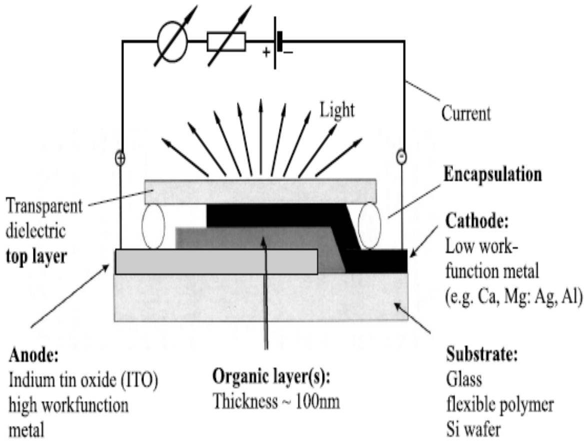

Fig.1 A cross-section through the simplest form of an organic light-emitting diode(OLED). One of the two metallic or metallic-conducting electrodes must be semitransparent to permit the luminescence to exit the device. Typical thicknesses of the organic layer(s) between the electrodes are between 1nm and 100 nm.

EQUATIONS

In this section we present a unified device model for OLEDs which includes charge injection, transport, and space charge effects in the organic material. The equations used are

1. Poisson Equation: It gives relation between Electric field and charge densities.

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$$\frac{\partial E(x)}{\partial x} = \frac{e}{\varepsilon\varepsilon_0}\left(p(x) - n(x)\right) \quad (1)$$

2. Drift and Diffusion term: The current composed of a drift and diffusion term.Here we have assumed mobility is dependent only on field according to Poole –Frenkel equation.

$\mu_n = \mu_0 \exp(E_0)$

where μ is zero field mobility ,E_0 is electric field

$$J_e(x) = e\mu_e(x,E).n(x).E(x)D(\mu)\frac{\partial n(x)}{\partial x} \quad (2)$$

3. Continuity equation:

$$\frac{\partial n(x)}{\partial t} = \frac{1}{e}\frac{\partial J_e(x)}{\partial x} - r(x).p(x).n(x) \quad (3)$$

Where
n = Density of Electrons
P = Density of Holes
E = Electric Field
r = Langevevin recombination rate :

$$r = \frac{e}{\varepsilon\varepsilon_0}.(\mu_e + \mu_p) \quad (4)$$

Solving simultaneously equations 1, 2 and 3 we get the rate equation comprising of exciton generation, diffusion and its recombination rate [1].

(A) Charge Density and Distance from Anode

The prefactor γ for the singlet exciton generation rate is typically taken to be 1/4 following the traditional spin statistics argument. Voltage applied=5Volts and distance from anode, X= 0nm to 100nm

Table1. Material Parameters Used for Device Simulation

S. No.	ETL NPB	ETL ALq3
1	γ =1/4	γ =1/4
2	E_0=5	E_{01}=5
3	d = $\gamma\sqrt{(E_0)}$	d_1 = $\gamma\sqrt{(E_{01})}$
4	$\mu_n=\mu_0 \exp(d)$	$\mu_n=\mu_0 \exp(d_1)$
5	$\mu_0 = 6\times 10^{-6}$	$\mu_0 = 6\times 10^{-6}$

Initially the holes from anode and electrons from cathode pile up and start penetrating into the adjacent layers. The decaying density of the two is due to the recombination of the two in the layers. Thus electron are injected from the right side and holes from the left side and exhibit a fall in their respective densities according to the recombination and a very few holes reach the opposite side cathode and similarly a very few electron to the anode side. Since the hole mobility is lower in Alq3 than electron, Alq3 acts as a electron transport layer and hindrance for the hole. As a result more and more electron and hole tend to recombine and the highest recombination density occurs at the interface. But here for the uniformity of the graph the two motilities of the hole and electron in the two layers are taken as a same constant.

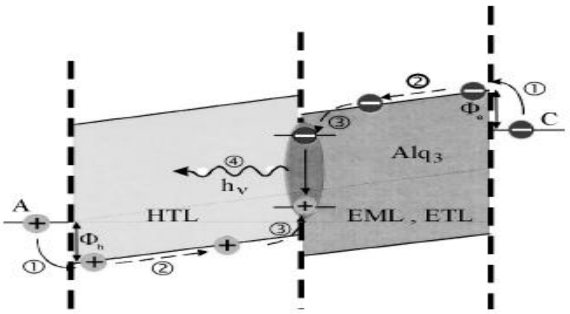

Fig.2 The structure and schematic energy diagram of a two-layer OLED. With a suitable choice of the layer thicknesses, recombination occurs in the emission layer (EML) Alq3 in the neighborhood of the HTL/Alq3 interface layer.Alq3 is simultaneously the electron transport layer (ETL). HTL is a hole transport layer. It can be made of e.g. NPB.

