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Effects of Carrier Mobility and defects on the Recombination Characteristic of P3HT: Graphene Bulk Heterojunction Solar Cell

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***Abstract*— Several extensive studies have been carried out for poly(3-hexylthiophene) (P3HT) mixed with carbon derivatives such as phenyl-C61-butyric acid methyl ester (PCBM) in organic solar cells, but few searches found on the blend of p3HT :graphene.**

We have used the Solar Cell Capacitance Simulator (SCAPS) and we have choose the effective medium model (EMM) to simulate the active layer lightly doped P, the appropriate parameters have been introduced in a platform of (SCAPS) Simulator. First we optimized the thickness of the active layer, where we model the characteristics of the solar cell: efficiency (η), open circuit voltage (Voc), short circuit current (Jsc) and fill factor (FF), next we varied the holes mobility and the defects density and we calculated the characteristics of the recombination rate according to these two variables.

***Keywords*—Organic Cell, Conjugated Polymer , poly(3-hexylthiophene) (P3HT), Graphene, SCAPS simulator.**

I. INTRODUCTION

In an attempt to solve energy and environmental problems, as an alternative feasible to oil combustion, the world of photovoltaics has evolved, mainly inorganic semiconductor cells [1].

Inorganic photovoltaic devices have been widely used since the 1970s because of their high power conversion efficiency [2].

Compared to inorganic photovoltaic devices, organic photovoltaic (OPV) devices have many advantages, including mechanical flexibility, the possibility of treatment in solution and a low specific weight [3],[4].

As a result, the exploration of organic photovoltaic devices has developed, especially solar cells with conjugated polymers.

In this work we chose P3HT (poly (3-hexylthiophene) a p-type semiconductor conjugated polymer is one of the most studied conjugated polymers that is suitable for organic solar cells because of its appropriate absorption spectrum and low-cost manufacturing potential [5].

Also it has properties such as high electrical conductivity and high solubility in different solvents [6] mixed with graphene, which is an excellent acceptor [7],[8] its mobility is remarkably high 1E4cm² / Vs, it is highly transparent [9] and its electrical conductivity is very high [10],[11] .

This blend of P3HT:Graphene constitutes the active layer of the studied organic cell.

We have used the effective medium model and the appropriate parameters have been introduced in a platform of the Solar Cell Capacitance Simulator (SCAPS).

II. THEORETICAL MODEL

The bulk heterojunction organic solar cell is composed of two materials which each have two orbitals called highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital(LUMO).

The P3HT is a first material, is an electron donor and has the lowest ionization potential (Ei).

The second material is a Graphene , is an electron acceptor and has the highest electron affinity (χa) [12].

After the donor material has absorbed light there is creation of electron-hole pairs called excitons, the latter diffuse towards the interface between the electron donor and acceptor material where an electron can easily be transferred between the LUMO of the donor material (higher in energy) and the LUMO of the acceptor material, the most important is that the exciton reaches an interface.

For this, it is necessary that the distance between the donor material and the acceptor material be less than 10nm. Once the interface is reached the exciton of the electron-hole pair dissociates into a polaron.

After the dissociation, the charges are transported to the electrodes The last step is the extraction of the charges Fig.1.

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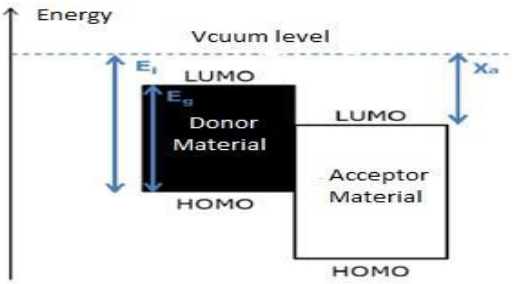

Fig. 1 Energy diagram of HOMO and LUMO orbitals of donor and acceptor materials. [12]

