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Simulation and Fabrication of P3HT:PCBM Solar Cell

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Abstract **- Poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl-C71 butyric acid methyl ester (PCBM) polymer solar cell is studied by using GPVDM simulations and experiments. The research focuses on the effects of active layer thickness on solar cell structures as bulk heterojunction (BHJ) (ITO/P3HT:PCBM/Al) as compared to a bilayer structure (ITO/P3HT/PCBM/Al). The optimal active layer thickness of 200 nm is obtained in the simulation for BHJ solar structure. The results also indicate that bulk heterojunctions exhibit slightly higher efficiency than bilayer solar cell with the same thickness, possibly due to a better and worthier total surface region for charge separation and reduced recombination between the electrons and holes. BHJ solar cell is fabricated in the experiment by using spin coating. The results show that higher spin speeds result in a thinner active layer, and the device coated at 2500 rpm had the highest power conversion efficiency of 0.91 % because of a higher I_{sc} and fill factor, despite a low absorption. The results suggest that bulk resistance, and morphology of the active layer play important roles in the carrier transport in the P3HT:PCBM solar cell.**

Keywords — Organic solar cell, simulation, fabrication, P3HT, PCBM

I. INTRODUCTION

Organic solar cells or organic photovoltaic (OPV) have several important advantages over the inorganics; such as the abundance of raw materials and the lower production cost. Also, less energy is required to produce an organic solar cell. In addition, organic solar cells can be manufactured on flexible, transparent, or coloured substrates for integration into a wide range of applications.

One of the most promising organic solar materials is the polymeric material: poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl-C71 butyric acid methyl ester (PCBM) [1]. The blend of both polymers (P3HT:PCBM) in solvent, coated as an active layer in between anode and cathode solar cell exhibited promising efficient of up to 5 % [2, 3]. The polymers act as the donor and acceptor in a bulk heterojunction (BHJ) configuration in the active layer. The blending allows the mix of the polymers to efficiently split the excitons into charge carriers as the exciton diffusion length in polymers like P3HT is only ∼10 nm [4]. Alternatively, the two polymers can be coated as two layers (P3HT/PCBM) in the solar cell, thus the name bilayer heterojunction solar cell [5]. High efficiency cell was also achieved through proper selection and control of the device fabrication process in bilayer structure. BHJ structure has a more complex nanoscale architecture while bilayer P3HT/PCBM devices are layered. In addition, BHJ structures offer the benefit of a simpler fabrication via solution process techniques such as spin-coating. Bilayer structures, in contrast, necessitate multilayer deposition and additional precautions to prevent intermixing between layers, making the fabrication more difficult [6, 7]. On the other hand, the mixing of the two components in the blend film, that is influenced by processing conditions, has a significant impact on the interpenetrating network in BHJ devices, that can warrant better charge transfer [5].

In the current work, polymer solar cell based on P3HT and PCBM are investigated firstly through device simulation to compare the performance of a BHJ to a bilayer device with the same thickness. Subsequently, solar cell devices with BHJ structures

are fabricated by spin-coating method with different spin-speed in order to obtain devices with different thicknesses.

II. METHODOLOGY

A. Simulation of P3HT:PCBM Solar Cell

GPVDM (General Purpose Photovoltaic Device Modelling), now known as OghmaNano, is a tool used to study the characteristic of P3HT:PCBM solar cell. The model describes trapped carriers using a non-equilibrium Shockley-Read-Hall formalism, thus enable the device based on disorder materials. In the first simulation, the active layer of a P3HT:PCBM bulk heterojunction (BHJ) solar cell of ITO/P3HT:PCBM/Al is varied from 50 nm - 400 nm. Subsequently, bilayer structure (1:1) ITO/P3HT/PCBM/Al with the optimized thickness is modelled and compared to the BHJ structure.

B. Fabrication & Characterization of P3HT:PCBM BHJ Solar Cell

Patterned ITO (20 Ω/□) coated glasses are ultrasonic cleaned with acetone, isopropyl alcohol and deionise water for 10 minutes each and then subjected to UV-ozone treatment for 10 minutes prior to coating of the active layer by spin-coating. Subsequently, a P3HT:PCBM mixture with a ratio of 1:1 was dissolved in chloroform at a concentration of 10 mg/ml. The resulting solution was then spin-coated onto the patterned ITO-coated glass substrates, which were subsequently annealed at 120 °C for 10 minutes. Four samples with various spin speeds (1000, 1500, 2000, and 2500 rpm) were prepared for the P3HT:PCBM layer. Following the preparation of the active layer, an aluminum (Al) layer with the thickness of 100 nm is thermal evaporated using a thermal evaporator (Edwards Auto 306) at a base pressure of 3×10^{-4} Pa, serving as the cathode electrode for the device.

