Solid State Science and Technology, Vol. 20, No 1 & 2 (2012) 102-108
ISSN 0128-7389

INVESTIGATION OF RECOMBINATION PROCESS OF P3HT:PCBM ORGANIC SOLAR CELL

Eng Kok Chiew[1,*], Muhammad Yahaya[2] and A. P. Othman[1]

[1]*School of Applied Physics,Faculty of Science and Technology,Universiti Kebangsaan Malaysia,43600 UKM Bangi,Selangor,Malaysia*

[2]*Institute of Microengineering and Nanoelectronis,Universiti Kebangsaan Malaysia,43600 UKM Bangi,Selangor,Malaysia*

**Corresponding author: engkok.chiew@yahoo.com*

ABSTRACT

A computational study on a recombination mechanism in a bulk heterojunction (BHJ) organic solar cells of P3HT:PCBM was done. Using the simulation tools SCAPS, the electrical performances of organic solar cells and the intensity-dependent current density -voltage (*J-V*) were simulated and compared with the actual experimental result. Various light intensity dependent simulations were performed, and the results found showed that the higher the light intensity, the higher the current in reverse bias, since more photo-generated charge carriers were available to participate in the current.

Keywords: Bulk Heterojunction; organic solar cells; simulation; SCAPS; recombination; P3HT/PCBM; modeling

INTRODUCTION

Bulk heterojunction (BHJ) organic solar cells [1] have been investigated extensively because of its low cost fabrication in large sizes for harvesting energy from sunlight and in desired shapes [2]. Although efficiency of BHJ organic solar cell have reached to about 8% of the efficiency approved by National Renewable Energy Laboratory[3]. Efforts to commercialize BHJ cells is a major challenge, first, there is a need to improve the efficiency of the cell and second, to optimize the photo generation processes. However, optimization process in the performance of the cell needs the basic understanding of the physics behind the operation of these devices. Theoretical studies and simulation will play a major role to optimize BHJ organic solar cell. Understanding of recombination mechanism in Organic Solar Cells (OSCs) is important to optimize BHJ OSCs as these cells shows low efficiency. The PV mechanism in OSC cell is still unclear, even though some research groups confirmed that bimolecular recombination is the most dominant in loss mechanism[4], but more researchers believed that monomolecular recombination dictates the performance of OSCs [5-8]. The complexity of bi-continuous interpenetrating networks in BHJ configuration limits the theoretical analysis about recombination in OSCs. Experimental studies using transient luminescence with ultrafast lasers are considered to be the most powerful tool to

Solid State Science and Technology, Vol. 20, No 1 & 2 (2012) 102-108
ISSN 0128-7389

explore recombination dynamics in semiconductor materials. Alas, luminescence quenching is dominant in OSCs because electrons excited by photon will transfer quickly from donor materials to acceptors in about 50fs [9]. Because of the difficulty in understanding recombination mechanism either by analysis in theory or experimental observations, numerical simulation offers a reasonable alternative to identify recombination kinetics in OSCs.

The most general strategy today is the so-called bulk heterojunction, which electron donors such as P3HT and electron acceptors such as PCBM combined to form a blended layer. In this system, separation of photo-induced excitons is much improved because electrons are transferred very fast and there exists a large interface between the 2 components [10]. In this paper, we investigate intensity-dependant current-voltage (J-V) characteristics of on poly(3-hexylthiophene) (P3HT) and[6,6]-phenyl C61-butyric acid methyl ester (PCBM) bulk heterojunction organic solar cell using the standard solar cell device simulator developed by University of Gent, new version of SCAPS [11] and compared with experimental data. We found that they are in good agreement with experimental results. In the second section, details of theoretical model that we used to describe recombination of the P3HT:PCBM bulk heterojunction organic solar cell is presented. In the third section we discuss the implementation of the simulation of recombination mechanism of the organic solar cells.

