Simulation of Organic Light Emitting Devices

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Abstract - ***The extracted features of organic material are used as input vectors for the standard equations, results in increasing the intensity of OLED. Simulation results helps in the analysis of identify the error and help us to use the device more accurately and has a better emission rate compared to the previous time analysis by MATLAB. We search for flexible and robust displays imparted greater momentum to the hectic research in the field of Organic and Polymer Light Emitting Diodes (OLEDs & PLEDs). Ease of fabricating multi color displays through affordable and cost effective techniques accelerated these investigations. Being an interdisciplinary area, understanding its physics and modeling have become unequivocally important for shaping tomorrow's device technology. By modeling PLEDs, analysis of quantum and power efficiencies is made possible from the current-voltage and luminance behaviors. Several approaches have been followed to generate device level behavioral models, like band based and exciton based models. Here the scope of Artificial Neural Networks (ANN) in device modelling is explored by fabricating and characterizing an MEH-PPV based device and simulating it by using MATLAB.***

Keywords: OLED, Exciton, Optimization, organic devices, 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 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. These 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, HUMO(highest unoccupied molecular orbital) and the LUMO(lowest unoccupied molecular orbital) of organic semiconductors. This are analogous to the valence and conduction bands of inorganic semiconductors.

II. SYSTEM MODEL

The Organic Light Emitting Diode consists 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. 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.

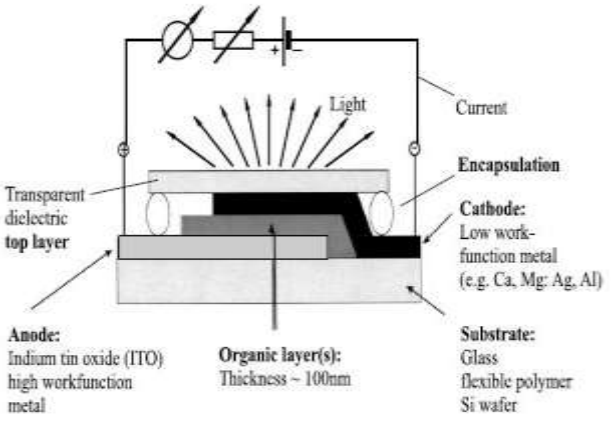


Fig.1 Show A cross-section through the simplest form of an organic light-emitting diode(OLED). One of the two metallic or metallic-conducting electrodes must be semitransparent to permit the luminescence to exit the device. Typical thicknesses of the organic layer(s) between the electrodes are between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

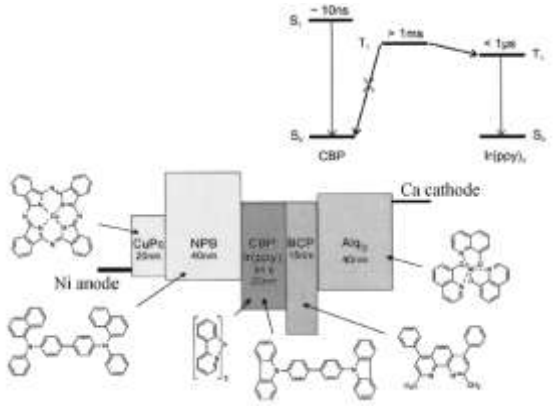


Fig.2 This fig shown The structure and energy diagram of a high-efficiency "phosphorescent" OLED made with several organic layers. The energy diagram on the upper right shows the non-radiative population of the triplet state of Ir(ppy)3, from which the electroluminescence is emitted. The diagram is drawn for an applied voltage of V = –VBI.

III. EXCITON ENERGY TRANSFER MODELLING

State-of-the art OLEDs are composed of several functional layers whose thickness obeys some optical or electronic criteria and which may be further complicated by dye doping, charge doping etc. The optimum harvesting of excitation energy by use of fluorescent and phosphorescent dye do pants remains a challenge. Here we attempt to give a simulation example of dual emitters in two layers EML1 and EML2 of a hypothetical 4-layer device structure. The rate equations for excitons is used here to model the energy transfer among different exciton species in a multilayer small molecule OLED as depicted in fig.

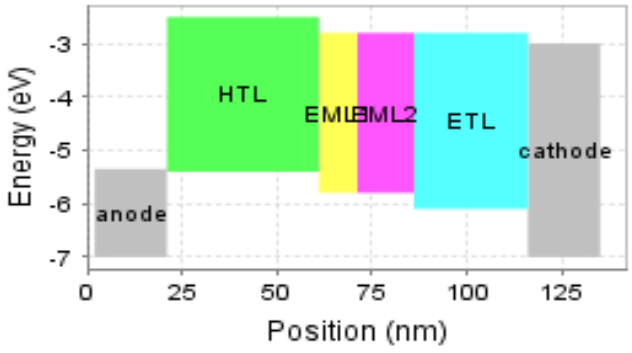


Fig.3 Energy level diagram of a 4-layer OLED with two emissive layers EML1 and EML2 with two exciton species each. charge-carrier mobilities is often very complicated and at low fields practically impossible. In 1970 Pai9 demonstrated that at high electric field E the mobility of photo injected holes in poly(N-vinylcarbazole! (PVK) can be described by

