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The evaluation of organic solar cell's properties based on polymer F8BT and fullerene derivative C60PCBM

Abstract. The paper included fabrication and characterization of the bulk heterojunction organic solar cell (BHJ OSC) based on poly[(9,9-di-noctylfluorenyl-2,7-diyl)-alt-(benzo[2,1,3]thiadiazol-4,8-diyl)] (F8BT) and fullerene derivative [6,6]-phenyl-C61-butyric acid methyl ester (C60PCBM). It was studied the influence of annealing the temperature range: 120°C-200°C on absorption properties of F8BT, C60PCBM and F8BT:C60PCBM films. The annealing of films and the encapsulation of OSC's was carried out under nitrogen atmosphere in glove boxes. Fabricated devices were examined in terms of basic operational parameters such as: open circuit voltage, short circuit current, fill factor, power conversion efficiency. Annealing process at 120°C resulted in power conversion efficiency about 0.053% and fill factor ratio about 31%. Encapsulation after fabrication improved the work parameters of the OSCs and extended their lifetime in relation to non-encapsulation devices.

Streszczenie. W ramach prac wytworzono i scharakteryzowano objętościowe heterozłączowe polimerowe, ogniwo fotowoltaiczne (OPV) oparte na poli [(9,9-di-n – oktylofluoren 12,7 - diylu) - alt - (benzo [2,1,3] tiadiazolo-4,8 - diylu)] (F8BT) oraz pochodną fulerenu [6,6] - fenylo - C61 - estru metylowego kwasu masłowego (C60PCBM). Zbadano wpływ wygrzewania warstw F8BT, C60PCBM oraz blendy F8BT:C60PCBM w zakresie od 120°C do 200°C na właściwości absorpcyjne. Wygrzewanie badanych warstw oraz hermetyzację OSC wykonywano w atmosferze azotu w komorach rękawicowych. Dla skonstruowanych urządzeń wyznaczono charakterystyki prądowo-napięciowe oraz podstawowe parametry użytkowe: napięcie obwodu otwartego, prąd obwodu zamkniętego, współczynnik wypełnienia równym 0,31%. Hermetyzacja po procesie wytwarzania spowodowała poprawę parametrów roboczych urządzeń oraz przedłużyła ich czas życia w stosunku do urządzeń niehermetyzowanych. (Ocena właściwości organicznego ogniwa fotowoltaicznego opartego na polimerze F8BT i pochodnej fulerenu C60PCBM).

Keywords: organic solar cell, photovoltaic, polymer F8BT, fullerene derivative C60PCBM, blend F8BT:C60PCBM, blend polymer/fullerene. **Słowa kluczowe:** organiczne ogniwo fotowoltaiczne, fotowoltaika, polimer F8BT, pochodna fulerenu C60PCBM, blenda F8BT:C60PCBM, blenda polimer:fulleren.

Introduction

Polymer solar cells are a promising new class of photovoltaic technology. The ability to deposit thin polymeric films over a large scale at low cost may provide polymer OSC an edge over rival technologies. Polymer solar cells are typically based on a bicontinuous blend of donor and acceptor materials [1]. It can be classified into two types in terms of acceptor materials. These are polymer/fullerene solar cells based on a blend of a conjugated polymer and a fullerene derivative such as [6,6]phenyl-C61 butyric acid methyl ester (C60PCBM) and polymer/polymer solar cells based on a blend of a donor polymer and an acceptor polymer. The organic solar cell have been mostly studied in recent years. The power conversion efficiency (PCE) of polymer/fullerene solar cells has been steadily improved and most recently exceeds about 10% [2-4]. For comparison, the PCE of polymer/polymer solar cells remains at ~2% [4-6]. The new idea to use solar radiation more effectively a useful approach is to stack multiple photoactive layers with complementary absorption spectra in series to make a tandem. These construction reach PCE at around 10-11% [2,4]. The newest materials exhibits reproducible PCE with relatively high external quantum efficiency (>80%) and high fill factor (~0.7) [2-4, 7-11]. Nowadays these device parameters are the highest in organic solar cells.

