Journal of New Technology and Materials
JNTM
Vol. 04, N°01 (2014)35-38

OEB Univ. Publish. Co.

Electrical characteristics of Organic Light Emitting Diode "OLED" finite difference modeling

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Received: 30 April 2014, accepted 26 May 2014

Abstract

In this paper, a finite difference modeling of single layer organic light emitting diode "OLED" based on MEH-PPV [**P**oly (2-**M**ethoxy, 5-(2'-**E**thyl-**H**exoxy)-1, 4-**P**henylene-**V**inylene)] and DP-PPV [**P**oly (2, 3-**DiP**henyl-**P**henylene-**V**inylene)] is presented through the simulation of the basic equations i.e. the time independent continuity equations, with a drift diffusion form for current density, coupled to Poisson's equation. Thus, several parameters are extracted from this model; J (V) characteristics for the two devices which are compared to the experimental results and the spatial distributions of the potential, the electric field and the carrier concentrations.

Keywords: OLED; simulation ; finite difference;MEH-PPV; DP-PPV; J(V) characteristics

1. Introduction

Organic light emitting devices have been remarkably improved since the announcement of the first Organic light emitting diode "OLED" in 1987[1]. These organic devices have a great potential indeed in various industries as are used in many applications such as lighting, handheld displays like smart phones, tablets and cameras and TV's of course. Even though this great development, OLED's are still lacking in some other areas related to the lifetime of these devices, the injection and transport mechanism which are not properly determined since the organic semiconductors have an amorphous structure unlike the inorganic ones that present a crystallized one.

To understand the operation principle of such devices, and before manufacturing them, we have to predict first their behavior by studying them trough what we know now as "Numerical modeling" [2], which is a powerful method of visualizing the dynamic behavior of physical systems of such devices. In this respect, we used an electrical model composed of Poisson's equation, coupled to the time independent continuity equations, with a drift diffusion form for the current density.

In this paper, we present the model that we worked on along with the boundary conditions [3] where a set of equations were solved using finite difference method. Simulation results of J (V) characteristics for different organic semiconductor materials and for various thicknesses were compared to experimental data from [4, 5], a spatial distribution of carrier density, potential and electric field are shown.

2. The device model

In this section, the electrical model is presented along with the boundary conditions; finite difference method was applied to solve the basic equations and Gummel iteration is used [6].

2.1. Governing equations

To fully understand the mechanism of the transport and the injection of electrons /holes, we use the inorganic semiconductor devices equations i.e. the time independent continuity equations, with a drift diffusion form for current density, coupled to Poisson's equation, for modeling the organic semiconductor based devices as follows:

$$\frac{\partial J_n}{\partial x} = G - R; \quad \frac{\partial J_p}{\partial x} = G - R, \qquad (1)$$

J_n (J_p) is the electron (hole) current density, G is the carrier generation rate which is very small for materials with an energy gap larger than 2 eV, and R is the carrier recombination rate, this latter is not that important for the single carrier structures [4] . In the following expressions of J_n and J_p, the diffusivities are dependent of the mobilities using Einstein relation.

$$J_n = q\,\mu_n \left(n.E + \frac{k_B T}{q}\frac{\partial n}{\partial x}\right);$$

$$J_p = q\,\mu_p \left(p. - \frac{k_B T}{q}\frac{\partial p}{\partial x}\right) \qquad (2)$$

Where $\mathbf{q}$ is the electronic charge, $\mathbf{n(p)}$ is the electron (hole) density, $\mathbf{E}$ is the electric field, $\mathbf{k_B}$ is Boltzmann's constant, $\mathbf{T}$ is the temperature and, $\boldsymbol{\mu_n(\mu_p)}$ is the electron (hole) mobility which is expected to be Poole-Frenkel electric field dependent:

$$\mu_{PF} = \mu_0 \exp\left(-\frac{q\varepsilon_a}{kT}\right)\exp\left(\frac{q\beta}{kT}\sqrt{E}\right) \qquad (3)$$

Where $\boldsymbol{\mu_0}$ is the temperature independent pre-factor mobility, $\boldsymbol{\varepsilon_a}$ is the thermal activation energy and $\boldsymbol{\beta}$ is the Poole-Frenkel factor.

