Electrical Simulation for Different Thickness Ratio of PCBM and PTAA in Bilayer Organic Solar Cells

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In organic solar cells, it is regularly observed that different thickness of active layer result in different competency of the device due to its behaviour of charge transportation and charge collection in such volume morphology of active layer. In this paper, heterojunction device based on poly(triarylamine) (PTAA) and [6,6]-phenyl- C_{61} –butyric acid methyl ester (PCBM) as active layer had been electrically characterized using general –purpose photovoltaic device model (GPVDM) software. A thickness ratio: 50:50, 100:50,150:50, and 250:50 nm of PTAA to PCBM and vice versa for PCBM to PTAA were evaluated in this simulation. This simulation displays a pattern of current-voltage (*I-V*) and current density-voltage (*J-V*) at different thickness for PTAA/PCBM heterojunction bilayer solar cells. The short circuit current density (J_{sc}), open circuit voltage (V_{oc}) and fill factor (*FF*) for each different thickness active layer device was also presented as well. The highest achievable efficiency, 9.283 % was observed at thickness ratio of 250: 50 nm (PTAA to PCBM) under light intensity of 10 mW/cm².

Keywords: heterojunction devices; PTAA; PCBM; GPVDM; solar cells

I. INTRODUCTION

Organic semiconductor materials have the capability of transporting charge carriers and had been studied since 1950. Organic material is accepted as active materials in semiconductor devices due to their notable of development in many photonic applications, such as organic field-effect transistors (OFET), organic light-emitting diode (OFET), and organic solar cells (OSC) (Chen *et. al.,* 2009). Organic semiconductors have special characteristics such as light in weight, simple of production, and the price is relatively low (Kawano, Sakai, Yahiro, & Adachi, 2009).

An organic semiconductor can be classified into two categories known as small molecules and polymers. Usually the organic small molecule is compound contain carbon atom that are bonded into stable individual molecular unit. Both PCBM/PTAA of active layer that used in the simulation are classified as small molecule (Lin *et. al.,* 2014). Recently, the heterojunction of electron donor molecule and functionalized fullerene as electron acceptors have revolutionizes over the silicon based photovoltaic cells (Ramrakhiani, 2017). In an experimental data, the bilayered of heterojunction of an electron donate and fullerene electron acceptor can be employed in organic photovoltaic

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device as its more straightforward, facilitating optimization as compared with bulk heterojunction PVC. However, the exciton dissociation efficiency in bilayer device is lower than that of reported bulk heterojunction photovoltaic cells (Ramrakhiani, 2017). Hence, a group of researchers had proposed few methods to produce bilayer solar cells with better characteristics includes increasing the interface area of electrons and holes diffusion and also enhancing exciton dissociation (He *et. al.,* 2011).

Aim of this GPVDM simulation is to investigate the relationship between thicknesses of active layers towards its electrical characteristics. Performance of solar cell was strongly depending on the thickness of active layers which is related to the inter diffusion of the charge from hole transport layer towards the electron transport layer. The most favourable morphological volume of donor and acceptor material ensures movement of charge carrier paths to both electrodes and thus confines the potential for charge recombination (Intaniwet *et. al.,* 2009; Narayan, 2012)]. Results of this simulation can be used to design an experimental in fabricating bilayer organic devices of high efficiencies with less production time and costs.

II. THEORETICAL EQUATIONS

Short circuit current density, J_{sc} (Ong & Levitsky, 2010) can be derived from equation (1)

$$J_{sc} = \frac{I_{sc}}{A} \qquad (1)$$

$$I_{sc} = qG\,(L_n + L_p) \qquad (2)$$

where I_{sc} is short circuit current, A is the area of the layer, G is the generation rate, L_n and L_p is the diffusion length for electron and hole.

However, the short circuit current density J_{sc} (Nath et al. 2011) can be theoretically determined as

$$J_{sc} = q\int_{\lambda} b_s(\lambda)\,QE(\lambda)\,d\lambda \qquad (3)$$

Where $b_s(\lambda)$ is the incident photon flux density and $QE(\lambda)$ is the quantum efficiency *(QE)* of the cells at given wavelength, λ. QE is the quantum efficiency refers to amount of carries collected at the electrode to the amounts of photons of given energy incident.

