

PAPER • OPEN ACCESS

Numerical studies of P3HT : PCBM organic solar cell with an additional polymer layer using drift diffusion model

To cite this article: K S Nithya and K S Sudheer 2019 *J. Phys.: Conf. Ser.* **1172** 012017

View the [article online](#) for updates and enhancements.



IOP | ebooks™

Bringing together innovative digital publishing with leading authors from the global scientific community.

Start exploring the collection—download the first chapter of every title for free.

Numerical studies of P3HT : PCBM organic solar cell with an additional polymer layer using drift diffusion model

K S Nithya¹ and K S Sudheer²

¹Research scholar, Department of physics, Christ College Iirinjalakuda, University of Calicut, Kerala, India

²Associate Professor, Department of physics, Christ college Iirinjalakuda,, University of Calicut, Kerala, India

E-mail: nithyasathian@gmail.com

Abstract. Solar energy can replace the conventional energy sources in the near future. Organic solar cells have been showing tremendous improvement in their device performance for the past few years. Organic materials with their semiconducting properties and mechanical aspects being similar to that of conventional plastic materials present an affordable alternative for new generation solar cells to wipe out the energy crisis. Among the various structures for organic solar cells, bulk heterojunction (BHJ) solar cells have attracted attention for their improved mechanism for electron-hole pair separation, mechanical flexibility etc. In this paper, organic solar cell based on P3HT : PCBM BHJ is studied and the influence of active layer thickness on the device performance is investigated using numerical simulations with the drift diffusion concept. We further analyse the variation of device parameters by adding an additional polymer active layer of donor material P3HT between the BHJ and PEDOT : PSS layer. The numerical simulations are performed using the general purpose photovoltaic device model. The device parameters are assigned with the intention of analysing a solar cell with high mobility and less recombination rate leading to high efficiency. The solar cell shows maximum power conversion efficiency (PCE) of 9.312% when the active layer thickness is 210 nm. On adding additional P3HT layer, the optimized cell shows maximum PCE of 11.13% under AM 1.5 G spectrum when the polymer active layer thickness is 15 nm and BHJ is 195 nm

1. Introduction

Polymer solar cells are a promising alternative for the high-cost inorganic photovoltaics[1-2]. Organic photovoltaics(OPV) is one of the major research areas among the opto-electronic studies[3-4]. Their evolution from a single layer cell to bilayer structure and eventually to a bulk heterojunction design is truly remarkable[5-7]. It was only in 1995 that the concept of BHJ arrived. Since the structure is a blend of two materials: donor and acceptor, it eases the exciton dissociation process by providing a pathway at the material interface. Thus the structure effectively reduces the distance to be travelled by the exciton before recombination by matching with the exciton diffusion length[8-9].



The standard structure of BHJ includes an anode of high work function, hole transport layer followed by the active layer and a cathode of low work function material. The most commonly used BHJ is the one with P3HT (Poly 3-hexylthiophene) as the donor layer and PCBM (phenyl C-61 butyric acid methyl ester) as the acceptor layer. The light is absorbed predominantly in the donor layer and P3HT serves as a perfect option due to its reduced bandgap [10-11]. The P3HT : PCBM organic solar cell has poly(3,4-ethylene thiophene) polystyrene sulphonate PEDOT : PSS as the hole transport layer which mainly functions to planarize the rough surface of ITO and preventing any local short circuiting. ITO and Al functions as the anode front electrode and cathode back electrode respectively. In this work, the parameters of standard P3HT : PCBM heterojunction is analysed at different active layer thickness using the drift diffusion numerical model. The general purpose photovoltaic device model is used as the simulation tool.

A pure polymer active layer of P3HT which happens to be the donor impurity is added between the hole transport layer and BHJ with total active layer thickness remaining a constant. In this paper, a detailed analysis is presented about the influence of additional polymer active layer on the device performance.

2. Numerical modelling and material parameters

P3HT : PCBM Organic solar cell with conventional structure is simulated at different active layer thickness. The device structure of the cell is demonstrated in figure 1. The optimum active layer thickness is found at 210 nm and keeping this value as a constant, we simulated the cell after adding an additional P3HT polymer active layer as depicted in figure 2. The increase in polymer layer is compensated by a decrease in the BHJ thickness.