Poisson's equation is:

$$\frac{dE}{dx} = \frac{q}{\varepsilon}\left(p - n + N_D - N_A\right) \qquad (4)$$

The electrostatic potential $\mathbf{V}$ is related to$\mathbf{E}$ by:

$$E = -\frac{dV}{dx} \qquad (5)$$

Where $\boldsymbol{\varepsilon}$ is the static dielectric constant, $\mathbf{N_D}$ is the donor density and $\mathbf{N_A}$ is the acceptor one.

2.2. Boundary conditions

Considering the boundary conditions for the potential:

$$V(0) = 0, \qquad V(L) = V_d - V_a \qquad (6)$$

Where $\mathbf{V_a(V_d)}$ is the application (diffusion) potential.

The diffusion potential is expressed as:

$$V_d = \frac{k_B T}{q}\ln\left(\frac{n_L}{n_0}\right) = -\frac{k_B T}{q}\ln\left(\frac{p_L}{p_0}\right) \qquad (7)$$

The equilibrium free carrier concentrations at the interfaces are [3]:

$$\mathbf{n_0} = N_c \exp\left(-\frac{\phi_{b1}}{k_B T}\right),$$

$$\mathbf{n_L} = N_c \exp\left(-\frac{E_g - \phi_{b1}}{k_B T}\right)$$

$$\mathbf{p_0} = N_v \exp\left(-\frac{\phi_{b2}}{k_B T}\right), \qquad (8)$$

$$\mathbf{p_L} = N_v \exp\left(-\frac{E_g - \phi_{b2}}{k_B T}\right)$$

Where $\mathbf{N_c}$ and $\mathbf{N_v}$ are assumed to be equal and correspond to the density of negatively and positively chargeable sites in the film, $\mathbf{E_g}$ the band gap energy, $\boldsymbol{\phi_{b1}(\phi_{b2})}$ is the electron (hole) energy barrier.

The following expressions of the three main equations; (1), (2) and (5) are obtained using the finite difference method [7]:

Poisson's equation:

$$V_{i+1} + V_{i-1} - 2V_i = \frac{h^2 q}{\varepsilon}\left(n_i - p_i + N_a - N_D\right) \quad (9)$$

Coupled continuity and drift-diffusion equations:

$$[-(V_{i+1} - V_i) + V_T]\,n_{i+1} + [(V_i - V_{i-1}) - 2V_T]\,n_i + V_T\,n_{i-1} = 0$$

$$[-(V_{i+1} - V_i) - V_T]\,p_{i+1} + [(V_i - V_{i-1}) + 2V_T]\,p_i - V_T\,p_{i-1} = 0 \qquad (10)$$

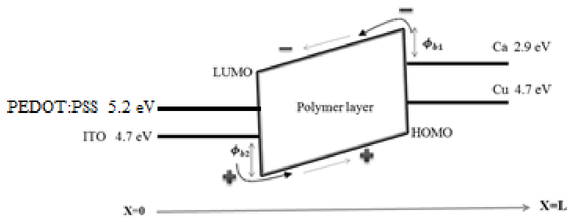

Fig.1 The model band diagram

3. Results and discussions

Fig.1 shows the band diagram of the device, where we consider a single layer organic diode based on: first: MEH-PPV [**P**oly (2-**M**ethoxy, 5-(2'-**E**thyl-**H**exoxy)-1, 4-**P**henylene-**V**inylene)], taking into account the electron and hole energy levels $\mathbf{E_c}$= $\mathbf{2.8\ eV}$ and $\mathbf{E_v}$ = $\mathbf{5.3\ eV}$, with the dielectric constant $\boldsymbol{\varepsilon_r}$= $\mathbf{3}$ and $\mathbf{n_0}$= $\mathbf{10^{21}\ Cm^{-3}}$. The organic layer is sandwiched between the anode ITO (Indium Tin Oxide) and the cathode Cu. The barrier for electron injection is **1.9 eV** and for hole injection is **0.2 eV**.
Second: DP-PPV with the electron and hole energy levels $\mathbf{E_c}$= $\mathbf{2.94\ eV}$ and $\mathbf{E_v}$ = $\mathbf{5.66\ eV}$, with the

dielectric constant $\mathcal{E}_r = 3$ and $n_0 = 10^{21}\ \mathrm{Cm}^{-3}$. The organic layer is sandwiched between the anode ITO and PEDOT:PSS [Poly (3,4-Ethylene Dioxy Thiophene): Poly(Styrene Sulphonate)], and the cathode Ca. The barrier for electron injection is **0.04 eV** and for hole injection is **0.46 eV**.