Fill factor is determined as

$$FF = \frac{V_{mpp} J_{mpp}}{V_{oc} J_{sc}} \qquad (4)$$

where V_{mpp} is the maximum power point in graph, J_{mpp} is the maximum power point for short circuit current. The stated equation resolving, and device modelling have been applied in research of (Narayan, 2012; T *et. al.,* 2016; Tsoi *et. al.,* 2011) for photovoltaic devices.

The power conversion efficiency *(η)* of organic solar cells can be expressed as

$$\eta = \frac{FF \cdot V_{oc} \cdot J_{sc}}{P_{in}} \qquad (5)$$

where, P_{in} is the light incident power density. V_{oc} is the open circuit voltage where the organic solar cells produced maximum voltage as the short circuit current density J_{sc} is zero under illumination is zero.

III. SIMULATION PARAMETERS

Figure 1 shows the structure of simulated bilayer solar cells. The device structure is split up into different materials consists small molecule as active layers. Electron transport material layer is the fullerene derivatives, [6,6]-Phenyl C_{61} butyric acid methyl ester, PCBM was reported to have higher efficiencies in organic solar cells and the Hole transport material layer, Poly(triarylamine), PTAA act as layer over which the electric model will be applied. Both thickness of active layer was manipulated using GPVDM software under 10 mW/cm² light intensity. First simulation of this configuration was focused on different thickness of PTAA at 50nm, 100nm, 150nm and 250nm respectively at fixed width of PCBM, 50nm. Next simulation was determining the electrical characteristics at different thickness layer PCBM, 50 nm, 100nm, 150nm and 250 nm at 50nm of PTAA. The depth of electrode ITO and Al were fixed at 100nm. The configuration of devices as shown in Table 1.
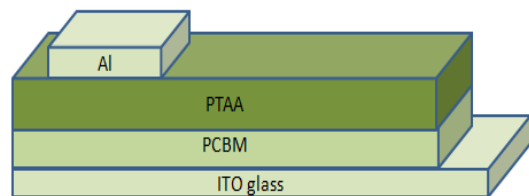

Figure 1. Structure of bilayer organic solar cells for GPVDM simulation

Table 1. The parameter configuration in applied GPVDM simulation of organic bilayer solar cell

PARAMETER	PARAMETER'S VALUE	UNITS
Electron trap density	1e25	$m^{-3} eV^{-1}$
Hole trap density	1e25	$m^{-3} eV^{-1}$
Electron Mobility	1e-6	$m^2 V^{-1} s^{-1}$
Hole mobility	1e-6	$m^2 V^{-1} s^{-1}$
Trapped electron to free hole	1e-22	m^{-2}
Trap hole to free electron	1e-22	m^{-2}
Free electron to trapped electron	1e-21	m^{-2}
Free hole to trapped hole	1e-21	m^{-2}
Device witdh	0.01	m