THEORETICAL MODEL

The basic principles of BHJ OSCs can be summarized as follows. Strongly bound excitons are being first in the conjugate polymers after excited by photons due to the low dielectric constant of organic materials. Afterwards, excitons will spread at the interface of donor/acceptor and then will get separated into the charge-transfer excitons (CTEs) whichwill occur either in geminate recombination or separate to free electrons and holes. After that, the free carriers will get transport of through the secluded phases and are finally correct by electrodes. Under certain circumstances and simplification, current-voltage (J-V) characteristics of OSCs will be simulated by models for classical semiconductor devices. Steady-state electrical behavior of classical semiconductor devices can be modeled by Poisson equation which is related to charge and electrostatic potential φ and continuity equations for electrons and holes as shown in the following [12]:

$$\frac{\partial^2 \varphi(x)}{\partial x^2} = \left(\frac{q}{\varepsilon}\right)[n(x) - p(x)], \quad (1)$$

$$\frac{\partial J_n(x)}{\partial x} = q(-G + R_n), \quad (2)$$

$$\frac{\partial J_p(x)}{\partial x} = q(G - R_p), \quad (3)$$

where describes electrical potential, q is the unit charge, is the dielectric constant of the semiconductor; n and p are electron and hole density, respectively; $J_{n(p)}$ is the electron/hole current density; G is the generation rate and $R_{n(p)}$ is the recombination loss. The equations are non-linear because of the continuity equations consist

recombination term which is non-linear in n and p. It consists of drift and diffusion currents, $J_{n(p)}$ as can be explained as:

$$J_n = -qn(x)\mu_n\left[\frac{\partial\varphi(x)}{\partial x}\right] + qD_n[\frac{\partial n(}{\partial} \quad (4)$$

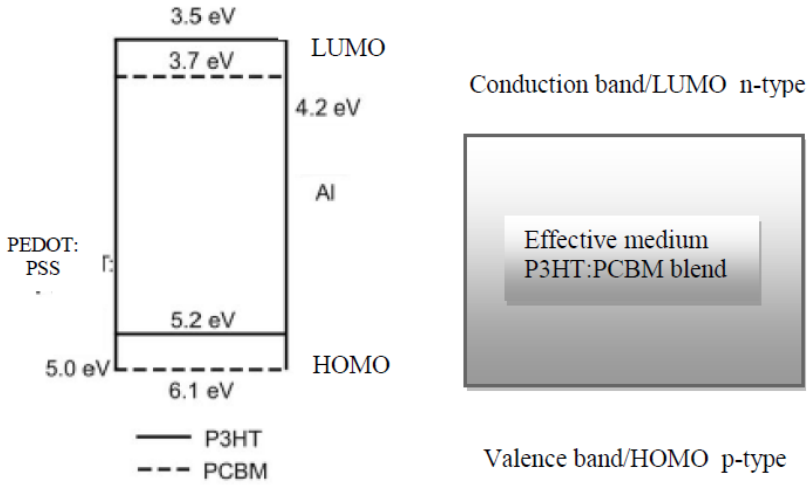
$$J_p = -qp(x)\mu_p\left[\frac{\partial\varphi(x)}{\partial x}\right] - qD_p[\frac{\partial p}{\partial} \quad (5)$$

where μ_n is the electron/hole mobility and $D_{n(p)}$ is the diffusion coefficient .
Several issues need to be dealt with to simulate BHJ OSCs using the model above due to their privileges properties. Firstly, is the spatially averaged dielectric constant of donor/acceptor blend and depends on the weight to donor-acceptor ratio of the materials. Secondly, effective carrier mobility (μ_e in acceptor and μ_h in donor) in BHJ configuration is different with value in their pristine phase, which is closely related with nano-morphology of disordered BHJ OSCs [13]. Thirdly, it was verified by experiment that the open circuit voltage(V_{OC}) is mainly defined by the difference between the highest occupied molecular orbital of the donor(E_{HO}^{d}) and the lowest unoccupied molecular orbital of the acceptor(E_{LU}^{a}) [14]. The effective band gap (E_g) in the simulation was expressed as $E_g = E_{LUMO}^{a} - E_{HO}^{d}$. Even though Einstein relation $\frac{D}{\mu} =$ possibly does not apply well in disordered materials [15], but it still can be assumed in the simulation for improvement without leading to substantial deviations.

The coupled differential equations were solved numerically by using Gummel iteration [16]. After the equations were solved successfully, characteristic of OSC (J-V) can fitted to experimental data by choosing suitable parameters, specially the loss recombination, $R_{n(p)}$. The comparisonresults of simulation with experimental data will estimate the enactive the loss recombination in OSCs.

To model J-V characteristics of P3HT:PCBM organic solar cell, P3HT:PCBM blend has been considered to be the effective medium semiconductor layer by electron mobility similar to electron mobility of PCBM and hole mobility and similar to hole mobility of P3HT respectively. The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) levels match the HOMO of P3HT and LUMO of PCBMrespectively. The schematic energy level diagram of the P3HT: PCBM organic solar cell and the effective medium model are shown in Figure 1.

