

SIMULATION OF POWER CONVERSION EFFICIENCY P3HT, PCBM BY VARYING ACTIVE LAYER THICKNESS

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Abstract

Organic solar cells technologies have gained more attention in recent years due to low cost of production and flexibility. The power conversion efficiency of organic solar cells has seen an evolution when compared to inorganic materials in the laboratory. In this manuscript, we used the general-purpose photovoltaic device model (GPVDM) software to study the effect of the layer thickness of the photoactive layer on the power conversion efficiency. The results obtained are compared to the experimental result obtained based on poly (3-hexylthiophene) (P3HT): [6, 6]-phenyl-C₆₁-butyric acid methyl ester (PCBM). The results obtained show that the power conversion efficiency depend on the photoactive layer thickness.

Keywords: organic solar cell; photoactive layer; power conversion efficiency.

Introduction

The Sun occupies by mass 99.8% of our solar system and comprises of nearly three-quarters of hydrogen, while the remaining 0.2% consists mostly of helium. The Sun is estimated to provide energy to the earth at 1.8×10^{17} W, while, annual energy consumption globally is estimated roughly to 1.7×10^{13} W [1]. Based on this estimate, only a small quota of energy released from the Sun will be needed to meet yearly energy consumption globally. The thermonuclear reaction occurs commonly within the innermost 25% of the sun's radius creating a temperature of about 1.5×10^7 K at the core and is accountable for massive power output in the form of blackbody radiation. The possibility for solar energy is vast; it is projected that the total power incident on the earth's surface from the Sun every year is 1.8×10^{17} W and this is corresponding to 1.5×10^{18} KWh yearly [2, 3]. The high cost encountered with the collection, conversion and storage of solar energy hinders its exploitation as an alternative energy source in various places. Radiation from the sun can be transformed into heat energy or electrical energy. It can be changed into electricity directly using solar cells. This process is known as the photovoltaic effect. Semiconductor materials used for manufacturing solar cells are used in naming them; these materials need to attain certain parameters which will aid absorption of sunlight. Regardless of the source of light, solar cell devices are described as photovoltaic and be classified as first, second and third generation cells.

New photovoltaic devices built on less expensive organic semiconductor materials have been fabricated for use to convert solar energy to electricity. These organic semiconductor materials utilized in fabricating organic solar cells (OSCs) hold the advantage of low cost of production. This has led to enormous acknowledgement and intense research interest in the design of OSCs as a substitute to silicon based solar cells [4-6]. Crystalline silicon solar cells are estimated to have high efficiencies relative to organic solar cells. Therefore, improving the absorbance of the organic semiconductor remains a hindrance [7, 8]. In order to attain high performance in OSCs several approaches have been adopted to address the challenge. It was proposed that the formation of conductive absorber medium, effective interfacial layers and fabrication of low band gap polymers are approaches that can be utilized [1]. There was work done on high-efficiency multi-junction polymer and hybrid solar cells by [9]

Also performance of P3HT:PCBM based organic solar cell has been compared with OC 1 C 10 PPV:PCBM based solar cell for two different cathode materials.[10]

Work was also done on cooperative power harvesting scheme, collecting power from two or more independent ambient energy sources into a single non-linear component. See [11]

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Modeling the short-circuit current density of polymer solar cells based on P3HT:PCBM blend reported in [12]. Similarly, Longterm stability of efficient inverted P3HT:PCBM solar cells was reported in [13]

A New Model for the Morphology of P3HT/PCBM Organic Photovoltaics from Small-Angle Neutron Scattering: Rivers and Streams was explored by [14]

In 2012 an experimental work was designed to provide quantitative thermodynamic information on the miscibility, inter diffusion, and depth profile of P3HT : PCBM thin films that are formed by thermally annealing initial bilayers. It was found that the resultant thin films consisted of a ‘bulk’ layer that is not influenced by the air or substrate surface. See [15]

In this manuscript, we shall be simulating the effect of varying the active layer thickness based on P3HT: PCBM organic solar cell on the power conversion efficiency while other parameters remain constant using the general-purpose photovoltaic device model simulation software and comparing it to experimental result.

Method

The general-purpose photovoltaic device model (GVPDM) simulation software was used in determining the PCE of the simulated device by varying the active layer thickness used in fabricating OSC devices. The layer structure of the P3HT: PCBM based BHJ-OSC is shown in Figure 1. The GVPDM simulation software is based on solving Poisson equation (1.0), electron and hole drift-diffusion equations (1.1 and 1.2) and the carrier continuity equations (1.3 and 1.4).

$$\frac{d}{dx} \epsilon_o \epsilon_r \frac{d\phi}{dx} = q(n - p) \quad (1.0)$$

$$J_n = q\mu_c n \frac{\partial E_c}{\partial x} + qD_n \frac{\partial n}{\partial x} \quad (1.1)$$

$$J_p = q\mu_h p \frac{\partial E_v}{\partial x} - qD_p \frac{\partial p}{\partial x} \quad (1.2)$$

$$\frac{\partial J_n}{\partial x} = q \left(R_n - G + \frac{\partial n}{\partial t} \right) \quad (1.3)$$

$$\frac{\partial J_p}{\partial x} = -q \left(R_p - G + \frac{\partial p}{\partial t} \right) \quad (1.4)$$

where q , D_n , D_p , n , p , J_n , J_p , ϵ_o , ϵ_r , ϕ , μ_c , μ_h , E_c , E_v , R_n , R_p and G are electronic charge, diffusion coefficient of electron, diffusion coefficient of hole, electron density, hole density, electron current density, hole current density, permittivity of free space, relative permittivity, voltage profile, electron mobility, hole mobility, free-electron mobility, free hole mobility, net recombination rate of electrons, net recombination of holes and free carrier generation rate respectively. The research was carried out by varying the thickness of the absorber layer (100, 120, 130 and 140 nm) while other material thickness was kept constant according to experimental values.