IV. RESULTS AND DISCUSSION

Figure 2 presents the I-V characteristics of the simulated device at different thickness of PCBM / PTAA. The device shows a highest current produced when thickness of PCBM at 250nm and PTAA at 50nm. PCBM can trap more electron charge to be diffused at electrode as the layer become thicker. However, at thickest layer of PTAA, the total current at 4V is slightly lower, 0.037 A, this indicate some of e^- is not able to be discharge at the electrode. The atomic structure of PTAA itself allowed the rate of exciton recombination become faster. However, as the thickness of PTAA increases, the photon is absorbed at higher rate causes the rate of exciton recombination at phases also increases (Lin et al., 2014). Both graph shown in figure 2 (a) and 2 (b) indicates that at 0.00 to 0.60 V, the current values was nearly to be constant where at V= 0, the I = -0.00208 A and -0.00187 A for PCBM and PTAA thickness at 250 nm respectively, this values is known to be the short circuit current. The point at V= 0.60 V, there was a sudden increase in current from both graphs represented as "knee" point (Ramrakhiani, 2017).
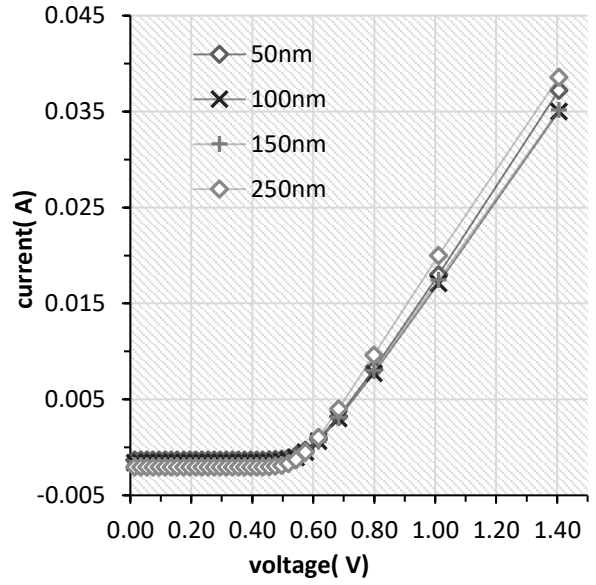

Figure 2(a). I-V characteristics of organic bilayer PCBM/PTAA at vary thickness of PCBM
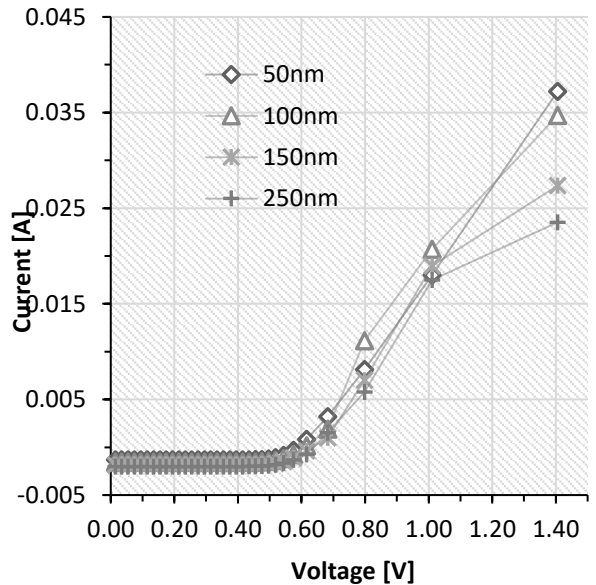

Figure 2(b). I-V characteristics of organic bilayer PCBM/PTAA at vary thickness of PTAA

Figure 3 shows the influence of layer thickness on J_{sc} for both configurations of solar cells. A thick layer enables more electron and holes trapping in film along with great photons absorbed to induce exciton dissociation at the interface (Kawano et al. 2009). The short circuit current density, J_{sc} for both configurations shows to have elevated value as thickness of active layer increases. It is observed the highest value of J_{sc} by 0.208 mA/ cm² at thickness ratio 250nm:50nm of PCBM to PTAA. In most of experimental data, thicker active film formed a reduction of short current density due to non-ideal surrounding environment during

the process of solar cells fabrication (T *et. al.,* 2016). In this simulation, the J_{sc} is increasing linearly with the active layer to indicate that almost all the photogenerated electron hole - pair contribute to J_{sc} since they are succeeded to be collected at electrode before the recombination occurs (Chopra, 2011)
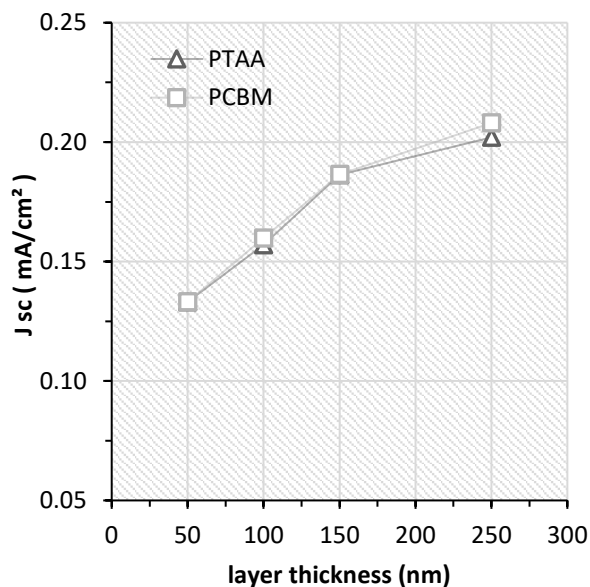