Drift-Diffusion Model:

The implemented physical models in Matlab cover all the key physical processes in OLEDs, charges injection, transport ,recombination, exciton diffusion, transfer and decay as well as light out-coupling and thin-film-optics. The key ingredients of our device model were outlined in reference . Our Matlab model that is dependent equations and highlight the coupling terms for electronic-optical and optical-electronic coupling. The Poisson equation and the (electron) continuity equation reads

$$\frac{dE(x)}{dx} = \frac{e}{\varepsilon \varepsilon_0}\left(p(x) - n(x)\right) \quad \text{..... .....……1}$$

The carrier transport model of the organic de- vice is described by drift–diffusion equations of current density coupled to the Poisson equation as follows:

$$\frac{d J_n}{dt} = q(R - G) \quad \text{.....2}$$

$$\frac{d J_P}{dt} = -q(R - G) \quad \text{.....3}$$

$$\frac{d}{dx}(\varepsilon_o \varepsilon_r)\frac{d\psi}{dx} = -q(p - n - n_r + p_r) \quad \text{.....4}$$

where Jn and Jp are the electron and the hole current densities respectively; q is the electron charge; R is the recombination rate; G is the generation rate expressed

$$R = \frac{q(\mu_n + \mu_p)}{\varepsilon_o \varepsilon_r} \quad \text{.....5}$$

$$G = \frac{q(\mu_n + \mu_p)}{\varepsilon_o \varepsilon_r}(n_e p_e) \quad \text{.....6}$$

with ne and pe being electron and hole equilibrium densities, respectively; n and p are the densities of free electrons and holes, respectively; ψ is the electrostatic potential; $\varepsilon_o \varepsilon_r$ is the permittivity of the organic material; n_t and p_t are the densities of trapped electrons and holes of the organic material; μ_n and μ_p are carrier mobilities, which are expected to be field dependent in the amorphous organic materials and given by Poole–Frenkel form

$$\mu = \mu_0 \exp \gamma\sqrt{E_0} \quad \text{.....7}$$

or

$$\mu_p = \mu_0 \exp \gamma\sqrt{E_0} \quad \text{.....8}$$

where μ_0 denotes the mobility at zero field. The field dependence γ through the coefficient g is comparable to the Poole-Frenkel effect.

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

The prefactor γ for the singlet exciton generation rate is typically taken to be 1/4 following the traditional spin statistics argument. Triplet excitons and guest molecule excitons can be treated analogous. We use the diffusion constant *DS=l2/*τ, with *l* being the diffusion length and τ the exciton lifetime. Charge injection is assumed to be thermionic and affected by image charge recombination.

Where

n = Density of Electrons
P = Density of Holes
E = Electric Field
r = Langevevin recombination rate :
Solving simultaneously equation using by MATLAB. we get the rate equation comprising of exciton generation, diffusion and its recombination rate .

IV. SIMULATION ANALYSIS

(A) Graph plot between Charge Density and Distance from Anode Graph A showing charge density profile of a bilayer OLED calculated with the MATLAB. Device models for the electronic and excitonic processes in OLEDs are solved by suitable numerical methods. Advanced optimization and fitting algorithms need to solve the electronic device model equations repeatedly ,rapidly and stable solvers model. In contrast to the optical OLED device simulations, the electronic device simulations have not yet achieved predictive power. Therefore, they must be applied to experimental OLED data in a descriptive manner. Electronic device simulation often deals with the study of the impact that physical models or parameters have on the device performance. The pre factor 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= 0 nm to 100nm.

TABLE1. MATERIAL PARAMETERS USED FOR DEVICE SIMULATION

Material/ Parameter	CuPc	NPD	Alq3
$\mu_{no}/(cm^2/Vs)$	6.9x 10^{-5}	1.1x 10^{-6}	8.0x 10^{-8}
$E_{no}/(V/cm)$	1.686x 10^{5}	1.111x 10^{5}	1.085x 10^{4}
$\mu_{po}/(cm^2/Vs)$	1.1x 10^{-6}	1.8x 10^{-5}	7.0x 10^{-10}
$E_{po}/(V/cm)$	1.235x 10^{4}	7.716x 10^{4}	1.235x 10^{4}

When a forward bias voltage of 5 V was applied, holes were injected from anode into the NPB/Alq3 layer and accumulated in the emissive layer due to band gap offset. The Alq3 layer adjacent to the cathode acts as an electron transporting layer and a hole blocker layer, where accumulation of holes in the emissive layer region caused electric field in Alq3 region to be higher than that of NPB layer .. The simulation shows, at steady state, the majority of holes is trapped in the emissive layer and recombines with the electrons coming from ETL.

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. These 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.