A UV-visible spectrometer is used to measure absorbance (Avantes AvaSpec-2048L). The morphology and thickness of the films are studied using an atomic force microscope (AFM) (Nanosurf). To assess the solar device performance, a solar simulator from Newport Oriel® Sol2ATM Class ABA is employed in a dark room, with illumination provided by AM 1.5 G (100 mW/cm2), and a Keithley 2400 SMU is used to determine I-V characteristics of the solar devices.

III. RESULTS AND DISCUSSIONS

A. Simulation of P3HT:PCBM Solar Cell

1. The Effect of Active Layer Thickness in BHJ Solar Cell

The thickness of the P3HT:PCBM (1:1) layer in BHJ solar cell is varied and the IV characteristics are shown in Fig. 1. The resultant device efficiency is shown in Fig. 2. The maximum efficiency of 4.66 % is obtained with an active layer thickness of 200 nm. The power conversion efficiency decreases as the active

layer thickness increases because of an increase in series resistance [8]. This effect becomes more pronounced beyond a thickness of 200 nm. It is widely known that a higher series resistance results in a lower fill factor, which lowers the efficiency. As a result, the series resistance is crucial for solar cells [9]. When the film is very thin, the incident light is not fully absorbed by the active film. On the contrary, if the active layer was too thick, the electrical properties will be affected. This is due to the lower open circuit voltage, so the thicker active layer does not guarantee higher efficiency [10]. A higher BHJ layer thickness can increase the short circuit current, but beyond a specific thickness, short circuit current will start to decrease [11]. The optimum thickness is about 100 - 250 nm.
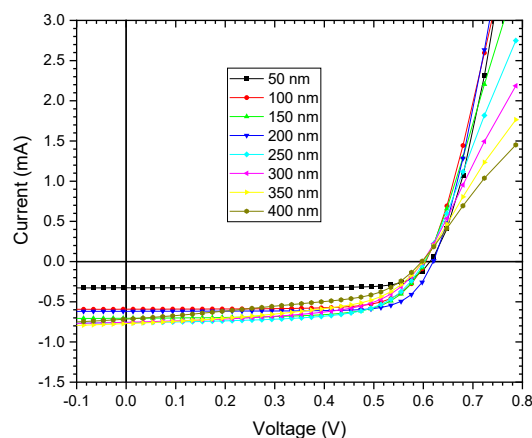

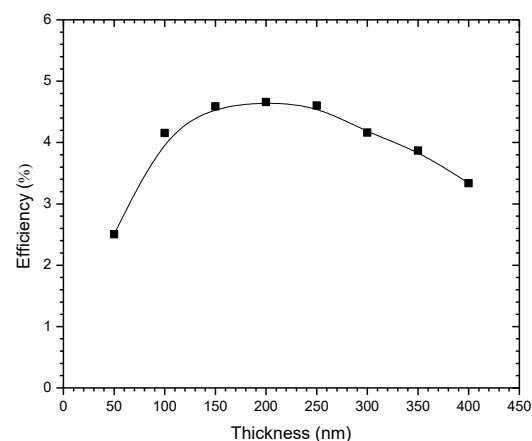Fig. 1. IV-characteristic of BHJ with different layer thickness.

Fig. 2. Efficiency of P3HT:PCBM BHJ solar cell with different thickness.

2. Comparison of BHJ and Bilayer Solar Cell

The performance of a bilayer solar cell is compared to a BHJ solar cell with an active layer of 200 nm. The ratio of the bilayer P3HT:PCBM remained 1:1 and each layer is 100 nm. In BHJ structure, the donor and acceptor are ordered into several domains through which holes and electrons can easily travel while the P3HT and PCBM layers formed a finite interface. The

simulated results are shown in Fig. 3. The bilayer solar cell exhibits an efficiency of only 3.29 % as compared to a BHJ solar cell (4.66 %) in Table I.

