Effect of Interface Thickness on Power Conversion Efficiency of Polymer Photovoltaic Cells

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We investigated the effect of the thicknesses of the interface layers (here, PEDOT:PSS and LiF) of polymer photovoltaic cells because variations in thickness strongly affect the power conversion efficiency (PCE). It was observed that the PCE rapidly increased with a PEDOT:PSS thickness of up to ~2,000 rpm and rapidly decreased when the PEDOT:PSS was thicker than ~2,000 rpm. A PCE of 6.648% was obtained at a specific PEDOT:PSS layer thickness of ~2,000 rpm, about 41.5% (from 4.698 to 6.648%) higher than the PCE with no PEDOT:PSS layer. In addition, the PCE slightly increased with an LiF layer thickness of up to ~0.5 nm and rapidly decreased when the LiF layer was thicker than ~0.5 nm. The maximum PCE was obtained at the LiF layer thickness of ~0.5 nm. In particular, the maximum values of PCE, J_{sc}, V_{oc}, and FF were obtained at 6.827%, 15.74 mA/cm^2, 0.665 V, and 0.652, respectively. The PCE increased 209.2% (from 2.028 to 6.827%), compared to the LiF layer thickness of ~5 nm.

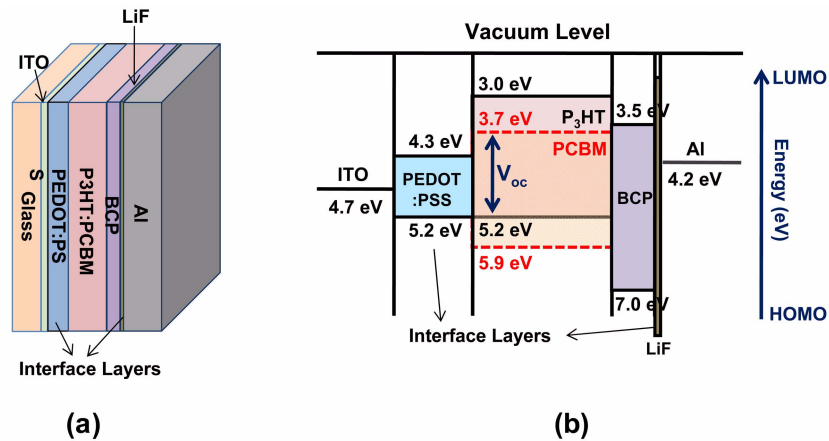**Keywords:** polymer photovoltaic cell, interface layer, PEDOT:PSS, LiF, power conversion efficiency

1. INTRODUCTION

Photovoltaic (PV) cells on organic materials (small-molecule and polymer materials) are strong candidates because of several important properties they have: large area, excellent mechanical flexibility, low production costs, and simple fabrication processes.[1-3] Therefore, many researchers have been trying to improve the power conversion efficiency (PCE) of organic photovoltaic (OPV) cells.[4-13] The PCE of an OPV cell can be determined by the following factors: the light absorption of the electron-donating material, the light absorption of the electron-acceptor material, transport of light-generated excitons from both layers to the donor-acceptor interface, efficiency of the hole/exciton breaking up into electron-hole pairs at the interface, transport of holes across the donating layer to the anodic electrode, transport of electrons across the acceptor layer to the cathodic electrode, quality of the contact between the donor layer and the anodic electrode, and quality of the contact between the acceptor layer and the cathodic electrode. Therefore, many researchers have tried to improve the PCE of OPV cells by modifying the donor, acceptor, blocking material, and PV cell structures.[11-18] However, the effects of the interface layer have not been sufficiently studied. Therefore, we studied the effect of the interface layer (here, PEDOT:PSS and LiF) to improve the PCE of the OPV cell.