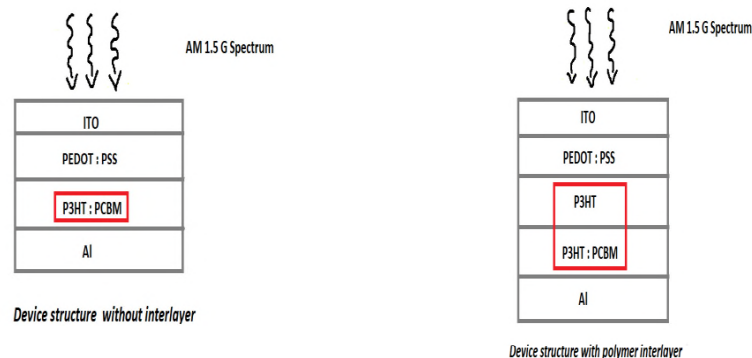


Figure 1. Device structure of pure BHJ organic solar cell.

Figure 2. Device structure with P3HT polymer interlayer.

The numerical simulation tool is general purpose photovoltaic device model. It solves the electrical model over the active layer material and details has been described elsewhere[12-17]. The drift diffusion equations for both charge carriers, electrons and holes are solved in position space. The equations are as follow:

$$J(n) = q\mu(e)n\frac{\partial E(l)}{\partial x} + qD(e)\frac{\partial n}{\partial x} \quad (1)$$

$$J(p) = q\mu(h)p\frac{\partial E(h)}{\partial x} + qD(h)\frac{\partial p}{\partial x} \quad (2)$$

Where J is the total current density, E_l and E_h corresponds to the energy levels of LUMO and HOMO respectively whereas μ is the mobility and n, p corresponds to the concentration of electron and holes while D denotes the diffusivity. The first term corresponds to the drift current density while second one shows the diffusion current density. The Shockley-Read-Hall recombination which has been already proved trustworthy for OPV is used to evaluate the carrier trapping and recombination processes inside the cell[18-27]. The input parameters used for the standard BHJ simulations are summarized in the following table 1.

Table 1. The parameters for the P3HT : PCBM organic solar cell simulation.

PARAMETERS	INPUT VALUE	
Electron trap density	3.8e26	m ⁻³ ev ⁻¹
Hole trap density	1.45e25	m ⁻³ ev ⁻¹
Electron tail slope	40e-3	eV
Hole tail slope	60e-3	eV
Electron mobility	2.48e-7	m ² v ⁻¹ s ⁻¹
Hole mobility	2.48e-7	m ² v ⁻¹ s ⁻¹
Relative permittivity	3.8	
Number of traps	20	
Free electron to trapped electron	2.5e-20	m ⁻²
Trapped electron to free hole	1.32e-22	m ⁻²
Trapped hole to free electron	4.67e-26	m ⁻²
Free hole to trapped hole	4.86e-22	m ⁻²
Effective density of electron states	1.28e-27	m ⁻³
Effective density of hole states	2.86e-25	m ⁻³

3. Results and Discussion

The device is simulated under AM 1.5 G spectrum. The thickness of anode, HTL and cathode are kept constant while the active layer (BHJ) thickness is varied. The numerical simulations are

performed for each thickness value without any polymer layer. The optimum thickness is found out. Keeping the total thickness of active layer at the obtained optimum value (thickness corresponding to highest PCE), P3HT layer is added between the HTL and BHJ as the additional active layer. The optical model is solved over all materials within the device and generation rate of the carriers throughout the solar cell is obtained. The schematic is given in Figure 3 and figure 4. The output parameters are given in table 2.

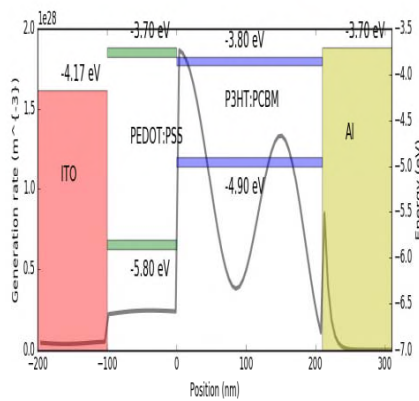


Figure 3. Optical model of pure BHJ organic solar cell.

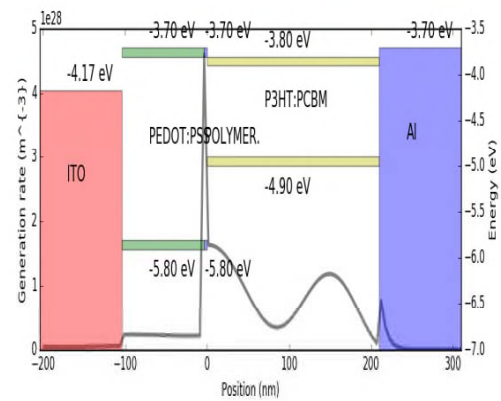


Figure 4. Optical model with P3HT polymer interlayer.