The equations that govern the studied model are the Poisson equation and the continuity equations for electrons and holes given by:

$$\frac{d^2\varphi}{dx^2} = -\frac{q}{\varepsilon_0\varepsilon_r}\left(p - n - N_A^- - N_D^+ + \frac{\rho_t}{q}\right), \qquad (1)$$

$$\frac{1}{q}\frac{dJ_n}{dx} = (G - R_n) \qquad (2)$$

$$-\frac{1}{q}\frac{dJ_p}{dx} = (G - R_p) \qquad (3)$$

where φ describes electrical potential, q is the unit charge, ε_0, ε_r is the dielectric constant of vacuum and the semiconductor respectively ; n and p are electron and hole density, respectively; $N_D^+ and\ N_A^-$ the density of ionized donors and acceptors, $\rho_t$the charge density of defects , J_n and J_p the electron and hole current density; G is the generation rate and *Rn(p)* is the recombination loss.

Equation 4 define the transportation of carriers:

$$J_n = -qD_n\frac{dn}{dx} + q\mu_n\frac{d\varphi}{dx}$$
$$J_p = -qD_p\frac{dp}{dx} - q\mu_p\frac{d\varphi}{dx} \qquad (4)$$

where $\mu_{n(p)}$ is the electron/hole mobility and Dn(p) is the diffusion coefficient .

The generation rate is given by:

$$G(\lambda, x) = \varphi_0\alpha(\lambda)exp\left(-x\left(\alpha(x)\right)\right) \qquad (5)$$

where φ_0 is the incident photon flux , x is a depth and α the absorption coefficient of the active material.

There are several recombination mechanisms in the organic cells in our work we took into account that of recombination by traps

III. METHODOLOGY

Several considerations must be taken into account when simulating the organic solar ones such as the dielectric constant ε which depends on the weight / donor / acceptor ratio of the materials, the effective mobility of the carriers (μn in the acceptor and μp in the donor) in the BHJ configuration is different from the value in their initial phase, which is closely related to the nano-morphology of the disordered bulk heterojunction organic cell.

The nanostructure p-n is represented by a single, lightly doped semiconductor layer P; we have considered the effective medium model (EMM) Fig.2,this effective medium will be characterized by an average of the properties of the materials n,p, it's supposed that the two materials are very well interpenetrated in the active layer, with a distance between all the points of the mixture and a donor / acceptor interface being less than the diffusion length of the excitons.

To create a driving force for the separation of the electron-hole pairs the contacts are considered to be selective, ie a contact accepts only the electrons and the other accepts only the holes[15].

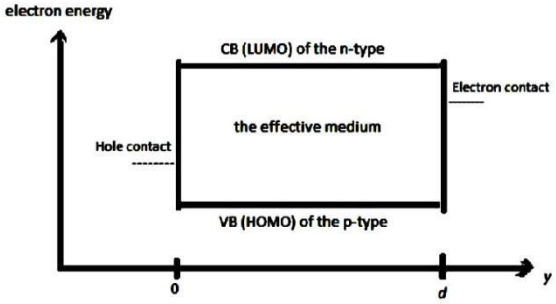

Fig.2 Schema of the effective medium model (EMM).

Parameters necessary for the simulation of the active layer are extracted from the literature such as the permittivity, the band gap as well as the absorption coefficient of the P3HT: graphene blend [6], subsequently are introduced on the platform of the simulator capacity of solar cells in one dimension (SCAPS-1D). Fig.3 and are given by Table 1.

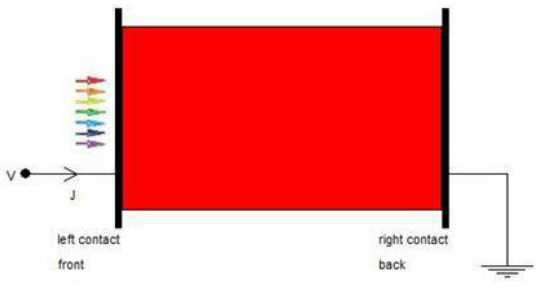

Fig.3 Solar cell active layer P3HT:Graphene

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Table 1 Parameters used in simulation

Parameter	Symbol	Value	Unit
Thickness	d	250	nm
Band gap	Eg	2.065	eV
Electron affinity	χ	3.4	eV
Effective densit of states	Nc,Nv	2E18	cm^{-3}
Electron mobility	μn	1E4	cm^2/Vs
Hole mobility	μp	Vari	cm^2/Vs
Dielectric constant	ε	6.3	

IV. Results and Discussion

Thickness is a very important parameter used to improve the properties of semiconductor devices, such as photovoltaic devices. The thickness of the active layer has been changed from 80 to 900 nm in order to determine the optimum thickness of the active layer according to the simulation shown in Fig.4.