In this paper we focus on a role of poly(9,9-dioctylfluorene-alt-benzothiadiazole) (F8BT) in organic solar cells. The polymer/polymer solar cells are mostly based on poly 3-hexylthiophene P3HT. The structure with P3HT and F8BT exhibits a device performance with PCE of less than 0.2% [12,13]. The difference in PCE is due to a character of acceptor materials. Both acceptor materials (F8BT and C60PCBM) are n-type semiconductors with high electron mobility ($\geq 10^{-4}$ cm² V⁻¹ s⁻¹) but F8BT has too high hole mobility ($\geq 10^{-3}$ cm² V⁻¹ s⁻¹) [12]. To reach good parameters of OSC is needed a high dissociation of excitons into free carriers. The process can be ensured only while the high

different between work function is guaranteed. In a blend P3HT:C60PCBM the LUMO–LUMO offset is 0.7 eV and in a blend P3HT:F8BT the LUMO–LUMO offset is 0.3 eV [7,8]. Generally 0.5 eV is considered to be enough for excitons to be dissociated into free carriers. This is an answer why blend polymer:C60PCBM had higher parameter of PCE. In this paper we have shown the OSC based on a blend F8BT and C60PCBM. In this active layer F8BT is a material to transport hole because of his high mobility and C60PCBM is material to electron transport. The value of work function between materials suggests that OSC can have good parameters.

Reagents, construction and measurements

For absorption measurement pristine film F8BT (Sigma-Aldrich), C60PCBM (Sigma-Aldrich) and a blend F8BT:C60PCBM (1:1 by weight) at a concentration of 20 mg mL⁻¹ were prepared onto quartz substrates by spincoating (1500 rotations/min for 20 s and 2500 rotations/min for 15 s) from a toluene (Sigma-Aldrich, HPLC) and a 1,2dichlorobenzene (Sigma-Aldrich, HPLC) solution.

For photovoltaic device fabrication ITO (Indium Tin Oxide) coated glass (Ossila, ~25 Ω /cm2) was cleaned with acetone and isopropanol alcohol four times and then dried with flowing nitrogen. On the top of the cleaned ITO coated glass. hole transport laver poly(3,4а ethylenedioxythiophene): (styrenesulfonate) poly (PEDOT:PSS) (Ossila, 1:2 methanol) was filtrated (PVDF 0.22 µm filter), spin-coated, removed from ITO connector pins and dried at 200°C for 10 min. The thickness of the PEDOT:PSS layer ranged from 40 to 50 nm. Next, the blend F8BT:C60PCBM film was spin-coated on the PEDOT:PSS layer (800 rotations/min for 180 s), softbacked at 50-60°C for 30 min and dried with various temperature in a range 120°C - 200°C. This temperature range was studied due to decrease of the electron mobility above 120°C to 160°C. It can be explained by conformational changes of the F8BT chain stacking below and above the glass transition temperature T_g . Between this temperature a rearrangement of the F8BT chains occurs into an energetically more favorable packing structure, which exhibits less overlap between BT units of neighboring polymer chains, making the electron hopping transport between those sites less favorable [14]. Additionally the film annealed at 120°C reveals an amorphous F8BT phase and a very flat surface with a root-mean-square (rms) roughness of about 0.5 nm. Annealing at temperatures between 160°C and 200°C does not change the morphology qualitatively. The rms roughness increases by an order of magnitude averaging 4.0 nm for 160°C and 4.5 nm for 200°C. This is possibly an indication of formation of a polycrystalline phase during annealing above T_g with yet very small grain size

[14]. Before spin-coating, the blend solution was stirred overnight, in a room temperature. The thickness of the polymers blend film ranged from 120 to 160 nm. Finally, the cathode, consisting of 1-2 nm thick LiF layer and ~50 nm thick aluminum layer, was deposited on the active layer by thermal evaporation ~6 × 10^{-7} Torr. During the last step, selected structures were encapsulated by epoxy (Ossila) and glass coverslip substrate and light-cured in UV light for 5 min. Encapsulated and non-encapsulated structures were used to comparison of operational parameters of the OSCs and their lifetime. The active area of devices was 4.5 mm² (see Figure 1.).



