

Adjusting optical resonance thickness to increase the conversion efficiency of polymer solar cells

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ABSTRACT

The derivatives of C₆₀, [6,6]-phenyl C61-butyric acid methyl ester (PCBM), and 3-hexylthiophene (P3HT) were dissolved in DCB solvent, then spin coated into an active layer for polymer solar cells. The experimental parameters were studied carefully to obtain the optimum power conversion efficiency (PCE). The primary process for generation of photocurrent in an organic photovoltaic device is the generation of bound electron–hole pairs (excitons) by absorption of energy (photons) from the optical electric field. Modeling was based on the assumption that the photocurrent generation process is the result of the creation and diffusion of photogenerated species (excitons), which are dissociated by charge transfer at the active layer. Improve organic optics absorb by insert organic layer (CuPc or C₆₀) at the active layer/Al interface. This research is divided into two components. First part, we use n-type C₆₀ as transmission layer. When an optimum thickness of C₆₀ is 5 nm, the J_{sc} of polymer solar cell can be increased from 7.26 mA/cm² to 7.7 mA/cm². The V_{oc} decrease is because the energy level of C₆₀ LUMO (lowest unoccupied molecular orbital) at 4.5 eV is higher than the 3.7 eV of PCBM. Second part, we use p-type CuPc as transmission layer. When an optimum thickness of CuPc is 3 nm, the short circuit photo-current density (J_{sc}) and open circuit voltage (V_{oc}) of polymer solar cell can be increased from 7.26 mA/cm² to 8.0 mA/cm² and 0.56–0.58 V, respectively. The reason is the same as C₆₀. The V_{oc} increase is because the energy level of CuPc LUMO (lowest unoccupied molecular orbital) at 3.1 eV is lower than the 3.7 eV of PCBM. The J_{sc} increase is because the 3 nm of CuPc leads to a constructive interference happened in the active layer and thus optical absorption increases. In this study we used 3 nm of CuPc at the active layer/Al interface to enhance the short circuit current density, and the efficiency was increased to 2.94%.

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1. Introduction

Poly(3-hexylthiophene) (P3HT) has an excellent nature of film formation and possesses good semiconductor properties. For example its containing a higher carrier mobility rate and therefore can be applied on the production of optoelectronic devices for flexible plastic substrates. In 1995 Heeger et al. used a mixture of MEH-PPV and PCBM to form a single-layer heterogeneous structure, in which PCE reached 1.5% [1]. In 2001 Sariciftci et al. used a mixture of MDMO-PPV and PCBM, and also LiF/Al as the cathode to improve the efficiency to 2.1% [2]. In 2005 Yang et al. took use of the self-organization effect and with slow growth treatment to reduce the resistance of devices connected in series resistance, which enhanced the carrier mobility rate and increased the efficiency to

4.37% [3]. In the same year Heeger et al. produced devices which PCE reached 5% [4]. It was done mainly by the use of P3HT/PCBM [poly(3-hexylthiophene)/[6,6]-phenyl C61-butyric acid methyl ester] to create *P–N* junction structures for solar cell devices [5,6]. In 2008, Chunfu Zhang et al. inserted the donor material, CuPc, between the active layer and anode. They demonstrated a simple tandem structure of organic photovoltaic cells for efficient light harvesting [7]. Because organic solar cells have the advantages of low cost, lightweight, deflectable, and can easily produce for large areas [8–10], they are in worth for further research. In this study, we reports effects of organic solar cells with difference organic material (C₆₀ or CuPc) and optical resonance thickness.

