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Optimized Device Structure of Organic Photovoltaic Cells using Low Band Gap Small Molecules in Dry Process

Kohei Yamamoto[1], Tetsuhiko Miyadera[1], Yutaka Matsuo[2], Tetsuya Taima[3] and Masayuki Chikamatsu[1]

[1] RCPV, AIST, Tsukuba Central 5-1, 1-1-1 Higashi, Tsukuba, Ibaraki 305-8565, Japan
[2] Univ. of Tokyo, 7-3-1, Hongo, Bunkyo-ku Tokyo 113-0033, Japan
[3] Kanazawa University, Kakuma, Kanazawa Ishikawa 920-1192, Japan

E-mail: ko.yamamoto@aist.go.jp

Abstract

Low band gap molecules have been used in photo active layer of organic photovoltaic cells to obtain higher open circuit voltage and to absorb light with longer wavelength for improving power conversion efficiency. Here we report on the effect of film quality of small molecules by optimizing the device structure of organic photovoltaic cells. 6-fold improvement of power conversion efficiency was obtained using the inverted structure compared to conventional structure.

1. Introduction

Organic photovoltaic (OPV) cells have many advantage, such as their light weight, flexibility, and low cost. Recently, organic photovoltaic cells were achieved to 13.7% in 2018 [1)]. For high performance of OPV cells, low band gap of organic semiconductor has been required [1, 2)]. Low band gap molecules have potential to obtain higher open circuit voltage (V_{oc}) and to absorb light with longer wavelength for increased power conversion efficiencies (PCEs) of OPV cells. The tetracene imide disulfide (TIDS) materials were reported to have long-wavelength absorptions of up to 886 nm in the thin films and high V_{oc} of 0.8 V by using solution process [3)]. In this work, we introduced N-(n-hexyl)-tetracene carboxylic acid 5,6-imide-11,12-disulfide (Hexyl-TIDS) as p-type organic semiconductor to optimize OPV device structure for improved OPV performance. There are two kinds of the OPV cell structures, which are called conventional structure and inverted structure. In conventional structure, p-type organic semiconducting layer such as Hexyl-TIDS is deposited on indium tin oxide (ITO) substrate. On the other hand, n-type organic semiconducting layer such as C_{60} is deposited on ITO substrate in inverted structure. Inverted OPV cells have air-stable properties [4)], however, the PCE of inverted OPV cells using small molecules is low, compared with conventional OPV cells [5)]. In this work, we try to achieve high PCE by optimized OPV cell structure.

2. Experimental

Fabrications of OPV cells

Figure 1 shows Hexyl-TIDS as p-type organic semiconductor and device structure used in this work. The conventional and inverted device structure is ITO / MoO_3 / Hexyl-TIDS / C_{60} / BCP / Al, and ITO / Zinc-Oxide (ZnO) / C_{60} / Hexyl-TIDS / MoO_3 / Ag in this work. Bare ITO was treated with oxygen plasma for 20 min before use. The MoO_3 (10 nm), C_{60} (30 nm), BCP (10 nm), Al (100 nm), and Ag (100 nm) were deposited in conventional vacuum deposition system. The Hexyl-TIDS (30 nm) was deposited by laser deposition system with 808 nm CW semiconductor lasers, which was modulated as a 10 Hz square wave to accomplish precise control and the evaporation rate was adjusted by tuning the duty ratio of the square wave. The ZnO layer (30 nm) was fabricated by spin coating using ZnO nano-particle solution in glove box under nitrogen gas.

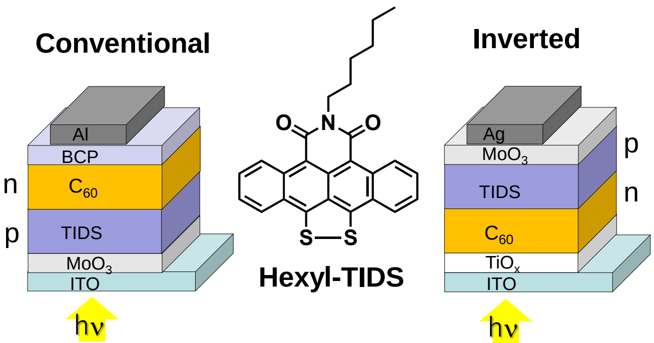

Fig. 1 Diagram of the cell structure and chemical structures of Hexyl-TIDS. The thickness of C_{60} and Hexyl-TIDS are 30 nm, respectively.

Method of Measurement

The current-density versus voltage (*J-V*) curve of the cells was measured under dark and simulated AM 1.5G solar illumination with a Keithley 2400 Digital Source Meter. IPCE spectra were collected by using a Xe lamp, which was integrated with a computer-controlled monochromator. UV-vis absorption spectra were measured by Shimadzu UV-3600 UV-vis-NIR scanning spectrophotometer.