Fig. 1. Schematic construction of the examined heterojunction organic solar cell ITO/PEDOT:PSS(~40nm)/F8BT:C60PCBM(~120-160nm)/LiF(1-2nm)/Al(~50nm) (left) and their size parameters with highlighted active area (right)

The optical absorption coefficient of pristine and blend films were measured using an UV-Vis absorption spectrometer (Specord M40). An atomic force microscope and profiler (Bruker, Dektak XT) were used to examine the surface and thickness of the pristine films and the blend film. The photovoltaic characteristics of devices under white light illumination (AM 1.5) were measured using a solar simulator installed in a glove box (Glove Box Technology Ltd.) based on a filtered lamp with output intensity of 100 mW/cm². The device performance was measured using a system equipped with sources and multimeters (Keithley 2400) and LabView software.

All procedures of fabrication and measurement were carried out in a nitrogen atmosphere in a clean room or a glove box.



Fig. 2. Absorption spectra of pristine F8BT (dash dot line), pristine C60PCBM (dash line) and blend F8BT:C60PCBM (solid line)

Experimental results

The absorption spectrum of pristine F8BT film extends partially into the visible, with the onset of absorption at about 375 nm. On the other hand, the PCBM weakly absorbs over all the visible range, with a very weak tail from transitions up to 800 nm. Above this value absorption was not observed. The absorption spectra of a blend F8BT:PCBM correspond to the superposition of the spectra of the two components, thus demonstrating the absence of a significant ground state interaction between the two materials. In particular, both F8BT and PCBM components in the blend are capable of absorbing light at 460 nm, with low efficiency. Therefore, at 460 nm the light absorption produces singlet excited states either in the polymer or in the PCBM (see Figure 2.).

Current - voltage (IV) characteristics were measured in a calibrated solar simulator with AM 1.5 illumination and power intensity of 100 mW/cm² (see Figure 3. and Figure 4.). The PCE is defined as the ratio of max output power to the light power incident on the active area of the device. The light power incident is standardized at 1000 W/m2 with a spectral intensity matching that of the sun on the earth's surface at an incident angle of 48.19° (AM 1.5). The devices without heat treatment show a poor performance with V_{OC} = 0.66 [V], I_{SC} = 1.15E-05 [A] and FF = 29 [%]. The PCE for this device is therefore 0.049 [%]. After thermal annealing at 120°C I_{SC} and FF slightly increase such as PCE = 0.053 [%]. After annealing at 160°C and 200°C, the devices exhibits decrease all work parameters. V_{OC} = 0.44 [V] and V_{OC} = 0.36 [V], I_{SC} = 9.32E-06 [A] and I_{SC} = 1.09E-05 [A], FF = 28 [%] and FF = 27 [%], PCE = 0.025 [%] and PCE = 0.023 [%] respectively (see table 1.).

Table 1. The comparison of the best performances obtained from tested solar cell ITO/PEDOT:PSS/F8BT:C60PCBM/LiF/AI under AM 1.5 illumination and power intensity of 100 mW/cm² without and with heat treatment at 120°C, 160°C and 200°C



Fig. 3. The IV characteristics obtained from organic solar cell ITO/PEDOT:PSS/F8BT:C60PCBM/LiF/Al under AM 1.5 illumination and power intensity of 100 mW/cm². Curves from device without thermal annealing (solid line) and device with heat treatment at 120°C (dash line), at 160°C (dot line) and at 200°C (dash dot line)



Fig. 4. The IV characteristics obtained from organic solar cell ITO/PEDOT:PSS/F8BT:C60PCBM/LiF/Al under AM 1.5 illumination and power intensity of 100 mW/cm² (solid line) and without illumination (dash line) with heat treatment at 120°C and PCE = 0.053 %

Summary

The bulk heterojunction organic solar cell based on a blend polymer F8BT and fullerene derivative C60PCBM (1:1 weight) was presented. The photovoltaic effect was observed in UV-Vis range spectrum. It was possible to obtain current - voltage characteristics of OSCs and their work parameters. Power conversion efficiency in the best case reached the level of 0.053 % and fill factor ratio about 31 % with thermal annealing at 120°C and encapsulation after fabrication. Encapsulation after fabrication improved the work parameters of the OSCs and extended their lifetime in relation to non-encapsulation devices.

We fully expect that the device performance can be further improved by the optimization of the material and the device fabrication.

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