2. Experimental

The sheet resistance and thickness of the ITO glass substrate were 5 Ω/□ and 280 nm respectively. Photo-lithography was used

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to define the anode plot. The glass substrate was then placed within an ultrasound washer, in sequence using acetone, methyl alcohol and deionized water (DI water) each for 8 min. The glass substrate was then blown dry by nitrogen and placed in an oven for 30 min. The substrate was then placed within a oxygen plasma washing machine. The surface of the ITO glass was cleaned in an oxygen plasma environment of oxygen flow rate 10 sccm, RF power 30 W. The substrate was then removed and spin coated a layer of PEDOT:PSS to repair the ITO surface to assist the holes transfer to the electrode. The substrate was then removed and placed in a N_2 glove box. The active layer material (P3HT:PCBM = 1:1, 1.7 wt%) was then dissolved in *o*-dichlorobenzene (DCB) and placed on a hot-plate at temperature 40 °C, rotation speed 150 rpm for 24 h. The P3HT:PCBM solution was then spin coated on the PEDOT:PSS layer. After the coating of the organic layer, the device was placed within a Petri dish of diameter 12.9 cm and height 4.5 cm. A vapor chamber was formed by placing the device and solution on a hot-plate, and covered with a Petri dish. Total growth time was 40 min. By slow growth treatment the active layer had a self-organization effect. Because the device was placed within a saturated vapor environment, thus no film formation will occur on the active layer and still in a solution state. By the self-organization effect P3HT and PCBM will self-organized. Sample placed on a hot-plate before annealing prior to organic layer evaporation, and placed within an organic evaporation to apply evaporated C_{60} or CuPc, to increase the short circuit photo-current density of the polymer solar cells. By vaporization for metal deposition LiF/Al was used as the cathode. The device area size is 0.04 cm². After the completion of device production, AM 1.5G 100 mW/cm² was used as sunlight simulation. A KEITHLEY 2400 was used for measuring the current–voltage characteristics of the polymer solar cells. The IPCE spectra were recorded by illuminating the sample with 100 W halogen lamp by PV measurement corporation (USA).

3. Results and discussion

3.1. Comparison of different optical resonance thickness of C_{60}

The inserting of the accepting material, C_{60} , between the active layer and cathode was to mainly change the C_{60} thickness, allowing the optical resonance region lie between the active layer and the thin film, allowing the short circuit photo-current density and efficiency increase. Table 1 and Fig. 1 are the characteristic curves and J – V curve plots for a device vaporization-coated with C_{60} thicknesses of 0 nm, 2 nm, 5 nm and 10 nm, respectively. When the C_{60} thickness increased to 2 nm, the short circuit photo-current density of the device increased from 7.26 to 7.53 mA/cm². From the literatures [11–13], it is known that the incident light optical resonance region would move between the active layer and thin film thickness. When C_{60} thickness increased to 5 nm, the incident light optical resonance region would create the maximum short circuit photo-current density for the device of 7.70 mA/cm² between the thin film thickness of the active layer. As C_{60} thickness increased to 10 nm, the optical resonance region would deviate from the active layer thin film, and caused the short circuit

Table 1

Device characteristics with different thicknesses of C_{60} .

C_{60} thickness (nm)	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	PCE (%)
0	0.56	7.26	63.71	2.59
2	0.55	7.53	62.30	2.58
5	0.54	7.70	60.61	2.52
10	0.53	7.53	58.88	2.35

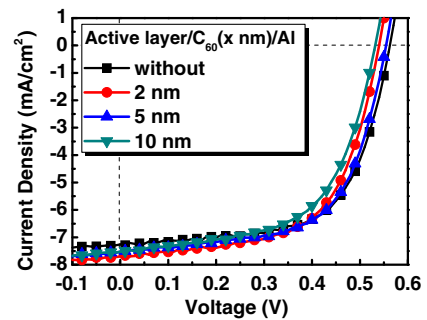


Fig. 1. J – V curve plots with different thicknesses of C_{60} .