(B) Exciton Density and Distance from Anode

The evolution of charges and excitons in the device is shown. From the profile, it can be inferred that it all depend on the location of charge accumulation layer that is by the internal barrier offered at the interface. Here for simplicity the density for hole and electron are kept same for uniformity of graph and mainly emphasis is given on the effect of the internal energy barrier. The importance of barrier lies in that the carrier leaves the device without recombination. Thus higher barrier leads to lower injection current and maximum recombination. This in turn improves the recombination efficiency.

(C) Exciton Density and Time Variations

In the Exciton density profile as a function of time, the holes penetrate from left side, penetrating NBp prior to the Alq3 layer. Simultaneously electrons enter into the device and combine to the holes at the NBP/Alq3 interface due to which the recombination exciton formation takes place and results in a rise of exciton density at the interface. But later on saturation prevails and the density remains constant.
The number of excitons increases until number of charges to be recombine grows. And that depends on that these charges do not diminish before the recombination. So increase in exciton growth depends on charge lifetime which in turn depends on supply voltage. Higher the supply voltage sooner saturation will be reached.

II. RESULT AND DISSCUSION

(A) Graph between Charge Density versus Distance from Anode

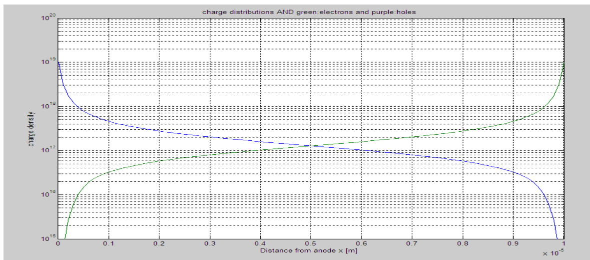

Fig 1: Green Colour Show of Electron and Purple Colour Show of Hole

Starting from an empty device we integrate until steady state is reached.

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Maximum of the generation rate is found in the half of the active layer that faces the incoming light. The charge density accumulates at the electrode where they are expected.

(B) Graph between Exciton Density versus Distance from Anode

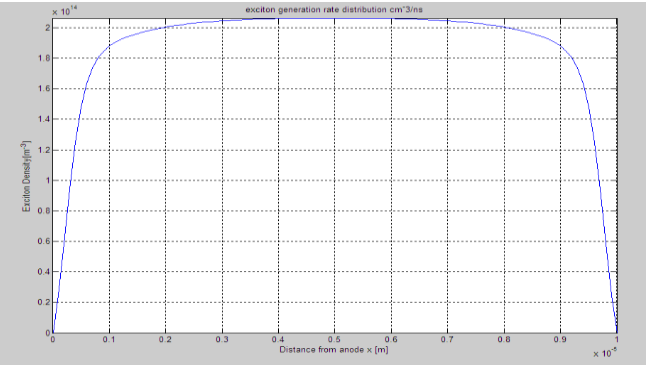

Fig.2: Shows Exciton Density

Electrons interpenetrate with holes that have entered the device in advance. The internal charge density is influenced by internal energy barriers, thus maximum density is observed in the middle.

(C) Graph between Exciton Density versus Time Variations

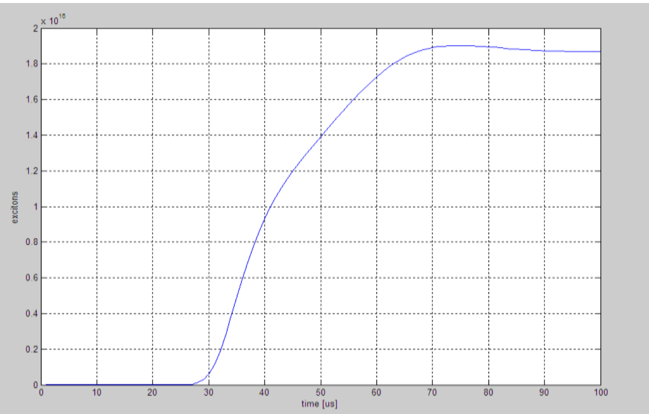

Fig3: Graph of Charge Distribution

Initially very high current is due to fast holes traversing the hole transport layer. This results in steep rise in recombination rate. The recombination rate then fallows steady state according to the applied voltage.

III. CONCLUSION

We have simulated both electrical and optical behavior of the OLEDS. Materials are chosen that the mobility of holes is higher in the HTL and less in ETL and vice versa for the electrons. Thus both holes and electrons tend to accumulate near the interference of the two materials. We successfully simulated theoretical equations including all parameters relating to influence its performance. Implementing these equations in MATLAB there is Good agreement between the simulated and the electroluminescence spectra observed in Alq3 based OLED devices.

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