Effects of exciton blocking layer and cathode electrode work function on the performance of polymer solar cells

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1. Introduction

Development of organic solar cells is very rapid [1,2]. This is due to the flexibility of synthesis routes of organic materials, which enable production of new materials with desired properties. Among the organic materials, polymers have interesting properties such as light weight, vast range of mechanical behavior, flexibility, solution process ability, high molecular weight, ease of functional group addition and so on. Polymer solar cells have become an interesting issue because of some advantages of this topic such as simple and cost effective coating methods, diversity of conjugate polymers, transparency, light weight, and flexibility [3,4]. Because of the low cost of polymer solar cells, they are a good alternative to traditional inorganic counterparts [5–7]. The main disadvantage of the polymer solar cells is their low power conversion efficiencies (PCEs) [8]. Due to the discovery of electron transfer from conjugated polymer to buckminsterfullerene [9] and the invention of the bulk heterojunction (BHJ) structure [10], the power conversion efficiencies of polymer solar cells were grew orders of magnitude and a realistic hope to reach higher efficiencies than traditional inorganic solar cells was created. Because of high absorption ratio of polymer semiconductors [11] and femto-second scale of charge transfer between polymer and fullerenes and internal quantum efficiency for charge generation of 0.95 [12], if the problem of charge collection is resolved, power conversion efficiencies about 15% will be
achievable [13]. After charge injection to fullerene phase, the resistances of electrons and holes transport to adjacent layers of electrodes, which are related to the morphology of bulk heterojunction structure, make some time for electrons and holes to recombine. For this reason, efforts have been devoted to manipulate the morphology of bulk heterojunction structure solar cells to achieve smaller transport resistances [14–16] using block copolymers [17], self-organization of polymer blends [18], polyaniline:polyvinylidene-fluoride composite as buffer layer [19], processing additives [20], and side chain manipulation [21]. Also, some post-treatments such as thermal annealing, solvent annealing, and electrical treatment [22] have been applied to improve the morphology of active layer. Another important resistance is the barrier of charge transport between active layer and electrodes. By inserting an exciton blocking layer, charge extraction can be improved. In this study, the effects of some important processing and post-processing treatments including the active layer film formation period, thermal annealing, electrical treatment, cathode work function modification, and exciton blocking layer type and thickness on the performance of poly(3-hexylthiophene-2,5-diyl) (P3HT);[6,6]-phenyl-C61-butyric acid methyl ester ([60]PCBM) solar cells were investigated.

2. Experimental

2.1. Materials

Patterned indium tin oxide (ITO)-coated substrates were purchased from Ossila Corp. with a sheet resistance of 20 Ω/□ and 150 nm in thickness. Poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS), P3HT (4002-EE), [60]PCBM (99%), o-dichlorobenzene (ODCB), and 1,8-diiodooctane were supplied from Sigma aldrich, Rieke Metals Inc., Solenne Inc., Merck, and Alfa Aesar, respectively. All materials were used as received.

2.2. Measurements and instruments

Atomic force microscopy (AFM) was conducted by a DualScope™ DS-95-50E/ Rasterscope C26. The thickness of PEDOT:PSS and active layers was measured by a Dektak profilometer and AFM, respectively. Current–voltage (I–V) characteristics of the solar cells were measured using an IVIUM CompactStat electrochemical analyzer under the illumination of AM1.5G, 100 mW cm⁻² using Luzchem Photoreactor Model LZC-SSR solar simulator. The calibration was done using a Thorlab calibrated photodiode. Each solar cell sample consisted of 6 pixels, which were evaluated separately, and I–V parameters of each sample were the average of them.

2.3. Sample preparation methods

After washing with detergents, the substrates were rinsed twice with distilled water and sonicated in isopropanol alcohol for 5 min. The substrates were dried with a nitrogen gun and exposed to UV-O₃ for 20 min. PEDOT:PSS was filtered by a 0.45 μm polyvinylidene fluoride (PVDF) membrane, and spin-coated on a clean ITO-coated glass at 2000 rpm for 1 min. The thickness of PEDOT:PSS layer was about 50 nm. The cathode strip was cleaned with a moistened cotton bud and heated at 125 °C for 15 min in a nitrogen-filled glove box. P3HT was dissolved in ODCB (10 mg/ml) by mixing at 50 °C for 2 h followed by mixing at room temperature for 12 h. After adding a specific amount of PCBM (P3HT:PCBM 1:2), the solution was mixed for 12 h at room temperature. Diiodooctane was added 1 h before coating. After filtering with a 0.45 μm polytetrafluoroethylene (PTFE) membrane, the solution was...
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