Figure 3. Device Short Circuit, J_{sc} at different thickness ratio of active layer

It is remarkable that the values of open circuit voltage also increase as the thickness layers for both configurations was increases, where thickest layer of PTAA gave significant effect to its electrical characteristics as compared with the thickest layer of PCBM. Open circuit voltage determined the voltage produced at solar cell junction when the forward biased current is zero. Figure 4 demonstrates the influence of layer thickness on open circuit voltage, V_{oc} of the simulated module. 0.616 V is the highest V_{oc} obtained from configuration of PCBM/ PTAA layers at thickness ratio of 50nm: 250nm. A study by Hsiang-Yu Chen et al. 2009 state that the values of V_{oc} was depends on the difference of HOMO level of e- donor and LUMO level of e- acceptor, lowering the differences will exhibit an increase the open circuit voltage (Chen et al. 2009). However, the V_{oc} in vary thickness of PCBM is lower compared to PTAA and the reasons by a smaller band gap is not very clear for this simulation. Large amount for crystalline volume fraction (F_c) was remarked to low values in Open circuit voltage of PCBM as compared with PTAA.
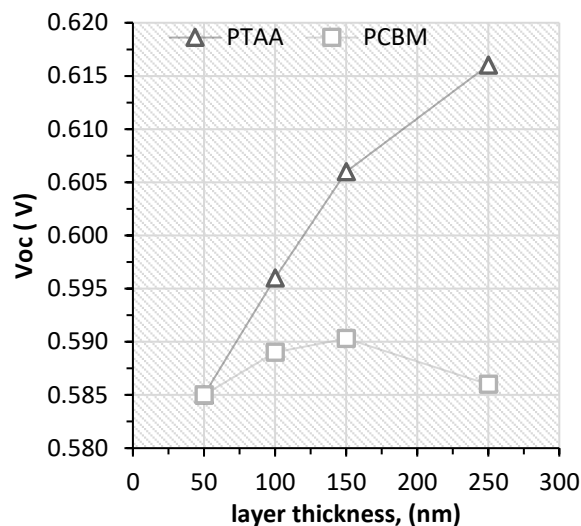

Figure 4. Device Open Circuit voltage, V_{oc} at different thickness ratio of active layer

Obviously, an increase in the thickness active layer both configurations had influenced the fill factor of the solar cells. At a thickness ratio 50nm:50nm for PTAA / PCBM, its yield 0.780 a.u of fill factor (*FF*) to provide more power under normal operating conditions. The variation in fill factor values indicates a change in series resistance of electron transport layer, where charge extraction at electrode increases as series resistance from a thin layer of PCBM was reducing (Narayan, 2012). The imbalanced charge extraction rates for the hole and the electrons also cause the fill factor, *FF* to decreases in thicker film (Lin et al. 2014). Figure 5 shows the influence of active layer thickness on fill factor, *FF* for both configurations of bilayer organic solar cells.
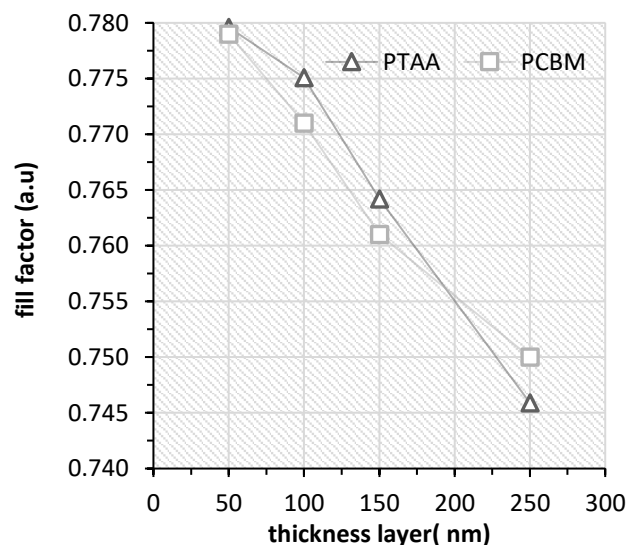