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2. EXPERIMENTAL PROCEDURE

Poly(3-hexylthiophene-2,5-diyl) (P3HT) and [6,6]-phenyl-C$_{61}$ butyric acid methyl ester (PCBM) were dissolved in chlorobenzene at a weight ratio of 2:1 and stirred on a hot plate at 50°C for more than 72 h in a glovebox before spin casting to form the blend layer. P3HT was selected as the electron-donating material and PCBM was used as the electron acceptor. To fabricate the PV cells, the ITO glass substrate was treated continuously with a 354-nm UV lamp for 60 s and then placed under a 200-W oxygen plasma flow for 30 s. An interface and hole injection layer of poly (3,4-ethylenedioxylenethiophene): polystyrene sulfonic acid (PEDOT:PSS, Baytron PVPAI 4083) was spin-coated (without PEDOT:PSS, 1000, 2000, and 3000 rpm) onto the ITO glass for 60 s after being filtered with a 5-μm pore PTFE syringe filter (Whatman) and then baked at 140°C for 10 min in a glovebox. The P3HT:PCBM blended solution was filtered using a 5-μm pore PTFE syringe filter. The P3HT:PCBM blended layer was then spin-cast at ~1,000 rpm for 60 s on the PEDOT:PSS layer and then baked at 150 for 10 min in a glovebox. A 2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline (BCP) layer was continuously deposited by thermal evaporation as a hole/exciton blocking layer on the P3HT:PCBM blended layer under a pressure of ~5 × 10^{-7} Torr and evaporated until it was ~12 nm thick. Finally, an Al electrode ~80 nm thick was deposited by thermal evaporation at a pressure of ~5 × 10^{-7} Torr. The evaporation rates of the BCP layer and

Fig. 1. Photovoltaic cell with P3HT:PCBM blended layer, BCP layer, and interface (PEDOT:PSS and LiF) layers: (a) cross-sectional structure schematic and (b) schematic energy band diagram.

the Al electrode were ~0.5 Å/s and ~5 Å/s, respectively. Figure 1 shows a schematic of the cross section and an energy band diagram of the OPV cell. All electrical measurements were performed under nitrogen (N_2) gas in a glovebox at room temperature. The photocurrent-density vs. voltage (J–V) was analyzed using an HP 4155C source-measure unit (SMU). The photocurrent was measured under AM 1.5 G solar illumination at 100 mW/cm^2 (1 sun) supplied using a Newport 150-W solar simulator. The light intensity was monitored with a silicon photodiode calibrated for the AM 1.5 G spectrum.

3. RESULTS AND DISCUSSION

To investigate the PCE dependence on the thickness of the PEDOT:PSS layer, OPV devices were fabricated with a sandwiched structure of varying PEDOT:PSS layer thicknesses and fixed P3HT:PCBM blended layer thickness (~1,000 rpm) and BCP layer (~12.0 nm) thickness between the anode (ITO) and reflective top electrode (Al).