Solid State Science and Technology, Vol. 20, No 1 & 2 (2012) 102-108
ISSN 0128-7389



(a) (b)

Figure1:(a) Schematic energy level diagrams of the PEDOT:PSS/ P3HT:PCBM/Al solar cell before the materials are brought into intimate contact; (b) the effective medium model which the intimate blend of an *n*-type material and a *p*-type material is represented by one single 'effective' material with 'average' properties

RESULTS AND DISCUSSIONS

The relationship between photocurrent density J_{ph} OSCs and the illumination intensity can be expressed as $J_{ph} \propto$. J_{ph} is obtained by subtracting the dark current from I-V curves at distinct light intensities.

Hence, stringent numerical simulation conducted was based on equations (1) to (5) to study photocurrent illumination intensity dependant. The simulation parameters of intensity dependant photocurrent $J_{ph} \propto$can be established in Table 1 and the simulation result is shown in figure 1 for recombination mechanism of P3HT:PCBM organic solar cell. The illumination intensity investigated here is around 1 sun intensity I_0, changed from $0.2I_0$ to $1.2I_0$ with step of $0.2I_0$, as loss mechanism under common operation condition (1 sun intensity) is extreme important in optimum OSCs. As shown in figure 2, characteristics of OSCs I-V curve was simulated under different illumination intensity at fixed recombination rate. The curve is in comparable to experimental results as reported by Liming Liu [17]. The results show that the higher the light intensity, the higher the current in reverse bias is since more photo-generated charge carriers are available to participate in the current.

Intensity dependence J-V curves was selected to study the loss recombination of BHJ OSCs because simulation on 1 set of experiment data (illumination intensity dependence J-V curves) cangive us reliable data to be compared with data from single experiment which can be easily simulated by manipulated suitable parameters.

Solid State Science and Technology, Vol. 20, No 1 & 2 (2012) 102-108
ISSN 0128-7389

Table1. Parameters used in the simulation with SCAPS on intensity-dependent photocurrent

Property	Symbol	Value
Band gap	E_g	1.05 [eV]
Electron affinity	χ	3.95 [eV]
Thickness of active layer	L	100 [nm]
Dielectric permittivity (relative)	ε_r	3
Effective density of state	N_c, N_v	1×10^{20} [cm^{-3}]
Electron mobility	μ_n	1.0×10^{-4} [$cm^2V^{-1}s^{-1}$]
Hole mobility	μ_p	1.0×10^{-4}[$cm^2V^{-1}s^{-1}$]

Recombination mechanism of P3HT:PCBM organic solar cell is show in figure 2. The illumination intensity investigated here is around 1 sun intensity I_0, changed from $0.2I_0$ to $1.2I_0$ with step of $0.2I_0$, as loss mechanism under common operation condition (1 sun intensity) is extreme important in optimum OSCs. From figure 2, we observed that the current density is proportional to the applied voltage of OSCs. The higher illumination intensity will gives rises of current density of carriers. However, this J-V curve will saturated after 0.6 V. By comparison with results reported by Liming Liu [14], our calculation show good agreement with them. Intensity dependence J-V curves was selected to study the loss recombination of BHJ OSCs because simulation on 1 set of experiment data (illumination intensity dependence J-V curves) can give us reliable data to be compared with data from single experiment which can be easily simulated by manipulated suitable parameters.