Table I: The performance of a BHJ solar cell as compared to a bilayer solar cell.

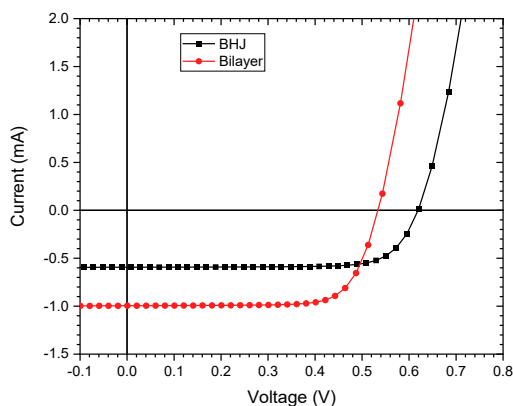| Model	V_{OC} (V)	J_{SC} (mA/cm^2)	Fill factor (%)	η (%)	Max Power (W/m^2)
BHJ	0.6191	0.09896	76.06	4.6606	46.6065
Bilayer	0.5385	0.08294	73.77	3.2950	32.9504

Fig. 3. The IV characteristics of a BHJ and a bilayer structure.

The best fill-factors are obtained when the transmitting times of electrons and holes are balanced between the two layers. This also demonstrates that electron conduction and extraction through fullerene limit the performance of bilayer and BHJ devices relying on the P3HT/PCBM material mixture. However, polymer-fullerene bilayers have a few advantages over BHJ devices, including reduced carrier recombination and thus improved control over the individual interface characteristics during OPV fabrication [5].

Contrasted with a simpler planar heterojunction, the BHJ structure gives a worthier total surface region for charge separation and reduced recombination, and these favourable circumstances ought to hypothetically mean significantly improved power conversion efficiency. Excitons must be created within their exciton diffusion lengths to the closest donor-acceptor interface for effective charge generation [4]. Recent research indicates that dispersion length for a few model conjugated polymers used in bulk heterojunction solar cells is in the range of 10 nm, implying that a nanometre-scale intermixing of the donor and acceptor moieties is required [2].

B. Fabrication and Characterization of P3HT:PCBM Solar Cell

1. Absorbance of P3HT:PCBM Layer

Figure 4 depicts the absorbance of a single mixed layer of P3HT:PCBM with a ratio of 1:1 at four different spin speeds. Three primary peaks are detected where the peaks at 300 and 335 nm are originated from PCBM and the third peak at 504 nm is due to P3HT. The intensity of the peak reduces with higher spin speed because of thinner films. The thicknesses of the layer are 121 nm, 96 nm, 82 nm and 78 nm respectively, measured by using AFM.
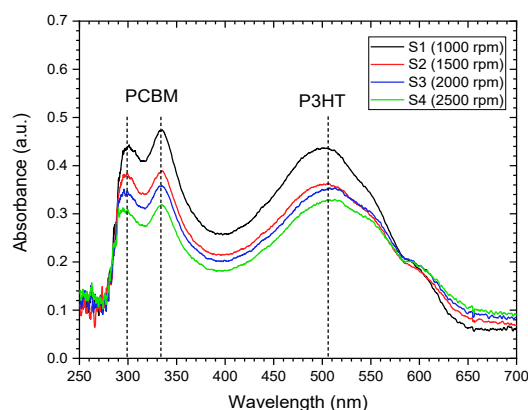

Fig. 4. Absorbance of P3HT:PCBM layer with different spin-speed and thickness S1(1000 rpm, 121 nm), S2 (1500 rpm, 96 nm), S3 (2000 rpm, 82 nm), S4 (2500 rpm, 78 nm).

2. Device Performance

Devices of ITO/P3HT:PCBM/Al with the 4 different thickness are tested using by using a solar simulator in Fig. 5. The performance is shown in Table II. S1 has the efficiency of 0.5495 %, followed by S2 (0.6101 %), S3 (0.8671 %) and S4 (0.910 %). The I-V characteristics are shown in Fig. 5. The open circuit voltages, V_{oc}, of all the devices are in the same range, while the short circuit current, I_{sc} is higher for S3 and S4 which are actually thinner. The low I_{sc} in S1 and S2 indicate a lower recombination, or lower electron and hole diffusion length. The fill factor also increases for S3 and S4.