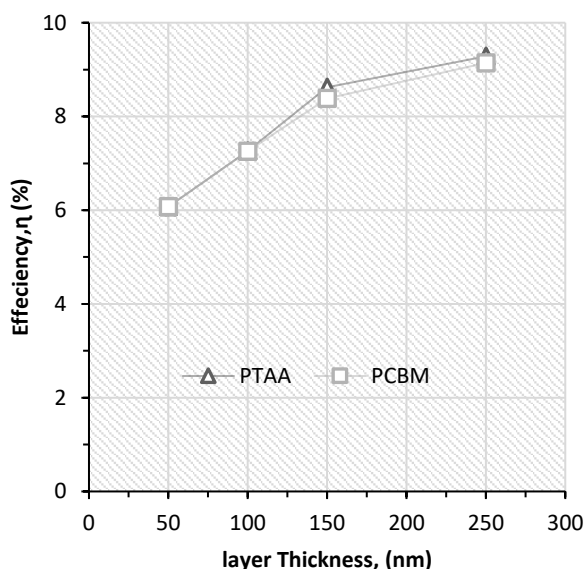Figure 5. Device fill factor at different thickness ratio of active layer

Figure 6. Device efficiency at different thickness ratio of active layer

The effect of active layer thickness on percentage efficiency had been analysed and shown in Figure 6. The thickest layer of hole transport material (PTAA 250nm with PCBM 50nm) had achieved the best efficiencies with 9.283%. This simulation shows that PCBM at thickest layer (PTAA at 50nm) also able to produces high efficiencies at 9.143% but slightly lower than the rate achieved by PTAA at 250 nm (PCBM at 50nm). The thicker active layer allows the formation of a continuous network throughout the entire active layers, created a maximum number of dissociate excitons and delayed the time of charge recombination due to its Columbic attraction at the interface. The combination of materials and different thickness used in this study reveals that depth of layer for holes transport material PTAA ratio can exhibit a better electrical characteristic compared with the changes in PCBM layer thickness. Table 2 and 3 shows the results of electrical simulation on performance of bilayer organic solar cells.

Table 2. The Electrical simulation at different thickness of PTAA at light intensity of 10mW/cm²

Thickness ratio PTAA to PCBM (nm)	J_{sc} (mA/cm²)	V_{oc} (V)	FF (a.u)	η (%)
50:50	1.330	0.585	0.780	6.075
100:50	1.560	0.597	0.775	7.626
150:50	1.860	0.606	0.764	8.670
250:50	2.000	0.616	0.746	9.283

Table 3. The Electrical simulation at different thickness of PCBM at light intensity of 10mW/cm²

Thickness ratio PCBM to PTAA (nm)	J_{sc} (mA/cm²)	V_{oc} (V)	FF (a.u)	η (%)
50:50	1.331	0.585	0.780	6.075
100 :50	1.598	0.589	0.771	7.260
150 :50	1.867	0.590	0.761	8.385
250 :50	2.080	0.587	0.750	9.143

V. CONCLUSION

Electrical characteristics of organic bilayer solar cell at different thickness ratio of PCBM/PTAA were analysed using the GPVDM solar cells software simulation. This software simulation is using numerical modelling reveals that the thicker layer of active layer yields a maximum efficiency of 9.283%. The change in the PTAA thickness shows more significant effect in the optical absorption when being compared to PCBM as its shows a higher value of open circuit voltage.

VI. ACKNOWLEDGEMENT

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