3. Result and Discussion

The *J-V* curves of OPV cells using conventional and inverted structure are shown in Figure 2. The corresponding values of short-circuit current density (J_{sc}), V_{oc}, fill factor (*FF*), PCE are shown in Table I. PCE of inverted OPV cell was improved up to 0.68% compared with 0.1 % of conventional OPV cell. Especially, the J_{sc} and *FF* of the conventional cell was very small value of 0.44 mA/cm^2 and 0.27, compared with inverted OPV cell.

Here we considered the reason of the increase in J_{sc} with inverted structure. The IPCE increased from range of 300 nm up to 850 nm with inverted structure, as shown in Figure 3.

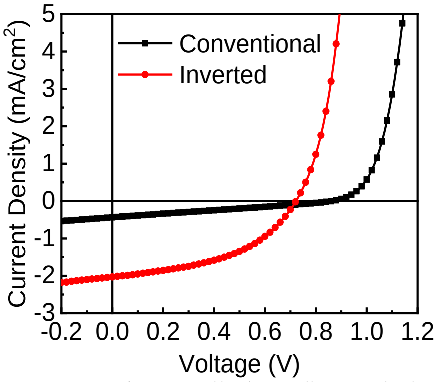

Fig. 2 *J-V* curves of OPV cells depending on device structure.

Table I Solar cell parameters calculated from *J-V* curves

	J_{sc} (mA/cm^2)	V_{oc} (V)	*FF*	PCE (%)
Conventional	0.44	0.86	0.27	0.10
Inverted	2.03	0.72	0.46	0.68

The UV-vis spectra of Hexyl-TIDS film with various condition are shown in Figure 4. In the black line, the Hexyl-TIDS film on MoO_3 without C_{60} have absorbance in range of 300 nm up to 350 nm, and 550 nm up to 850 nm. The C_{60} have absorbance in the range of 350 nm up to 550 nm shown as the red line.

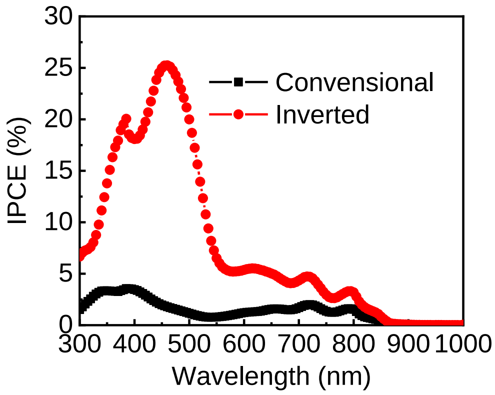

Fig. 3 IPCE spectra depending on device structure.

The IPCE was increased on absorbance range of Hexyl-TIDS and C_{60} by using inverted structure with same thickness, compared with conventional structure. The absorbance value of Hexyl-TIDS was increased on C_{60} condition more than on MoO_3 condition in range of 550 nm up to 850 nm. The reason of increasing IPCE on C_{60} absorption range can be optical interference effect using inverted structure. For inverted structure condition, we considered the molecular orientation of Hexyl-TIDS layer was optimized by C_{60} layer. Therefore, the deposition sequence of n-type and p-type organic semiconducting layers is important to obtain high PCE of OPV cells.

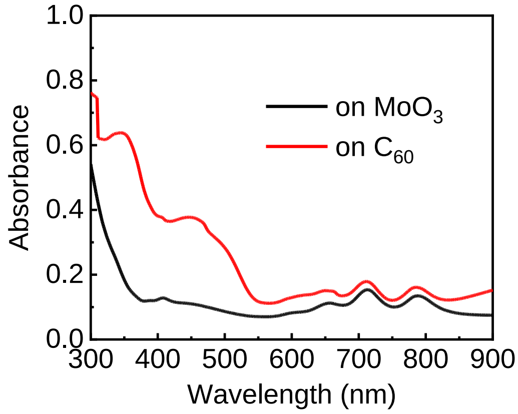

Fig. 4 UV-Vis absorption spectra of Hexyl-TIDS film on MoO_3 (black) and C_{60} (red). Thickness of Hexyl-TIDS film is 30 nm in both condition.

4. Conclusion

We investigated the effect of device structure for the performance of OPV cells based on low band gap small molecules. For increasing the IPCE of Hexyl-TIDS absorption range, we considered the molecular orientation of Hexyl-TIDS layer was optimized by C_{60} layer. The inverted structure can be optical interference effect with increasing IPCE value on C_{60} absorption range. As the result, PCE of inverted OPV cell was improved up to 0.68% compared with 0.1 % of conventional OPV cell. Especially, the J_{sc} and *FF* of the conventional cell was increased to 2.03 mA/cm^2 and 0.46, compared with conventional OPV cell.

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