Figure 2 shows the characteristics of the OPV device as a function of the thickness of the PEDOT:PSS layer. Figure 2(a) shows the photocurrent density vs. voltage (J-V) curves for OPV devices with varying PEDOT:PSS layer thicknesses. The short-circuit current (J_{sc}) varied with the thickness of the PEDOT:PSS layer while open-circuit voltage (V_{oc}) did not. The dependency of V_{oc} and J_{sc} on the thickness of the PEDOT:PSS layer is shown in detail in Figs. 2(b) and (c). The variation of V_{oc} was about 1.56% (from 0.635 V to 0.645 V), as shown in Fig. 2(c). V_{oc} is determined by the energy gap between the donor (P3HT) material's highest occupied molecular orbital (HOMO) level and the acceptor (PCBM) material's lowest unoccupied molecular orbital (LUMO) level (see Fig. 1(b)). The energy level between the donor (P3HT) material's HOMO level and the acceptor (PCBM) material's LUMO level was fixed. For this reason,
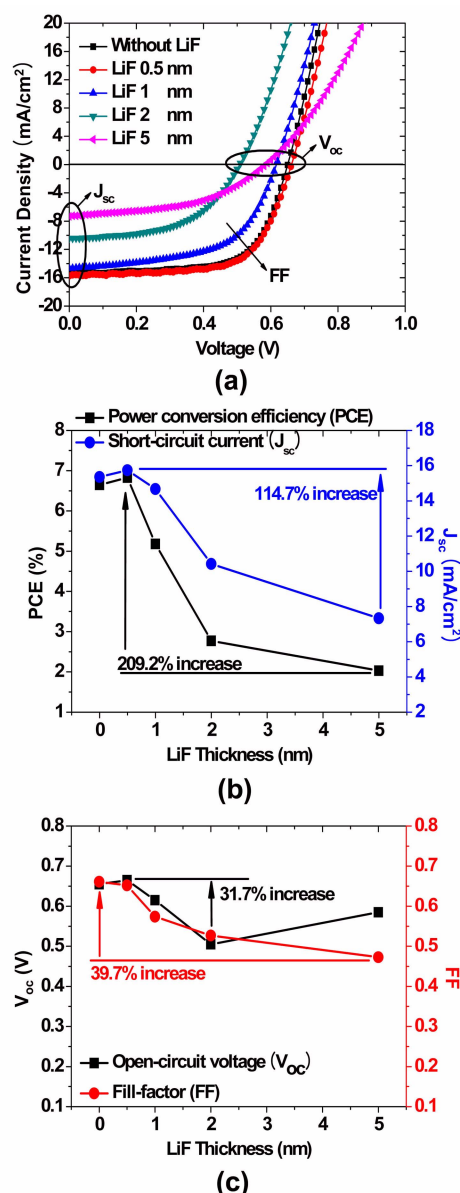
the variation in V_{oc} was uniform. However, J_{sc} sharply increased with the PEDOT:PSS layer thickness up to ~2,000 rpm and then suddenly decreased with further increase in the PEDOT:PSS layer thickness, as shown in Fig. 2(b). The PCE dramatically increased with the thickness of the PEDOT:PSS layer up to ~2,000 rpm and then suddenly decreased as the thickness of the PEDOT:PSS layer continued to increase. Figures 2(b) and (c) show that PCE had a tendency similar to that of J_{sc} rather than that of V_{oc} with varying of the PEDOT:PSS layer thickness. Since J_{sc} dominantly affected the PCE in changing the thickness of the PEDOT:PSS layer, the maximum PCE (6.648%) at a specific PEDOT:PSS layer thickness (~2,000 rpm) could be obtained, improving the PCE by about 41.5%, (Fig. 2(b)). This trend is likely associated with interface characteristics and carrier injection, depending on the thickness of the PEDOT:PSS layer. Therefore, if there is no PEDOT:PSS layer or if that layer is too thin, polymer photovoltaic cells would perform poorly because the interface characteristics between the ITO and the P3HT:PCBM blended layer are poor. In addition, if the PEDOT:PSS layer is too thick, i.e., less than 1,000 rpm, the interface characteristics would be fairly good, but PCE would be reduced because the high resistance of PEDOT:PSS layer makes carrier injection difficult. Therefore, It should be noted that obtaining maximum PCE requires optimal thickness of the PEDOT:PSS layer.

By fabrication of OPV devices with a sandwiched structure with fixed PEDOT:PSS layer thickness (~2,000 rpm), a P3HT:PCBM blended layer (~1,000 rpm), a BCP layer (~12.0 nm), and varying thicknesses of LiF layers (0, 0.5, 1, 2, 5 nm) between the anode (ITO) and reflective top electrode (Al), we investigated the PCE dependence on the thickness of the LiF layer. J_{sc} was varied with the thickness of the LiF layer while V_{oc} did not change significantly. The dependence of V_{oc} and J_{sc} on the thickness of the LiF layer is shown in Figs. 3(b) and (c). The variation of V_{oc} was about
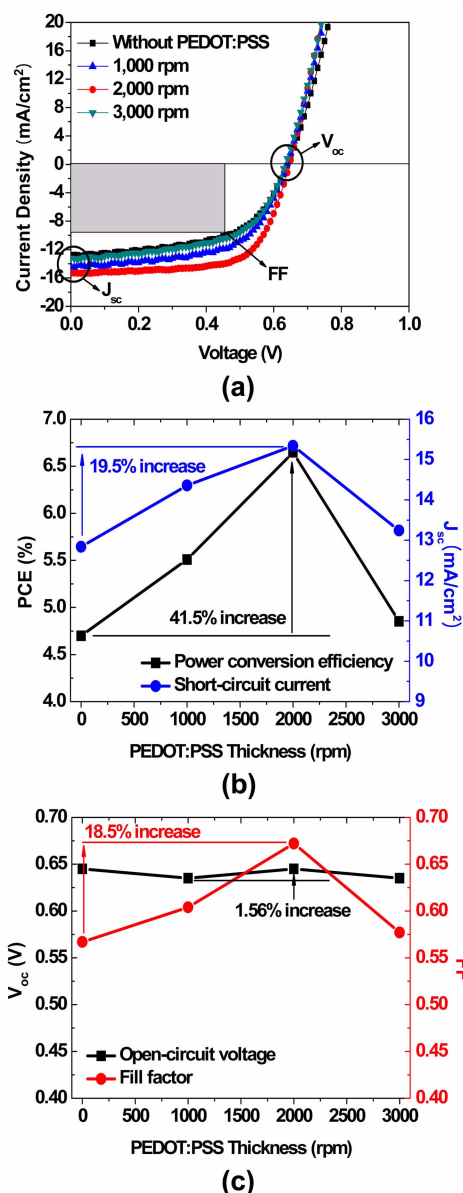
Fig. 2. Dependence of polymer photovoltaic cell performance on interface layer thickness (here, PEDOT:PSS layer): (a) The photocurrent-density vs. voltage (J-V), (b) variation of J_{sc} and PCE, and c) variation of V_{oc} and FF.

