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Parametric Analysis of P3HT:PCBM Based Nano Structured Organic Solar Cell

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Abstract*-In recent years, due to the light weight, low production cost and large scale application, organic solar cell has become one of the most researched topic in renewable energy field. In this paper, the electrical and the optical characteristics of poly-3-hexylthiophene:phenyl-C61-butyric acid methyl ester (P3HT:PCBM) are analyzed. Drift-diffusion equations are used for describing the free carrier transport characteristics and the trapped carrier which are independent of quasi-Fermi level are also taken into account. Considering the effective mobility, higher order recombination rates are numerically calculated. Photon density with respect to the position in the device is also calculated which shows considerably higher recombination rate*.

Keywords: Organic Solar Cell, Free Carrier Transport, Trapped Career, Photon Density

1. INTRODUCTION

Organic solar cell is one of the most promising and the strongest candidate for improved efficiency photovoltaic in the field of renewable energy. Remarkable improvement of efficiency in different types of organic solar cell has been seen in the previous decades. Recently large amount of solar cells are installed in different parts of the world commercially, for energy harvesting. Though major shares of the present market are captured by silicon based solar cell, the market share of the organic solar cell is increasing dramatically. In this paper, the parametric analysis of one of the strongest candidates of organic matter for organic solar cell i.e. P3HT: PCBM is done for the further improvement of this kind of solar cells.

2. RELATED WORKS

Organic solar cells simulation as well as practical implementation has been done by many researchers. In this paper only the recent and notable researches are cited. One of the most important parameters is the recombination rate and the modelings of non geminate recombination as well as convergence with experimental results are done by some researchers [1]. Simulations of dark and light J-V curves as well as the transient photocurrent at different conditions are found in some literature [2]. Distribution model of trapped career states (DoS) of the specific cell is from time of flight (ToF) based photo current measurement techniques are also analyzed [3]. Organic solar cell efficiency is increased by introducing polymer interlayer in some papers [5]. The significance of charge extraction when the transient voltages are increasing linearly is also analyzed in some literature [4]. The loss mechanisms and the parameters that are related to the loss mechanisms are discussed in literature [6].In literature [7], investigation of the buffer layer of specific oxides for the improvement of the extraction rate is done. Practical implementation and the analysis of life time of the organic solar cell is done in research [8] and [9]. With respect to the absorption spectrum, spectral response behavior of the single layer organic semiconductor device is analyzed in [10].

3. SIMULATED MODEL

The simulation for the parametric analysis of the P3HT: PCBM based organic solar cell is done in five major parts. The 3D view of the simulated nanostructured solar cell is shown in the following figure

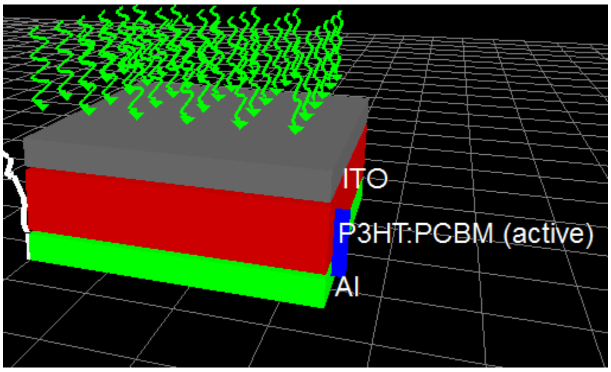

Fig.1: 3D structure of the organic solar cell

The major parts of the simulation are discussed briefly in the following subsections.

3.1Optical Analysis:

In the proposed structure, glass substrate, Aluminum contactors, active layers i.e. P3HT:PCBM is considered. The actual thickness of the organic solar cell is 225nm where as the aluminium contact and ITO has thickness of 125nm and 100nm respectively. The photon density at the different parts of the structure can be found in the following figures