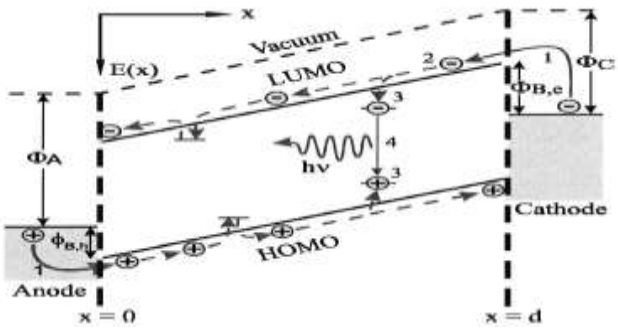


Fig 4. Show The structure and schematic energy diagram of a two-layer OLED. With a suitable choice of the layer thicknesses, recombination occurs in the emission layer (EML) Alq3 in the neighbourhood of the HTL/Alq3 interface layer.Alq3 is simultaneously the electron transport layer (ETL). HTL is a hole transport layer. It can be made of e.g. NPB.

(B)Graph Plot Between Exciton Density And Distance From Anode:

Graph B show of recombination rate in the device. The rate is biggest in interface between Alq3 and NPD as the hole and electron mobility are bigger at mid position and maximum amplitude showing in 20nm to 80nm. The recombination rate is Alq3 is more than NPD. So that Alq3 is a good as an emission layer in the structure. Graph B compares the simulated carrier recombination rate in the control bi-layer device. When electrons injected from cathode arrive this region, direct recombination process occurs which leads to the high recombination rate. It can be observed that the recombination rate and magnitude higher than in the control device and clearly confined within the emissive layer.

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. Then 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. we can improves the recombination and efficiency.

(c) exciton density and time variations:

In the Exciton density profile as a function of time, the holes penetrate from left side, penetrating NPD prior to the Alq3 layer. Simultaneously electrons enter into the device and combine to the holes at the NPD /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.

The delay time for EL is entirely determined by the arrival of electrons at the internal interface and varies with applied bias, as expected. While the fast initial rise can be attributed to the establishment of a high recombination rate density at the Alq3 side of the internal interface, the slow later rise is due to increasing penetration of holes into the Alq3 layer.

V. SIMULATION/EXPERIMENTAL RESULTS

(A)Graph Between Charge Density Versus Distance From Anode:

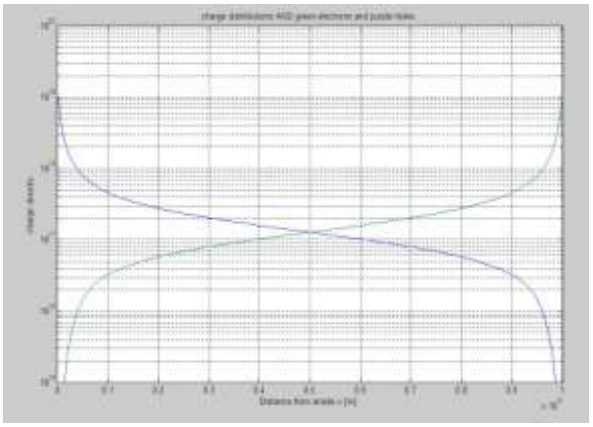
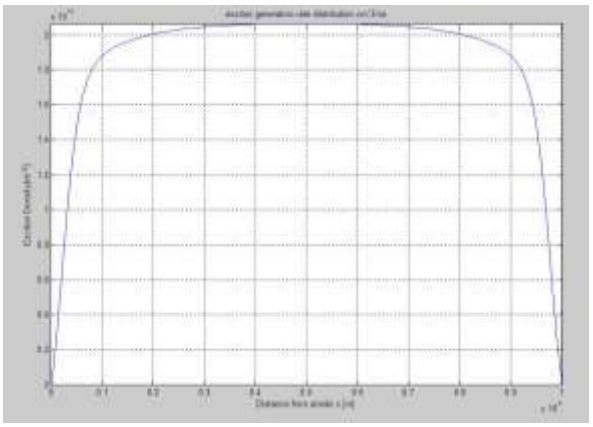


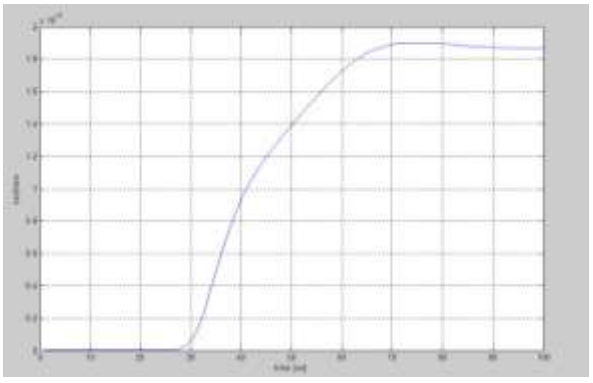
Fig : Green Colour Show of Electron and Purple Colour Show of Hole

(B) Graph Between Exciton Density Versus Distance From Anode:

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 Time Variations Versus Exciton Density:



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.

V. CONCLUSION

This simulator has a reliable and predictive character and is thus ideally suited to characterize and optimize OLED structures for display and lighting applications. The optical device simulator is extended by electronic device models which have a descriptive and instructive character.

We have simulated both electrical and optical behaviour 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 and NBD based OLED devices.

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