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K. S. Nithya, and K. S. Sudheer

Studies on P3HT: PCBM Organic Solar Cell with an Additional PC70BM Small Molecule Active layer at Optimum Thickness: A Numerical Simulation Approach

K S Nithya[1, a)] and K S Sudheer[2]

[1] *Research Scholar, Christ College, Irinjalakuda, University of Calicut, Kerala, India*
[2] *Associate Professor, Christ College, Irinjalakuda, University of Calicut, Kerala, India*

[a)] *Corresponding author: nithyasathian@gmail.com*

Abstract. Organic solar cells have been showing remarkable improvement for the past few decades. The cost-effective advantage along with the abundance of solar energy makes them, a potential candidate to wipe out the global energy crisis. In this paper, the most widely used bulk heterojunction of poly3-hexylthiophene: phenyl-C61-butyric acid methyl ester (P3HT: PCBM) is numerically simulated using the continuum drift diffusion model at different active layer thickness under AM 1.5 G spectrum. The maximum power conversion efficiency (PCE) of 6.345 % is obtained when the bulk has a thickness of 210 nm. Keeping this value as a constant, an additional PC70BM small molecule active layer is added compensated by decreasing the bulk thickness. General purpose photovoltaic device model is used as the numerical simulation tool. In the work, we demonstrate that a small molecule interlayer between the bulk heterojunction and Al electrode layer shows an increase in the power conversion efficiency of the organic solar cell and improves the device performance of P3HT: PCBM cell significantly. We further demonstrate that the fill factor of the device with the small molecule interlayer is far better than the device with bulk alone. A comparative study of organic solar cell parameters such as fill factor, open circuit voltage and short circuit current of the device with and without the interlayer are demonstrated in the work.

INTRODUCTION

For the last two decades, Organic Photovoltaics (OPV) has gained a lot of attention thanks to their low-cost and easy availability of materials.[1, 2] The evolution of OPV from a single layer geometry to the bulk heterojunction (BHJ) structure has been noteworthy, distinguishing themselves as a feasible solution for global energy demand.[3, 4] BHJ consists of a mixture of two materials; the donor and the acceptor. Due to the availability of donor-acceptor interface, the generation rate of excitons i.e. electron-hole pairs in the device and the higher probability for exciton dissociation at the boundary is an additional advantage for the design.[5-7] The charge carrier separation which happens to be the defining factor in the device performance is notably high in BHJ compared to the bilayer structure.The most popular BHJ today is a blend of poly(3-hexylthiophene 2,5-dyl) P3HT and phenyl- C61-Butyric acid methyl ester). The device structure has poly(3,4-ethylenethiophene) polystyrene sulfonate (PEDOT:PSS) as the hole transport layer while ITO and Al as the anode and cathode respectively. In this work, the standard P3HT : PCBM organic solar cell is numerically simulated at different active layer thickness using the general purpose photovoltaic device model to obtain optimum thickness value. An additional PC70BM small molecule layer, which happens to be the same material as that of the acceptor is added between the BHJ and Al electrode, The numerical simulations of the new structure is performed keeping the total active layer thickness at optimum value and varying the thickness of both the BHJ and the small molecule layer.

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NUMERICAL MODELLING AND PARAMETERS

The standard P3HT : PCBM organic solar cell is schematically demonstrated in fig 1.1(a). 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 PC70BM small molecule active layer as depicted in fig 1.1(b). The increase in small molecule layer is compensated by a decrease in the BHJ thickness. The device is simulated under AM 1.5 G spectrum.

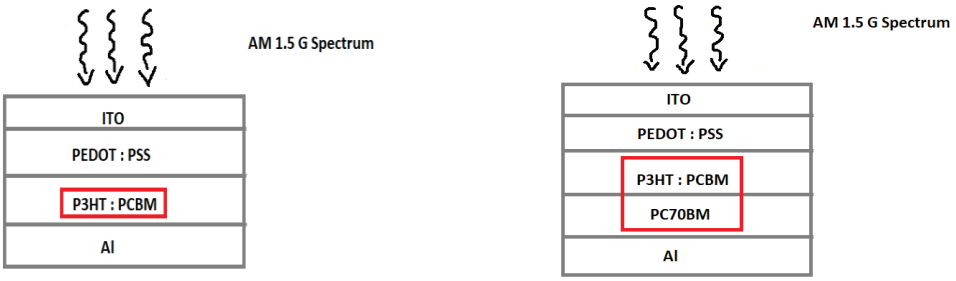

FIGURE 1. Device structure (a) without interlayer (b) with pc70bm interlayer

General purpose photovoltaic device model is the numerical simulation tool.[8-14] The continuum drift diffusion model has the active layer material being simulated by the electrical solver in the position space. The drift diffusion equation for both the charge carriers is given below:-

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

where J is the total current density, E*l* and E*h* corresponds to the energy levels of HOMO and LUMO 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 carrier trapping and recombination mechanism in the model is based on the Shockley-Read-Hall recombination process that has been widely accepted for BHJ analysis.[15-24]

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
Hole mobility	2.48e-7	m^2 v^{-1} s^{-1}
Hole mobility	2.48e-7	m^2 v^{-1} s^{-1}
Effective density of electron states	1.28e-27	m^{-3}
Effective density of hole states	2.86e-25	m^{-3}