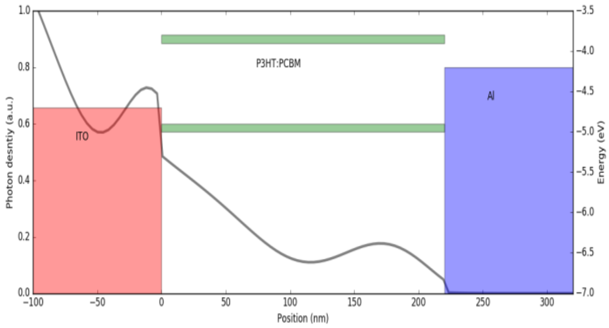

Fig.2: Photon Density on the solar cell

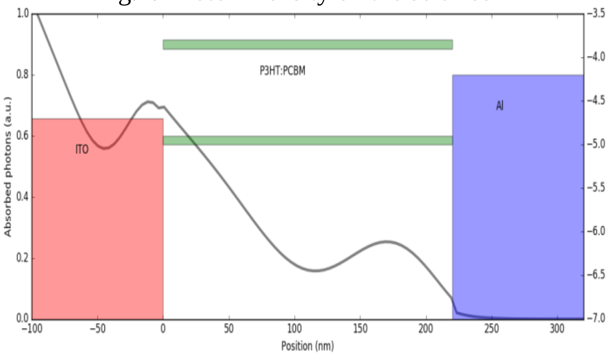

Fig.3: Absorbed Photon Density in the solar cell

From the above figures it is found that the photon density in the solar cell and the absorbed photon density in the solar cell is not same. As the photon density and the absorbed photon density is different, then the photon distribution will also be different .This is described details in the subsection 3.5.

3.2 Modeling of Free Carrier Transport

In this analysis, anode is considered as transparent and the cathode is considered as black body. Let the total operating thickness is d. Then the anode front end is x=0 and the cathode end point is x=d. The free space permittivity and P3HT:PCBM relative permittivity are ϵ_0 and ϵ_r respectively then for free carrier , poisons equation of voltage profile φ will be

$$\frac{d}{dx}(\epsilon)\frac{d\varphi}{dx} = q(n-p)$$

where q represents elementary charge of electron and $\epsilon = \epsilon_o\epsilon_r$. Electrons and holes both are considered as free career. For the determination of the characteristics of these free carries it is necessary to characterize the effective diffusion coefficient and effective mobility. For this continuity equation of these carriers must be developed. The continuity equation for the hole and carrier can be presented as

,

$$\frac{\partial Jn}{\partial x} = q(Rn - G + \frac{\partial n}{\partial t})$$

$$\frac{\partial Jp}{\partial x} = q(Rp - G + \frac{\partial p}{\partial t})$$

Here R represents recombination rate and G represents carrier generation.

Solving Drift- Diffusion equation the expression for electron current and hole current density can be found

$$J_n = q\,\mu_e n_f\frac{\partial E}{\partial x} + q\,D_n\frac{\partial nf}{\partial x}$$

$$J_p = q\,\mu_h p_f\frac{\partial E}{\partial x} - q\,D_p\frac{\partial pf}{\partial x}$$

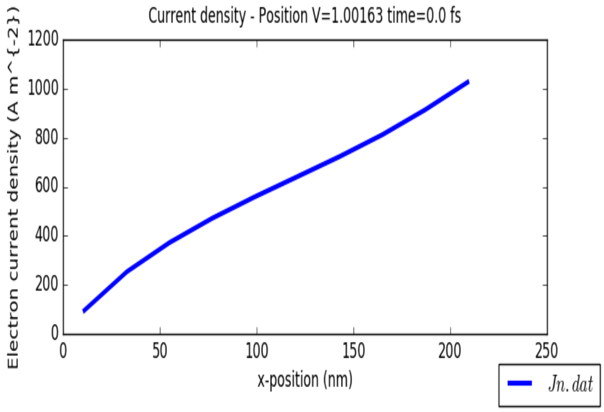

Fig .4: Electron Current Density

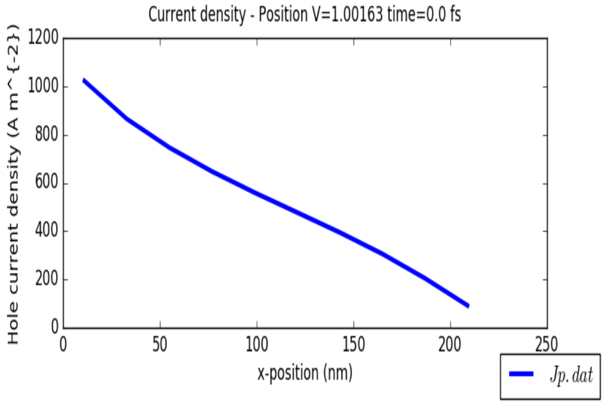

Fig.5: Hole Current Density

From the above two figures, it is clear that hole and electron current density inversely proportional. As the hole current density decreases, the electron current density increases accordingly. The density of electron and hole current must be considered for developing the trapped carrer model, recombination model as well as for efficiency calculation.