The optimized value of the layer is indicated at ~300 nm. In conclusion, with the increase in the thickness of the active laye r beyond 300nm, the values of the effeciency "eta", short-current circuit "Jsc" remain almost constant, whereas the open-circuit voltage "Voc" continues to increase with increasing active layer thickness and the fill factor 'FF' gradually decreases. All the performance parameters vary in a better direction with thickness increasing.

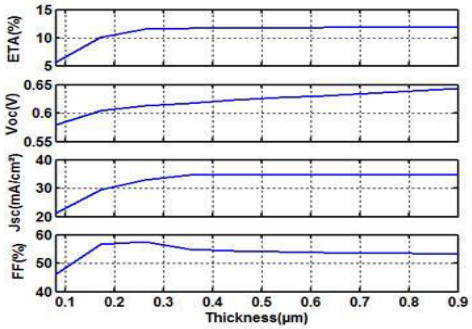


Fig.4 Optimizing the thickness active layer

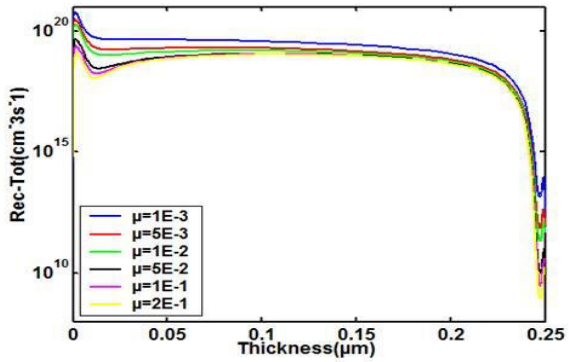
In this research paper, we found the recombination rate of solar cell at different charge mobility and different charge defects concentration. In BHJ solar cell, in which the blend is treated as one effective medium with an effective band- gap given by LUMO (lowest unoccupied molecular orbit) of acceptor and HOMO (highest occupied molecular orbit) of donor [13].

The recombination occurs mostly near semiconductor and electrode interface and there is less recombination in the bulk.

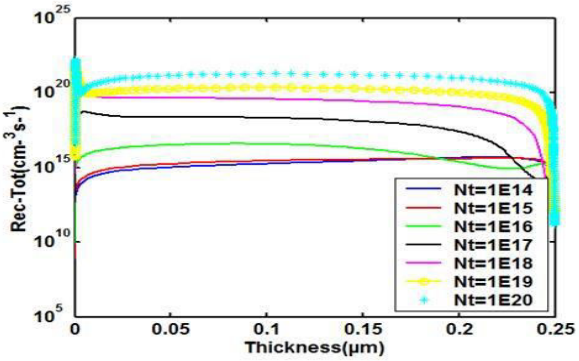
Figure6(a) shows the variations of total recombination in P3HT/Graphene solar cell with the mobility changing from 1E-3 to 0.2 cm²/Vs ,that basically decreases with increasing mobility. It can be seen in fig.6(b) the influence the defects charge concentration on the recombination rate,that increases proportionally with defect s density.

The recombination near the electrode can be regarded as dark carrier recombination[14].

This mixture of materials P3HT(donor) and GRAPHENE(acceptor), allows to increase the interfacial zones between the two, and consequently to reduce the recombination problems of photogenerated excitons far from the interface



(a)



(b)

Fig.6 Recombination rate:(a) effect of mobility ;(b) effect of defects

V. Conclusion

The ITO / P3HT: GRPHENE / Al architecture P3HT solar cell is designed and analyzed using a solar cell capacity simulator.

Absorbent layer thickness, defect density and hole mobility influence solar cell performance

Hence this simulation work will provide the handy information in fabricating P3HT:Graphene solar cells to reasonably choose material parameters and to achieve the good performances.

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