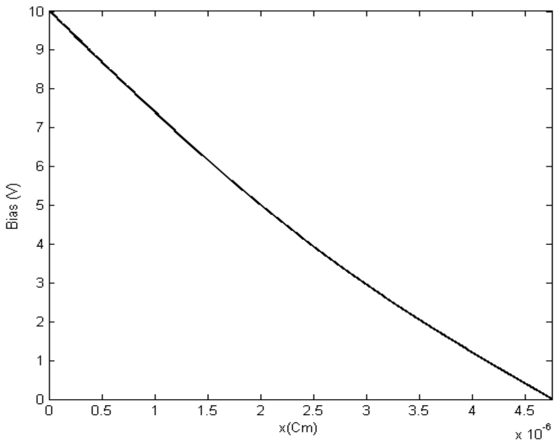

Fig.2 Spatial distribution of the potential

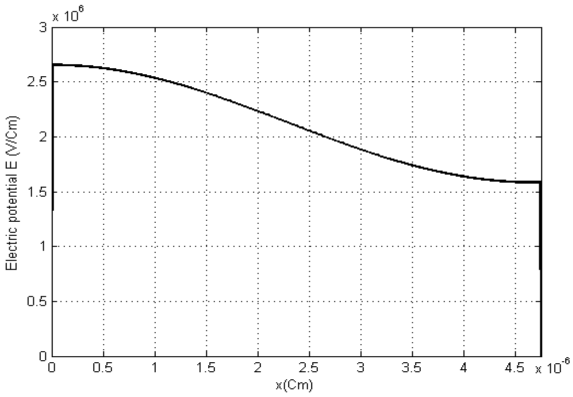

Fig.3 Electric field distribution

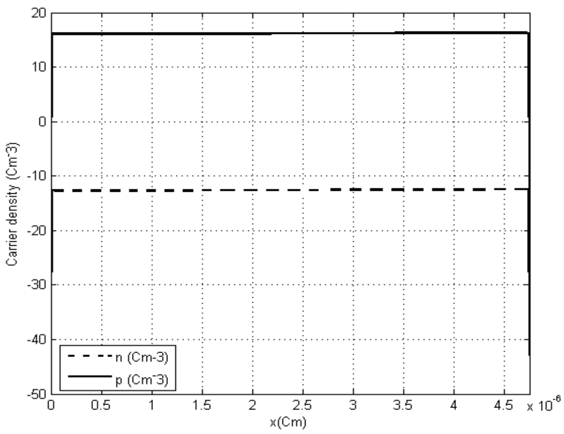

Fig.4 Carrier density ditribution for holes and electrons (ITO/MAH-PPV/Cu)

Fig.2 and Fig.3 present the spatial distribution of the potential and the electric field respectively for ITO/MEH-PPV/Cu device with a thickness of 45.7 nm.

Fig.4 shows the spatial distribution of the carriers density for both holes and electrons where the density of holes is much greater compared to electrons. In fact, the holes barrier injection is too small that these carriers pass through this barrier, in the opposite of the electrons where only few of them can traverse through this barrier.

Using this model, we can also calculate the J-V characteristics for ITO/MEH-PPV/Cu device for different thicknesses where these results shown in Fig.5, Fig.6, and Fig.7 are compared with experimental ones from [4].