3.3 Trapped Carrier Model

In case of organic solar cell not all the carriers are free. There are some trapped carriers. Now in the carrier balance equation there are four parameters, they are electron capture rate (r_{ec}), electron escape rate(r_{ee}), hole capture rate(r_{hc}), hole escape rate(r_{he})

$$\frac{\partial nt}{\partial t} = r_{ec} - r_{ee} - r_{hc} + r_{he}$$

The escape rate from electrons and holes are

$$E_n = v_{th}б_n N_c exp(\frac{Et-Ec}{kT})$$

$$E_P = v_{th}б_P N_v exp(\frac{Ev-Et}{kT})$$

3.4 Recombination Model

The average drift velocity which is gained by the charged particle is directly proportional to the applied electric field. The proportionality constant is known as mobility. The mobility of a carrier describes the characteristics of the movement of carrier in presence of electric field. For developing the recombination model, it is important to analyze the mobility of the carrier. But in case of organic solar cell there are four kinds of carriers. They are free electrons, trapped electrons, free holes and trapped holes. In this model average mobility of electrons and holes are taken into account. Now if the average mobility of the electrons and holes are taken as $\mu_e(n)$ and $\mu_n(n)$ then it can be expressed as .

$$\mu_e(n) = \frac{\mu e\, nf}{nf+ntr}$$

$$\mu_n(n) = \frac{\mu h\, pf}{pf+tr}$$

It is assumed that the electrons and the holes have Brownian motion. When the opposite charge carriers are close to each other's electrostatic field, recombination occurs. Though sometime cases it is found that the free charge carriers neglects the influence of trapped states, if variable mobility of the charged carrier is considered then Langevin recombination rate can be used. Now the Langevin recombination rate can be expressed as

$$R_{free} = qk_r \frac{(\alpha \mu e(n) + \beta \mu h(n))NtPt}{2\epsilon}$$

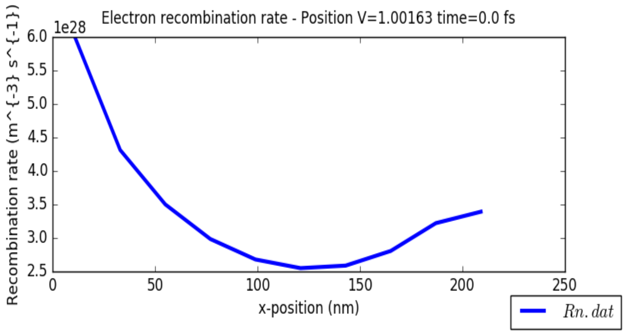

Fig.6: Electron recombination rate

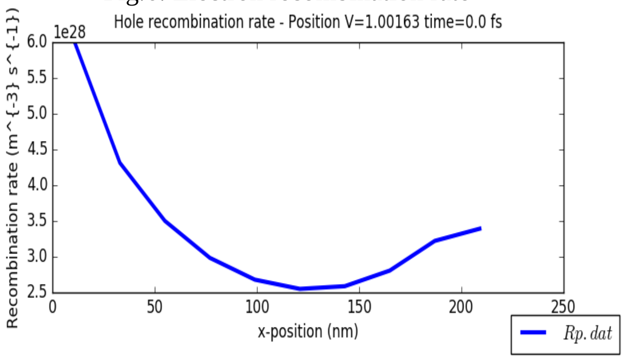

Fig.7: Hole recombination rate

3.5 Efficiency Calculations

One way to calculate efficiency is to analyze photon distribution and absorbed photon distribution.These two distributions are almost identical. All results are calculated considering AM1.5. The results will be almost identical as these results even if AM1.2 is considered.