RESULTS AND DISCUSSION

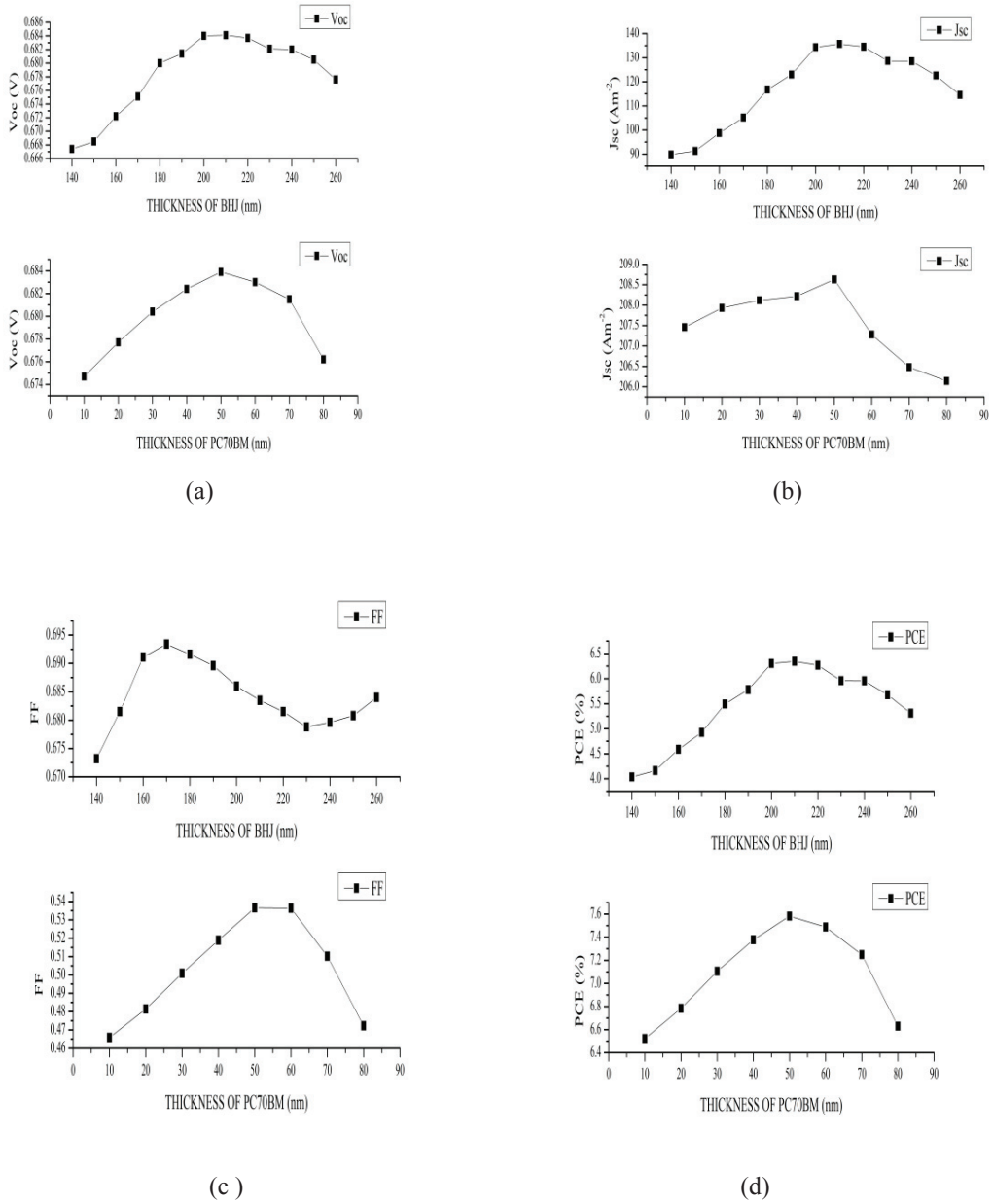

FIGURE 2. (a) Variation of Open Circuit Voltage (Voc) (b) Variation of Short Circuit Current density (Jsc) (c) Variation of Fill Factor (FF) (d) Variation of Power Conversion Efficiency (PCE)

The open circuit voltage is not affected with the new layer since it depends on the Homo and Lumo level. The short circuit current density shows a maximum value of 208.63 Am^{-2} when PCBM comprises 50 nm of the total active layer thickness compared to the previous maximum of 135.641 Am^{-2} when the entire BHJ comprises the 210 nm thickness. However, fill factor shows a decrease in the peak value with PC70BM layer. Power conversion

efficiency had a maximum of 6.345 % at 210 nm BHJ thickness. It shows a remarkable increase with a peak value of 7.582 % with BHJ contributing 160 nm of thickness and PC70BM forming the remaining 50 nm thickness.

CONCLUSION

In this work we demonstrate that the parameters of BHJ are affected by change in the active layer thickness. The addition of PC70BM small molecule in the active layer increases the short circuit current density and thereby increases the efficiency to a maximum value of 7.582 % when P3HT : PCBM forms 160 nm of the active layer and PC70BM form the remaining 50 nm thickness.

Our study indicates that the device performance of P3HT: PCBM organic solar cell increases with the addition of PC70BM small molecule layer.

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