Table 2. Photovoltaic parameters of BHJ with polymer layer.

Thickness of BHJ (nm)	Thickness of polymer (nm)	Voc (V)	Jsc (A m^{-2})	FF	PCE (%)
210	0	0.6560	227.20	0.6560	9.312
205	5	0.6980	226.53	0.6869	10.87
200	10	0.6917	228.25	0.7026	11.09
195	15	0.6892	228.75	0.7062	11.13
190	20	0.6874	228.47	0.7071	11.10
180	30	0.6843	226.55	0.7075	10.97
170	40	0.6814	224.02	0.7099	10.83
160	50	0.6780	221.98	0.7130	10.74
150	60	0.6782	221.23	0.7150	10.71

3.1 Effect of polymer layer on open circuit voltage(V_{oc})

The origin of open circuit voltage comes from the subsequent splitting of electron and hole quasi-fermi energy levels followed by light illumination on the device[28]. It decreases with the increasing disorder of the organic material that brings down the electron quasi-fermi level and lifting up the hole quasi-fermi level. The variation of V_{oc} with thickness is shown in figure 5 and figure 6. It can be seen that the open circuit voltage doesn't shows much variation when the thickness is changed. The additional layer doesn't significantly change the value of V_{oc} since the parameter mainly depends on the LUMO and HOMO level of the active layer material.

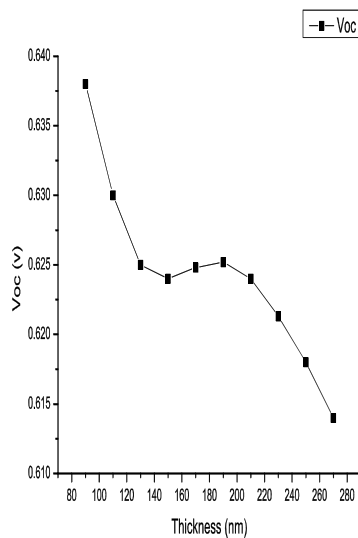


Figure 5. Variation of V_{oc} with thickness Of BHJ.

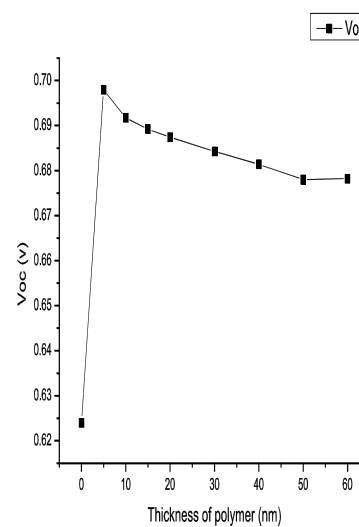


Figure 6. Variation of V_{oc} with thickness of polymer.

3.2 Effect of Polymer on Short Circuit Current Density(J_{sc})

The short circuit current density is a defining factor for the device's efficiency. It depends on the absorption property of donor material. The value of J_{sc} shows significant increase with the addition of polymer suggesting that the carrier photogeneration increased with the polymer layer. The maximum value is obtained when the polymer active layer thickness is 15 nm. On further increasing the thickness, J_{sc} decreases gradually. The schematic showing the variation is given in figure 7 and figure 8.

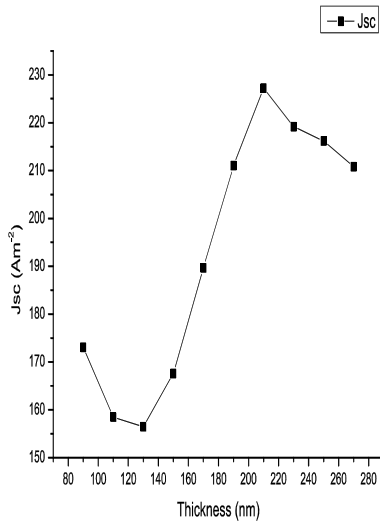


Figure 7. Variation of Jsc with thickness Of BHJ.

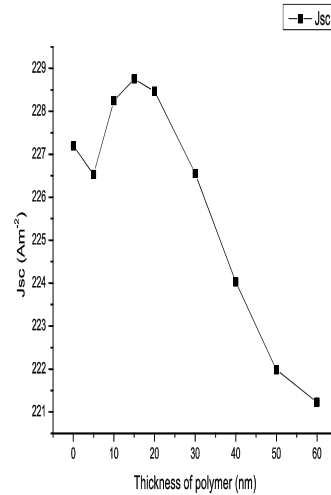


Figure 8. Variation of Jsc with thickness of polymer.