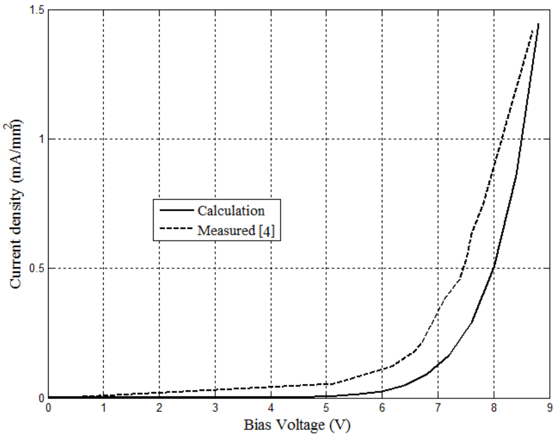

Fig.5 Current density versus bias voltage for 45.7 nm ITO/MEH-PPV/Cu device

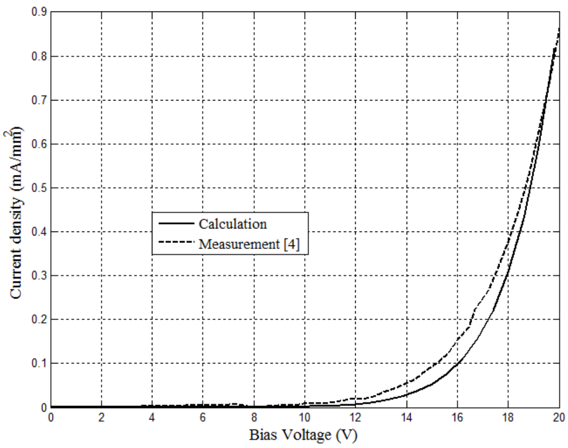

Fig.6 J(V) characteristics for 120 nm (ITO/MEH-PPV/Cu)

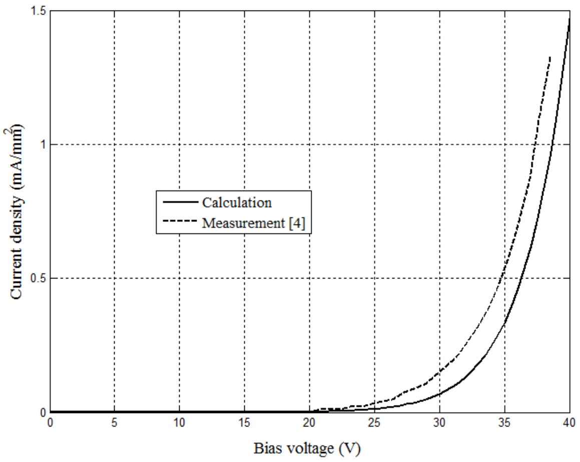

Fig.7 J(V) Characteristics for 210 nm (ITO/MEH-PPV/Cu)

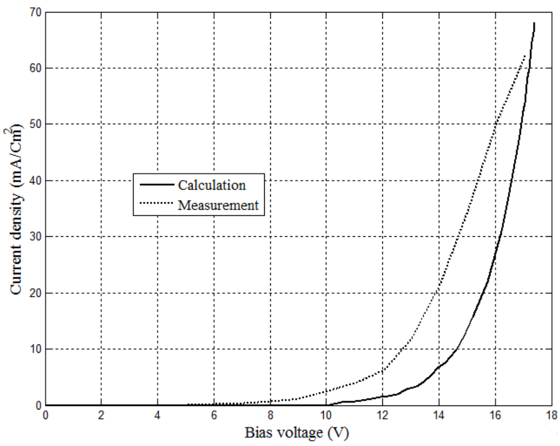

Fig.8 J(V) characteristics for 50 nm (PEDOT:PSS/ DP-PPV/ Ca

We applied the model used previously on PEDOT: PSS/DP-PPV/Ca device. Fig.8 shows a comparison of calculated and measured J-V characteristics of a 50-nm- thick DP-PPV diode [5].

4. Conclusion

In this study, finite difference method was applied for modeling the basic equations that control the operation principle of an OLED. The hole density is much greater than that of the electrons. From the J-V characteristics, the turn-on voltage increase with the thickness of the polymer layer and in the two devices based on MEH-PPV and DP-PPV, the same behavior was noticed and a shift between the experimental data and the calculated results was observed.

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