Fig. 3. Dependence of polymer photovoltaic cell performance on interface layer thickness (LiF): (a) photocurrent-density vs. voltage (J-V), (b) variation of J_{sc} and PCE, and c) variation of V_{oc} and FF.

37.6% (from 0.505 to 0.665 V), as shown in Fig. 3(c). This indicates that V_{oc} is almost independent of the thickness of the LiF layer, the same quality as that found in the donor (P3HT) and acceptor (PCBM) materials. However, J_{sc} slightly increased with an LiF layer thickness of up to ~0.5 nm and then abruptly decreased as the thickness of the LiF layer increased. In addition, J_{sc} was varied about 114.7% (from 7.33 to 15.74 mA/cm^2) with the change in the thickness of the LiF layer, as shown in Fig. 3(b). As a result, the maximum PCE (6.687%) at a specific LiF layer thickness (~0.5 nm) could be obtained, improving the PCE by about

209.2%, (Fig. 3(b)). This trend is likely associated with the dependence of the interface characteristics and carrier injection on the thickness of the LiF layer. Therefore, polymer photovoltaic cells without LiF perform poorly because the interface characteristics between the BCP layer and the Al electrode are poor. In addition, if the LiF layer is too thick, i.e., more than 1 nm, the interface characteristics would be fairly good, but PCE would be reduced because the high resistance of the LiF layer makes carrier injection difficult. Therefore, obtaining maximal PCE requires an optimal LiF layer thickness. By optimizing the thickness of the interface layers (PEDOT:PSS and LiF), a maximum PCE of 6.827 %

was obtained in our experiment, indicating that the PCE of organic photovoltaic (OPV) devices strongly depends on the thickness of the interface layers.

4. CONCLUSIONS

The dependence of PCE of OPV devices on the thickness of the interface layers (PEDOT:PSS and LiF) was investigated. The PCE peaked at a PEDOT:PSS layer thickness of ~2,000 rpm, improving PCE by about 41.5%. In addition, the PCE peaked at an LiF layer thickness of ~0.5 nm, improving PCE by about 209.2%. The effect of the thickness of the interface layers on PCE was determined by the change in J_{sc} rather than in V_{oc} (Figs. 2 and 3). An optimally thick PEDOT:PSS layer (here, ~2,000 rpm) was a good interface between the ITO and the P3HT:PCBM blended layer, and a ~0.5-nm-thick LiF layer was a good interface between the BCP and the Al electrode layers. This suggests optimal interface layer thickness can improve the performance of PV cells. To conclude, we observed PCE values of 6.827% in OPV cells with a structure of transparent bottom electrode (ITO), an interface layer (PEDOT:PSS, ~2,000 rpm), a polymer donor (P3HT) layer blended with a small molecule acceptor (PCBM), a small-molecule blocking layer (BCP, ~12.0 nm), an interface layer (LiF, ~0.5 nm), and a reflective top electrode (Al, ~80 nm).

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