Result and Discussion

Using the general-purpose photovoltaic device model (GVPDM) simulation software the current density (J) – voltage (V) curve (Figures 1 to 4) the photovoltaic parameters for the simulated devices was obtained using the simulation parameters in Table 1. The low mobility of carriers in polymer has hindered the absorber medium thickness (≤ 100 nm) resulting in limited optical absorption [2, 4] Therefore, one approach to improving the absorption of photons and overall power conversion efficiency can be derived by understanding the effect of the absorber layer thickness. A summary of the photovoltaic parameters is presented in Table 1. A decrease in power conversion efficiency is observed as the thickness of the active layer (P3HT: PCBM) is increased. The decrease in efficiency can be attributed to the decrease in current density (J_{sc}) which is linked to the combination of carriers and extraction of the carriers at the respective electrodes. Increasing the thickness of the active layer is stated to improve the absorption of photons but will limit the efficiency obtained due to the low mobility of carriers in polymers.

Table 1: Simulation parameters

Layer	Thickness (nm)
ITO	130
PEDOT: PSS	140
P3HT:PCBM	100, 120, 130 and 140
LiF	0.40
Al	60

Table 2: Photovoltaic parameters for simulated solar cells

Thickness (nm)	V_{oc} (V)	J_{sc} (A/Cm ²)	FF	PCE (%)
100	0.61	79.55	76.52	3.72
120	0.60	80.81	75.16	3.68
130	0.60	81.41	74.47	3.66
140	0.60	83.40	73.47	3.89

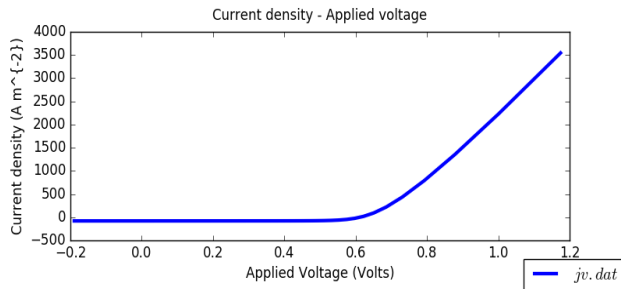


Figure 1: Current density – voltage curve for the simulated device (100 nm)

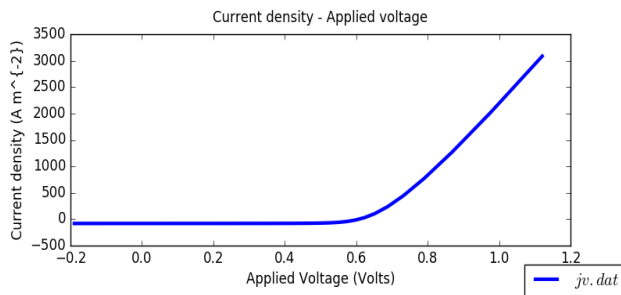


Figure 2: Current density – voltage curve for the simulated device (120 nm)

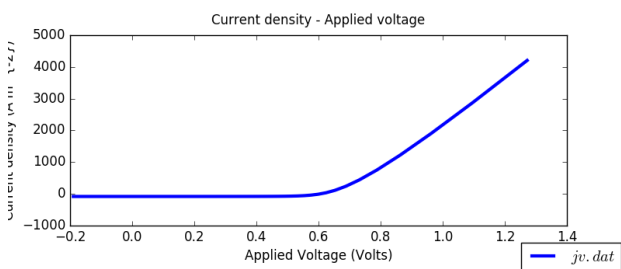


Figure 3: Current density – voltage curve for the simulated device (130 nm)

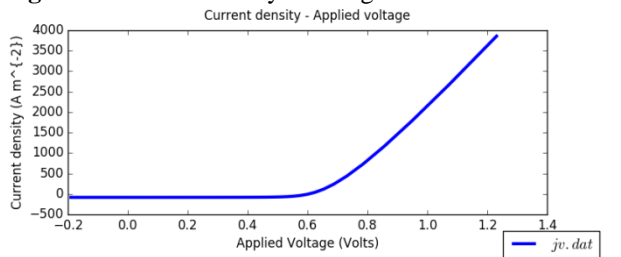


Figure 4: Current density – voltage curve for the simulated device (140 nm)

Conclusion

In this research work, the electrical stimulation of the bulk heterojunction (P3HT: PCBM) organic solar cell has done. The J-V characteristics curve of organic solar cell varies with thickness of the absorber layer. In this study, we obtained the maximum short circuit current at 83.40 A/cm^2 due to maximum dissociation probability. If the mobility increased or decreased, the dissociation probability decrease and the short circuit current also decrease leading to reduction in power conversion efficiency. The optimum efficiency of organic solar cell is obtained 100 nm.

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