3.3 Effect of Polymer on Fill Factor(FF)

Fill factor is the measure of quality of the solar cell. It is the ratio of maximum power output and the product of open circuit voltage and short circuit current. The fill factor is defined by

$$FF = \frac{P(m)}{V_{oc} \cdot I_{sc}} \quad (3)$$

where $P(m)$ is the maximum output power, V_{oc} is the open circuit voltage and J_{sc} is the shortcircuit current density. FF decreases with thickness but it is observed to be increasing while adding the polymer layer. This could be due to an increase in the average shunt resistance of the cell. The variation is shown in Figure 9 and figure 10.

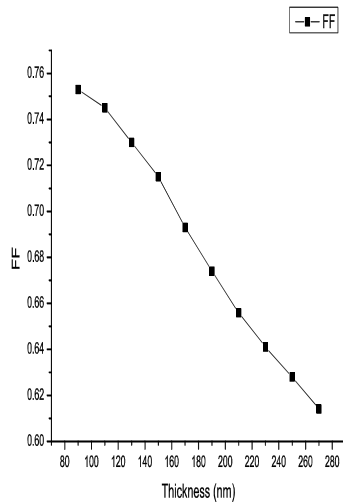


Figure 9. Variation of FF with thickness Of BHJ.

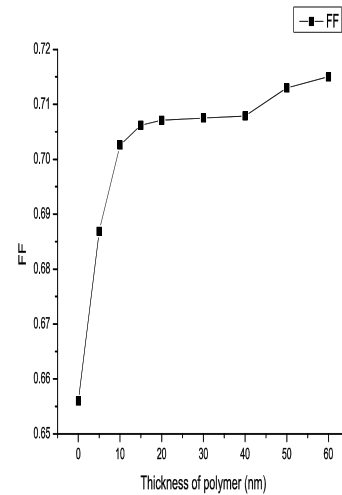


Figure 10. Variation of FF with thickness of polymer.

3.4 Effect of Polymer on Power Conversion Efficiency(PCE)

The efficiency of organic solar cell depends on open circuit voltage, short circuit current density and fill factor.

$$PCE = \frac{FF.Voc.Jsc}{P(in)} \quad (4)$$

Where P(in) is the incident power under AM 1.5 G Spectrum.

The maximum efficiency is obtained at 210 nm with the value 9.312 %. There is a significant increase in the efficiency with the addition of polymer layer. It reaches a maximum of 11.13 % when the polymer layer thickness is 15 nm and decreases gradually after that. The variation is shown in figure 11 and figure 12.

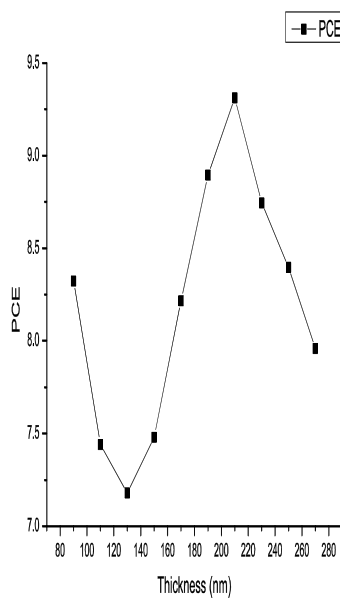


Figure 11. Variation of PCE with thickness Of BHJ.

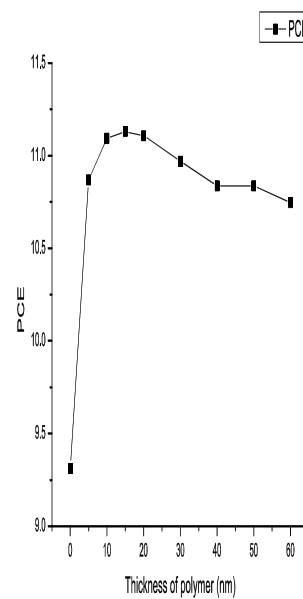


Figure 12. Variation of PCE with thickness of polymer.

4. Conclusion

In this work we demonstrate that the parameters of BHJ is effected by change in the active layer thickness. When the active layer has a thickness of 210 nm, the PCE reaches the maximum value of 9.312%. The addition of a pure polymer which happens to be the same material as that of the donor as the active layer increases the short circuit current density and thereby increases the efficiency to a maximum value of 11.13%. On further increasing the polymer thickness, PCE starts to decrease while the fill factor is showing a steady increase with the addition of polymer.

Our study indicates that the device performance of P3HT : PCBM organic solar cell increases with the addition of polymer active layer.

Acknowledgements

One of the authors, K S Nithya acknowledges KSCSTE for providing the research fellowship for funding this work.

