Enhancing the Fill Factor in Polymer Photovoltaic Cell by Using a Hole Transporting Layer

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1. Introduction

Control of charge carrier transport at heterointerfaces in multilayer structures is one of the most important issues in the improvement of organic photovoltaic cells (OPVs). Up to now, the most frequently used buffer layer in organic poly(3,4-ethylene solar cells is dioxythiophene):poly(styrene sulfonate) (PEDOT:PSS). Due to its high transparency, high work function, smooth morphological properties and good conductivity, the hole collection of the indium tin oxide (ITO) anode can be facilitated via the PEDOT:PSS layer from the highest occupied molecular orbital (HOMO) of a photoactive film [1,2]. However, the interface between ITO and PEDOT:PSS is not stable and the chemical reaction between ITO and PE-DOT:PSS can result in degraded device performance [3–5].

In this work, we demonstrate that a thin film of transition metal oxides of vanadium oxide (V_2O_5) and organic material of copper phthalocyanine (CuPc) is a promising buffer layer and hole transporting layer (HTL), respectively, in the polymer OPV cells. The fill factor (FF) and power conversion efficiency are enhanced in this work.

2. Experiments

The polymer PV cells in this study consist of a layer of P3HT/PCBM blend thin film sandwiched between ITO and a metal cathode. The device architecture is shown schematically in Fig. 1(a), and energy level diagrams of different materials used in the device fabrication are shown in Fig. 1(b). The OPV cells used in this study were fabricated as follows. ITO-coated glass substrates were sequentially washed by sonication in detergent, water, acetone, isopropanol and water for 20 min. A bulk-heterojunction layer was spin-cast onto the buffer layer PEDOT:PSS at a coating speed of 3500 rpm for 60 s. For the buffer layer, PE-DOT:PSS and V₂O₅ were used. A PEDOT:PSS layer of about 25 nm thickness was obtained by spin coating an aqueous solution onto ITO coated glass substrates, followed by baking at 140 °C for 5 min under a N₂ atmosphere. V₂O₅ and CuPc layers were thermally evaporated onto ITO substrates sequentially under a vacuum of 10⁻⁶Torr. The active layer thin films of a P3HT:PCBM 1:0.8 weight-ratio solution, P3HT was first dissolved in 1,2dichlorobenzene to which PCBM powder was subsequently added. The blend was then stirred for about 24 h at 40 °C in the glove box before spin coating. Finally the cathode, evaporate of 7 Å of LiF and 150 nm of Al, was thermally deposited on top of the active layer in a deposition chamber in the glove box under a vacuum of 10^{-6} Torr.

The evaporation rate and thickness of the film was determined using an oscillating quartz thickness monitor (Sycon STM-100). The active area of the device, defined by shadow mask, was 0.24 cm². The current-voltage (I-V) curves were measured by a Keithley 2400 source meter. Sample was illuminated using an AM 1.5 G simulated solar spectrum from a filtered Xe arc lamp source. The light intensity of which was measured by a calibrated silicon detector.

3. Results and discussion

The OPVs structures in this study are summarized as follows:

Cell 1: ITO/ P3HT:PCBM/LiF/Al Cell 2: ITO/PEDOT:PSS/P3HT:PCBM/LiF/Al Cell 3. ITO/V₂O₅/P3HT:PCBM/LiF/Al Cell 4: ITO/V₂O₅/CuPc/P3HT:PCBM/LiF/Al

The J-V characteristics under illumination for the OPV devices are shown in Fig. 2. The summary of various device parameters for all types of devices made in this study is given in Table I. Cell 2 with a buffer layer of PE-DOT:PSS exhibits a power conversion efficiency of 2.09% and FF of 41.5%. The short-current density (J_{sc}) and open-circuit voltage (V_{oc}) are 8.39 mA/cm² and 0.6 V, respectively. A buffer layer efficiently prevents the recombination of charge carriers at the active layer/ITO interface. Considering Cell 1 without a buffer layer, P3HT:PCBM directly contacts with ITO. It is possible for active layer to transfer hole to ITO electrode, thereby increasing the recombination rate of photogenerated charges. Open-circuit voltages (V_{oc}) is the same for all devices with different buffer layers, irrespective of the work function of the buffer material, which were V₂O₅ (4.7 eV), and PEDOT:PSS (5.2 eV). It has been understood that the Voc corresponds to the active layer difference between the donor HOMO and the acceptor LUMO levels [6].Instead of PEDOT:PSS, V2O5 is introduced as a buffer layer in Cell 3. Comparing with Cell 2, Cell 3 shows an increased J_{sc} from 8.39 mA/cm² to 14.89 mA/cm². We also find the surface morphology of V_2O_5 is better than PEDOT:PSS. A smooth interface between V₂O₅ and P3HT:PCBM will benefit current spreading in Cell 3.

By inserting a 5 nm CuPc hole transporting layer (HTL), Cell 4 (ITO/V₂O₅/CuPc/P3HT:PCBM/LiF/Al) gives rise to a significant increase in fill factor (FF) from 28.8% to 62.2%, and exhibits a very low J_{sc} of 5.64 mA/cm². The FF values for the present devices are very high, being comparable to those reported for bulk-heterojunction OPV using

Table I. Organic characteristics for device with different type of buffer layer and HTL under illumination at an intensity of 100 mW/cm²

Device structure: ITO/Buffer layer/HTL	$J_{sc} (mA/cm^2)$	$V_{oc}(V)$	FF (%)	PCE (%)
Cell 1:ITO only	4.46	0.25	23.5	0.26
Cell 2:ITO/PEDOT:PSS	8.39	0.6	41.5	2.09
Cell 3:ITO/ V_2O_5 (10nm)	14.89	0.6	28.8	2.57
Cell 4:ITO/V ₂ O ₅ (5nm)/CuPc (5 nm)	5.64	0.6	62.2	2.11

polycrystalline CuPc [7]. Introducing CuPc HTL will contribute to the series resistance (R_s) of the device and may result in lower current. An increase in shunt resistance (R_{sh}) will also enhance the FF of the device. By analysising the energy diagram shown in Fig. 1(b), CuPc has a higher work function (5.3 eV) than ITO (4.7 eV) and V₂O₅ (4.7 eV). It means the hole could transfer easily from active layer to anode. CuPc has usually been used as a hole injection layer in OLEDs [8] to speed up the hole injection from the anode to active layer. The similar effect can be found in the OPV proposed in the study.

4. Conclusions

In summary, bulk-heterojunction OPVs using a buffer layer material of V_2O_5 and a HTL material of CuPc show higher performance relative to that using PEDOT:PSS materials. High FF of 62.2% has been obtained in Cell 4 and its structure is ITO/V₂O₅/CuPc/P3HT:PCBM/LiF/Al. The buffer layer plays an important role in preventing an unwanted chemical reaction between the ITO and the active layer. By analysising the energy level diagram, CuPc has a higher ability to transfer the carrier from active layer to anode. The elevated shunt resistance also makes contribution to the improvement in FF, leading to a significant improvement in power conversion efficiency. Films' thickness including V_2O_5 and CuPC will be optimized in the near future. The characteristics should be greatly improved.

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Fig. 1 (a) The device structure of the OPV. (b) Scheme of the energy levels of the materials involved in the OPV.



Fig. 2 The *J-V* characteristics of the devices under 100 mW/cm² white light illumination in air.