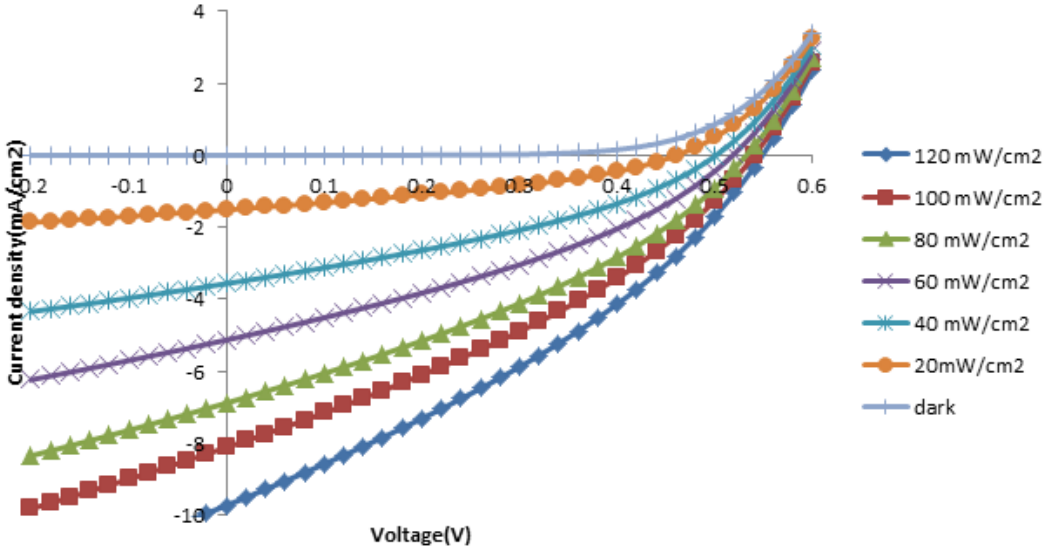


Figure 2: SCAPS simulation of the I-V curves of a Al/LiF/P3HT : PCBM /ITO/PEDOT-PSS solar cell, for varying illumination intensity

CONCLUSION

In summary, recombination mechanism in P3HT:PCBM organic solar cell have been investigated by simulation intensity depandant J-V curve and comparison between experimental and simulation of J-V curve characteristicsunder different illumination intensities found that monomolecular recombination mechanism dominates in BHJ OSCs. Further investigation of the physical mechanism of the monomolecular recombination mechanism will lead to better understanding of the internal physical operation of organic solar cell more thoroughly and hence improving the performance.

ACKNOWLEDGMENTS

This work has been carried out with the support of Operational Research University Fund (OUP) grant:UKM-OUP-NBT-29-141/2011. We are grateful to Professor M Burgelman for supplying his version of SCAPS.

REFERENCES

[1] G. Yu, J. Gao, J.C. Hummelen, F. Wudl, A.J. Heeger, *Science* **270** (1995) 1789–1791
[2] S.E. Shaheen, C.J. Brabec, N.S. Sariciftci, F. Padinger, T. Fromherz, J.C. Hummelen, *Applied Physics Letters* **78** (2001) 841–843.
[3] Information on http://www.pvtech.org/news/_a/new_polymers_push_solarmers_opv_efficiency_to_record_8.13/
[4] L.J.A. Koster, V.D. Mihailetchi, P.W.M. Blom, *Applied Physics Letters* **88** (2006) 052104-1–052104-3.
[5] R.A. Street, *Applied Physics Letters* **93** (2008) 133308–133311.
[6] M. Hallermann, E. Da Como, J. Feldmann, M. Izquierdo, S. Filippone, N. Martin, S. Juchter, E. von Hauff, *Applied Physics Letters* **97** (2010) 023301–023303.
[7] R.A. Street, M. Schoendorf, *Physical Review B,* **81** (2010) 205307-1–205307-12.
[8] I. Riedel, J. Parisi, V. Dyakonov, L. Lutsen, D. Vanderzande, J.C. Hummelen, *Advanced Functional Materials* **14** (2004) 38–44.
[9] C.J. Brabec, N.S. Sariciftci, J.C. Hummelen, Plastic solar cells, *Advanced Functional Materials* **11** (2001) 15–26.
[10] Information on http://www.light.t.u-tokyo.ac.jp/english/photovoltaic/Introduction.html
[11] M. Burgelman, P. Nollet and S. Degrave, *Thin Solid Films,* **361-362**, 2000, 527–532
[12] S.M.Sze, Physics of Semiconductor Devices, 2nd Edition, Wiley, London, 1981.
[13] V.D.Mihailetchi, H.X.Xie, B.deBoer, L.J.A.Koster, P.W.M.Blom, Charge transport and photocurrent generation in poly(3-

hexylthiophene):methanofullerene bulk-heterojunction solar cells,Advanced Functional Materials **16** (2006) 699-C708

[14] C.J. Brabec, A. Cravino, D. Meissner, N.S. Sariciftci, T. Fromherz, M.T. Rispens, L. Sanchez, J.C. Hummelen, *Advanced Functional Materials* **11** (2001) 374-380

[15] Y.Roichman, N. Tessler, *Applied Physics Letters* **80** (2002) 1948-C1950

[16] H.K. Gummel, *IEEE Transactions on Electron Devices* **11** (1964) 455–465

[17] Liming Liu, Guangyong Li, *Solar Energy Materials & Solar Cells* **95** (2011) 2557–2563