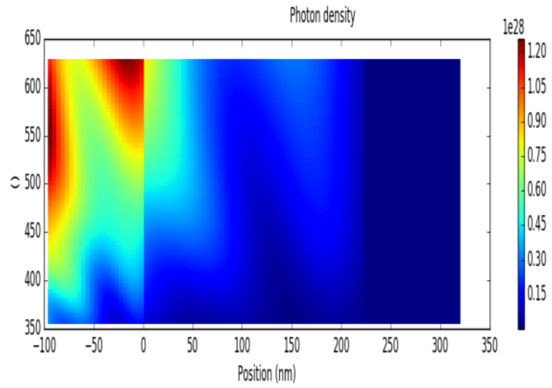

Fig.8: Photon Density

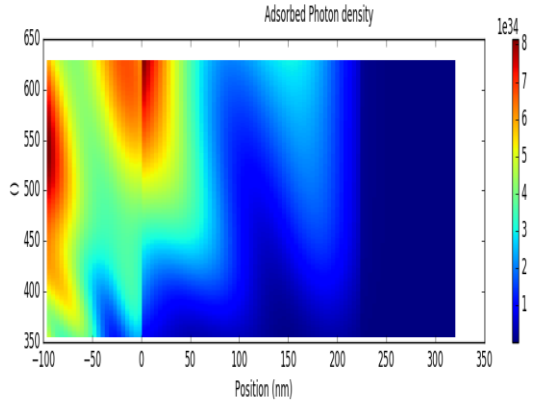

Fig .9: Absorbed Photon Density

This means that most of the photon that is incident on the solar cells are absorbed accordingly which is an important measure of efficiency. It is also observed from the above mentioned figure that in the photon density in the transition point of ITO and the effective layer is almost smooth which indicates the negligible amount of loss of photon.

Another important measure of efficiency of solar cell is the amount of reflected light. The less light is reflected, the more photon is absorbed. The reflected light with respect to the light wavelength is given in the following figure.

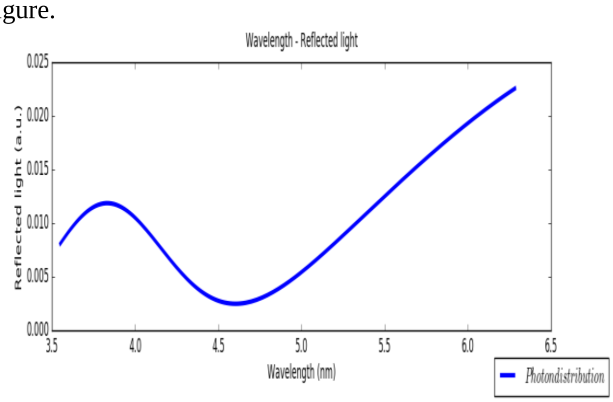

Fig.10: Reflected Light Characteristics

From the figure it is obvious that the light of 4.57nm is reflects the list and after the increase of 4.57nm, the amount of reflected light increases almost linearly.

4. CONCLUSION

Form the above parametric analysis it is seen that though the generation rate of the carriers with respect to the position of the organic solar cell is almost piecewise linearly decreasing, the electron and hole recombination rate is less compared to the inorganic solar cell due to the significant amount of trapped carriers. But this inconvenience can be overcome by finding the appropriate buffer layers in the anode in further research which alternatively responsible for the creation of larger amount of defects paving the way for more hole extraction even though the loss of work function i.e. interface field.

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6. REFERENCES

[1] R. C. I. MacKenzie,T . Kirchartz, G. F. A. Dibb, and J. Nelson “Modeling Nongeminate Recombination in P3HT:PCBM Solar Cells”*Journal of Phycal Chemistry*, vol.115 , no.19 , pp.9806 - 9813 , 2011.

[2] R. C. I. MacKenzie , C. G. Shuttle , M. L. Chabinyc ,and J. Nelson“Extracting Microscopic Device Parameters from Transient Photocurrent Measurements of P3HT:PCBM Solar Cells” *Journal of Advanced Energy Material*, vol.2 no.6 , pp.662-669 ,2012.