photo-current density of the device reduce to 7.53 mA/cm². In addition, the open circuit voltage was found to decrease as the C_{60} thickness increased. The reason was because the open circuit voltage of the device was determined by the energy gap of $HOMO_{Doner}$ – $LUMO_{Accept}$ [14]. From the energy gap plot for solar cells in Fig. 2, it could be seen that the energy gap for $HOMO_{Doner}$ – $LUMO_{Accept}$ before any vaporization-coating of C_{60} was 1 eV; once C_{60} was introduced, since the LUMO of C_{60} is higher than its PCBM, the energy gap of $HOMO_{Doner}$ – $LUMO_{Accept}$ decreased to 0.8 eV, and thus the energy gap for $HOMO_{Doner}$ – $LUMO_{Accept}$ reduced 0.2 eV, and causing the open circuit voltage of the device to drop. The curve fill-factor also decreased as the C_{60} thickness increased. There were two main reasons for this phenomenon: first, the total thickness of the device increased, which caused the series resistance to increase and thus the curve fill-factor to slightly decrease. The second reason was that the created excitons as the polymer solar cell receives sunlight from distributed from the active layer in all directions. When the excitons distributed to the donor–acceptor interface, the existing inside electric field would cause the excitons separate into electrons and electron holes. Valid currents are generated by collecting with electrodes. However, as the excitons move to the interface of the active layer and C_{60} , since the LUMO of C_{60} when compared with the active layer is higher, it would cause the excitons move to the C_{60} layer, and resulting with the loss of the excitons. This causes current leakage of the solar cell, and reduced the curve fill-factor of the device. When the vaporization-coating of C_{60} was 2 nm, the device obtained the optimal characteristics: the open circuit voltage was 0.55 V, the short circuit photo-current density was, 7.53 mA/cm², the curve fill-factor was 62.30%, and the efficiency was 2.58%.

3.2. Comparison of different optical resonance thickness of CuPc

Since C_{60} material would cause the open circuit voltage and curve fill-factor of the device to decrease, and causing the device's

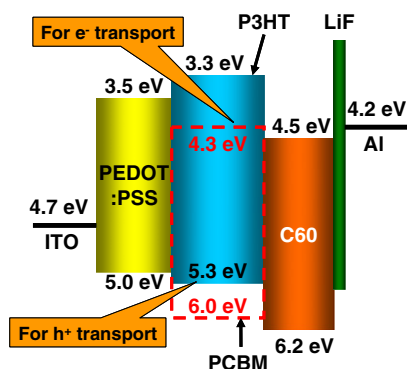


Fig. 2. Energy gap between the active layer and cathode with the coating of C_{60} .

efficiency unable to rise, therefore CuPc was used to replacing the coating between the active layer and cathode. As the LUMO of CuPc is higher than C₆₀, the current leakage of the device was reduced and the open circuit voltage increased, which increased the efficiency of the polymer solar cell. Table 2 and Fig. 3 are the characteristic curves and *J*–*V* curve plots for a device vaporization-coated with CuPc thicknesses of 1 nm, 3 nm and 6 nm respectively. When the CuPc thickness was 1 nm, the incident light optical resonant maximum was adjusted and shifted into the active layer. But due to the LUMO of CuPc is lower than that of PCBM as shown in Fig. 4, the electrons need to jump over a barrier in order to be transported to the cathode. Therefore, the short circuit current density of the device with 1 nm CuPc decreased to 6.49 mA/cm². When the CuPc thickness increased to 3 nm, the incident light resonant maximum was just located in the central region of active layer which resulted in a maximum short circuit current density of 8.00 mA/cm². When the CuPc thickness increased to thicker than 3 nm, the photo-induced electrons were more difficult to be transported to the cathode and the incident light optical resonant maximum may deviate from the center region in the active layer. Therefore the device with 5 nm CuPc has lower short circuit current density than that with 3 nm CuPc. In addition, with the increasing of the vaporized CuPc thickness, the open circuit voltage of the device was determined by the gap energy of HOMO_{Donor}–LUMO_{Accept}. From the energy gap plot for solar cells in Fig. 3, it could be seen that the original energy gap for HOMO_{Donor}–LUMO_{Accept} before any vaporization-coating of CuPc was 1 eV; once CuPc was introduced, since the LUMO of CuPc is lower than its PCBM, the energy gap for HOMO_{Donor}–LUMO_{Accept} increased to 1.8 eV, and thus the open circuit voltage of the device increased (see Fig. 4). The curve fill-factor also slightly decreased as the CuPc thickness increased. The main reason was the total thickness of the device caused the series resistance to increase and thus the curve fill-factor to slightly decrease. Fig. 5 displays the IPCE results of photovoltaic cells fabricated with difference organic material. The IPCE maximum of 42.7% at 510 nm was observed for ITO/PEDOT:PSS/active layer/LiF/Al. The IPCE of photovoltaic cells was observed to be 48.1% at the same wavelength for ITO/PEDOT:PSS/active layer/C₆₀/LiF/Al, due to the excitons move to the C₆₀ layer, and resulting with the loss of the excitons. The IPCE of polymer solar cells was increased to 47.3%

Table 2
Device characteristics with different thicknesses of CuPc.