References

- [1] H. Hoppe and N. S. Sariciftci, "Polymer solar cells," *Adv. Polym. Sci.* **214**, 1–86 (2008).
- [2] K. M. Coakley and M. D. McGehee, "Conjugated polymer photovoltaic cells," *Chem. Mater.* **16**(23), 4533–4542 (2004).
- [3] B. A. Gregg and M. C. Hanna, "Comparing organic to inorganic photovoltaic cells: Theory, experiment, and simulation," *J. Appl. Phys.* **93**, 3605–3614 (2003).
- [4] S. E. Shaheen, C. J. Brabec, N. S. Sariciftci, F. Padinger, T. Fromherz, and J. C. Hummelen, "2.5% efficient organic plastic solar cells," *Appl. Phys. Lett.* **78**, 841–843 (2001).
- [5] M. A. Green, K. Emery, Y. Hishikawa, W. Warta, E. D. Dunlop, *Prog. Photovolt: Res. Appl.* 2014, **22**, 701.
- [6] Z. He, C. Zhong, S. Su, M. Xu, H. Wu, Y. Cao, *Nat. Photonics* 2012, **6**, 593.
- [7] Y. Liu, J. Zhao, Z. Li, C. Mu, W. Ma, H. Hu, K. Jiang, H. Lin, H. Ade, H. Yan, *Nat. Commun.* 2014, **5**, 5293.
- [8] M. C. Scharber and N. S. Sariciftci, "Efficiency of bulk-heterojunction organic solar cells," *Prog. Polym. Sci.* **38**, 1929(2013).
- [9] G. Yu, J. Gao, J. C. Hummelen, F. Wudl, and A. J. Heeger, "Polymer photovoltaic cells: Enhanced efficiencies via a network of internal donor-acceptor heterojunctions," *Science*, **270**, 1789 (1995).
- [10] O. V. Mikhnenko, P. W. M. Blom, and T.-Q. Nguyen, "Exciton diffusion in organic semiconductors," *Energy Environ. Sci.* **8**, 1867–1888 (2015).
- [11] M. T. Dang, L. Hirsch, and G. Wantz, "P3HT:PCBM, best seller in polymer photovoltaic research," *Adv. Mater.* **23**, 3597–3602 (2011).
- [12] R. C. I. MacKenzie, C. G. Shuttle, M. L. Chabinyk and J. Nelson, *Adv. Energy Mater.*, 2012, **2**(6), 662–669.
- [13] M. Hilczler and M. Tachiya, *J. Phys. Chem. C*, 2010, **114**(14), 6808–6813.
- [14] C. Groves and N. C. Greenham, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 2008, **78**(15), 155205.
- [15] L. J. A. Koster, V. D. Mihailetschi and P. W. M. Blom, *Appl. Phys. Lett.*, 2006, **88**(5), 052104.
- [16] R. A. Street, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 2011, **84**(7), 075208.
- [17] A. Wagenpfahl, C. Deibel and V. Dyakonov, *IEEE J. Sel. Top. Quantum Electron.*, 2010, **16**(6), 1759–1763.
- [18] H. Bassler, *Phys. Status Solidi B*, 1993, **175**, 15–55.
- [19] B. Bohnenbuck, E. von Hauff, J. Parisi, C. Deibel and V. Dyakonov, *J. Appl. Phys.*, 2006, **99**(2), 024506.
- [20] Y. Roichman and N. Tessler, *Appl. Phys. Lett.*, 2002, **80**(11), 1948–1950.
- [21] F. F. Stelzl and U. Würfel, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 2012, **86**, 075315.
- [22] N. Tessler and Y. Roichman, *Org. Electron.*, 2005, **6**(56), 200–210.
- [23] W. Shockley and W. T. Read, *Phys. Rev.*, 1952, **87**(5), 835–842.
- [24] L. Tzabari and N. Tessler, *J. Appl. Phys.*, 2011, **109**(6), 064501.
- [25] W. Tress, K. Leo and M. Riede, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 2012, **85**, 155201.
- [26] R. C. I. MacKenzie, T. Kirchartz, G. F. A. Dibb and J. Nelson, *J. Phys. Chem. C*, 2011, **115**(19), 9806–9813.
- [27] A. Foertig, J. Rauh, V. Dyakonov and C. Deibel, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 2012, **86**, 115302.
- [28] K. Vandewal, K. Tvingstedt, A. Gadisa, O. Inganäs, and J. V. Manca, "On the origin of the open-circuit voltage of polymer-fullerene solar cells," *Nat. Mater.*, **8**, 904–909 (2009).