[3] R. C. I. MacKenzie, C. G. Shuttle, G. F. Dibb, N. Treat, E. Hauff, M. J. Robb, C. J. Hawker, M. L. Chabinyc, and J. Nelson “Interpreting the Density of States Extracted from Organic Solar Cells Using Transient Photocurrent Measurements” *Journal of Physical Chemistry*, vol.117, no.24 , pp.12407-12414 , 2013

[4] R. Hanfland, M. A. Fischer, W. Brutting, U. Wurfel, R. C. I. MacKenzie “Supplementary information for - The physical meaning of charge extraction by linearly increasing voltage transients from organic solar cells” University of Nottingham, Technical Rep. , 2013.

[5] F. Deschler, D. Riedel, B. Ecker, E. Hauff, E. D. Como and R. C. I. MacKenzie “Increasing organic solar cell efficiency with polymer interlayers”*Journal of Physical Chemistry Chemical Physics*, Vol. 15 , No. 3 , pp.705-712, 2013.

[6] R. C. I. MacKenzie , V. S. Balderrama , S. Schmeisser , R. Stoof , S. Greedy , J. Pallarès , L. F. Marsal , A. Chanaewa , and E. von Hauf“Loss Mechanisms in High Efficiency Polymer Solar Cells” *Journal of Advanced Energy Material*, vol.6 no.4 , pp. ,2015

[7] B. Dasgupta, W. P. Goh, Z. E. Ooi, L. M. Wong, C. Y. Jiang, Yi Ren, E. S. Tok, J. Pan, J. Zhang and S. Y. Chiam, “Enhanced Extraction Rates through Gap States of Molybdenum Oxide Anode Buffer”*Journal of Physical Chemistry*, vol.117 no.18 , pp.9206-9211 ,2013.

[8] Y. Gao , R. C. I. MacKenzie , Y. Liu , B. Xu , P. H. M. van Loosdrecht ,and W. Tian “Engineering Ultra Long Charge Carrier Lifetimes in Organic Electronic Devices at Room Temperature” *Journal of Advanced Material Interfaces*, vol.2 , no.4 , pp. ,2015.

[9] Y. Liu, R.. C. I. Mackenzie, B. Xu, Y. Gao , M. G.Fabra, D. Grant, P. H. M. van Loosdrecht, and W. Tian “Organic semiconductors with a charge carrier life time of over 2 hours at room temperature” *Journal of Materials Chemistry C*, vol.3 , no. , pp.12260-12266 ,2015.

[10] S. Kumar and S. S. K. Iyer, “Spectral Response Behavior in Single-Layer Organic Semiconductor Devices in Relation to its Absorption Spectrum” *IEEE Journal Of Photovoltaics*, Vol. 7, No. 2,pp.558-565, Mar. 2017

7. NOMENCLATURE

Symbol	Meaning	Unit
T	Temperature	(K)
ϵ_o	Permittivity of free space	Dimentio-nless
ϵ_r	Relative Permittivity	Dimentio-nless
ϵ	Effective Permittivity	Dimentio-nless
φ	Voltage Profile	
q	Elementary charge	Coulmb
n	Electron Concentration	m^{-3}
p	Hole Concentration	m^{-3}
J_n	Electron Current Density	Am^{-2}
J_p	Hole Current Density	Am^{-2}
R_p	Recombination rate of hole	$m^{-3}s^{-1}$
R_n	Recombination rate of electron	$m^{-3}s^{-1}$
G	Carrier generation rate	$m^{-3}s^{-1}$
μ_e	Electron mobility	$m^2V^{-1}s^{-1}$
μ_h	Hole mobility	$m^2V^{-1}s^{-1}$
n_f	Free electron concentration	m^{-3}
p_f	Free hole concentration	m^{-3}
D_n	Electron diffusion coefficient	

D_p	Hole diffusion coefficient	
n_t	Trapped carrier concentration	m^{-3}
v_{th}	Thermal Velocity	m^{-3}
$б_p$	Electron trap cross section	m^2
$б_n$	Hole trap cross section	m^2
N_c	Effective free electron density state	$m^{-3}eV^{-1}$
N_v	Effective free hole density state	$m^{-3}eV^{-1}$
α	Langevin reduction parameter	Dimensionless
β	Langevin reduction parameter	Dimensionless