The results suggest that experimental physical parameters to influence the performance of the solar cell significantly. For a simple single layer device, the property of the active layer is then crucial. The thicknesses of S3 and S4 obtained are closed to the optimum thickness reported (85 nm) where the contact resistance and bulk resistance are optimum [9]. Another possible contributing factor to a better efficiency of the thinner S3 and S4 despite higher absorbance could be due to the surface morphology of the active layer. Figure 6 shows the surface morphology of the S1 (121 nm) and S3 (82 nm). Sample S3 has higher roughness than S1.

The efficiency of P3HT:PCBM solar cell was influenced by the morphology and the interface which in turn depends strongly on the preparation method [12]. In the report, the change in morphology was caused by the degree of annealing. In the current work, all the samples are annealed at the same condition; but during the spin-coating process, the speed influences the thickness of the resulting film through centrifugal force, while the extent of spin dewetting determines the ultimate morphology of the film [13]. The results also show that rougher surface provided a larger contact area at the interface for carrier collection.

Table II: The characteristic of a ITO/P3HT:PCBM/Al solar cell with different spin speed and thicknesses.

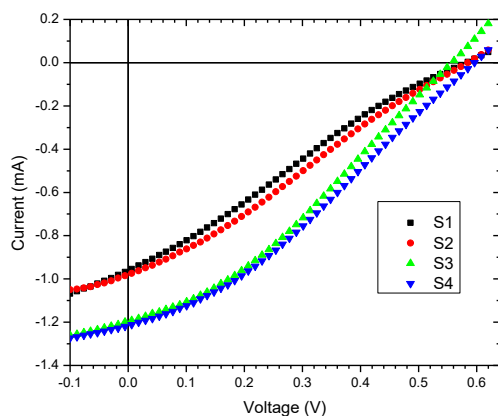| Sample	Thickness (nm)	V_{OC} (V)	I_{SC} (mA)	Fill factor (%)	H (%)	P (mW)
S1	121	0.5810	0.960	24.63	0.5495	0.274
S2	96	0.5839	0.978	26.71	0.6101	0.298
S3	82	0.5566	1.193	32.64	0.8671	0.395
S4	78	0.5960	1.211	31.51	0.910	0.420

Fig. 5. The I-V curve for different spin speed on a single layer device.

(a)

(b)
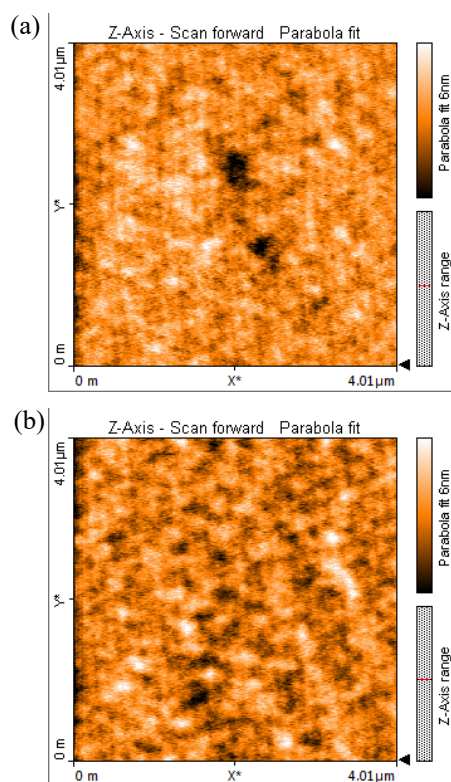
Fig. 6. AFM images of (a) S1 (R_{rms} = 0.88 nm) and (b) S3 (R_{rms} = 0.97 nm).

IV. CONCLUSION

The results of device simulation of P3HT:PCBM organic solar cell show that the optimum thickness for a BHJ solar cell to be at 200 nm. The efficiency for a 200 nm BHJ solar cell is also higher than that of a bilayer cell with the same thickness.

P3HT:PCBM solar cells with different thicknesses are fabricated by spin-coating. Although the absorbance of the thinner devices (78 nm - 82 nm) are lower, they exhibit higher I_{sc} and fill factor, and thus higher efficiency. The results suggest that properties of the active layer, in terms of contact and bulk resistance, and morphology play important roles in the carrier transport upon light absorption.

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