CuPc thickness (nm)	V _{oc} (V)	J _{sc} (mA/cm ²)	FF (%)	PCE (%)
0	0.56	7.26	63.71	2.59
1	0.57	6.49	63.53	2.35
3	0.58	8.00	63.36	2.94
6	0.58	7.22	62.80	2.63

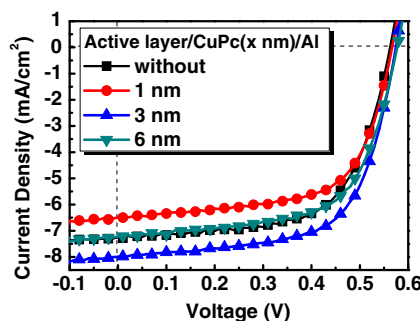


Fig. 3. *J*–*V* curve plots with different thicknesses of CuPc.

Table 3
The comparisons of J_{sc} from I–*V* curves with those from IPCE measurements.

	J _{sc} of I– <i>V</i> (mA/cm ²)	J _{sc} of IPCE (mA/cm ²)
Without	7.26	5.40
C ₆₀ -2nm	7.53	6.08
CuPc-3nm	8.00	6.16

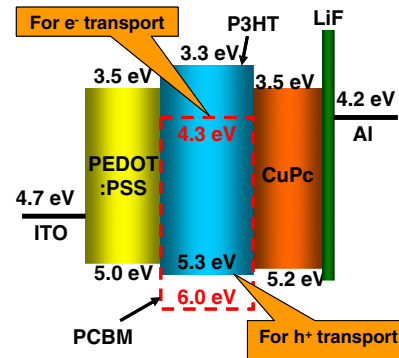


Fig. 4. Energy gap between the active layer and cathode with the coating of CuPc.

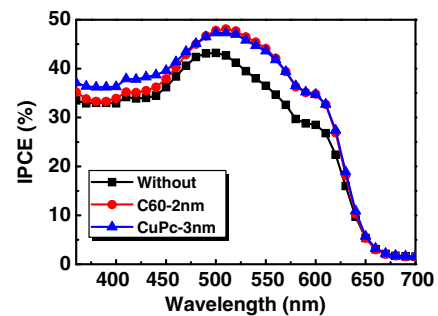


Fig. 5. Incident photon-to-current conversion efficiency (IPCE) curves for the optical resonance material photovoltaic cells fabricated.

at the same wavelength for ITO/PEDOT:PSS/Active layer/CuPc/LiF/Al, due to two reason: (1) increase in the Incident photon-to-current conversion efficiency as a result of the optical resonance present in the active layer, (2) the excitons inability to move to the CuPc layer, resulting in no loss of excitons. Table 3 shows the comparisons of J_{sc} from I–*V* curves with those from IPCE measurements.

When the vaporization-coating of CuPc was 3 nm, the device obtained the optimal characteristics: the open circuit voltage was 0.58 V, the short circuit current density of 8.00 mA/cm², the curve fill-factor of 63.36%, and conversion efficiency of 2.94%.

4. Conclusion

In the study, the inserting of an optical resonance thin film between the active layer and cathode could increase the short circuit photo-current density and efficiency of the device. In addition, the LUMO of the optical resonance thin film may not have a large difference with the difference between PCBM and LUMO; as an over-high LUMO would cause the open circuit voltage and curve fill-factor to decrease, and an over-low LUMO would require the created electrons of the polymer solar cell device to jump over a

barrier to reach the cathode. When an optimum thickness of CuPc is 3 nm was chose, the short current (J_{sc}), open voltage (V_{oc}) and power conversion efficiency (PCE) of a polymer solar cell can be increased from 7.26 mA/cm² to 8.00 mA/cm², and 0.56–0.58 V, and 2.58–2.94%, respectively.

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