International Journal of Applied Power Engineering (IJAPE)
Vol. 14, No. 1, March 2025, pp. 138~145
ISSN: 2252-8792, DOI: 10.11591/ijape.v14.i1.pp138-145

Organic solar cells: a study on material selection and fabrication precision

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Article Info

Article history:

Received Apr 24, 2024
Revised Aug 25, 2024
Accepted Oct 23, 2024

Keywords:

Efficiency
Organic solar cells
P3HT:PCBM
PCDTBT:PCBM
PTB7:PCBM

ABSTRACT

The accelerating development of renewable energy technologies is imperative for addressing the problems of climate change and resource depletion. Solar energy, ideal for distributed power generation and more environmentally friendly, is integral to the progression of solar technology. Organic solar cells (OSCs) have become a key innovation in this domain, offering a promising alternative to traditional solar technologies. OSCs have received a lot of interest in the preceding years owing to their capacity to increase efficiency, affordability, and longevity. However, a dearth of research and development activities aimed at improving organic photovoltaic systems exists. This work details the laborious process of building a Bulk heterojunction (BHJ) OSC, describing the manufacturing stages and subsequent device characterization. OSCs were created in this work using three active layer materials: P3HT:PCBM, PTB7:PCBM, and PCDTBT:PCBM. The comparative analysis revealed significant efficiency disparities, with PCDTBT:PCBM exhibiting superior performance and electrical properties, while challenges were encountered with aged materials, emphasizing the relevance of meticulous material handling and the use of cutting-edge fabrication machinery in achieving efficient solar cell production.

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1. INTRODUCTION

As society shifts toward environmentally sensitive and sustainable energy sources, solar power has come under the limelight, gaining popular interest in the preceding years [1]-[3]. Continuous advances in photovoltaic technology are being made, pushing the frontiers of creativity in the design of innovative solar cell technologies and structures. Both the scientific and industrial communities are working to improve the efficiency, cost, and durability of existing solar technology. While silicon-based solar cells have traditionally received the most attention, interest has recently shifted to cutting-edge 3rd generation solar cell technology.

The main emphasis of this study is on bulk heterojunction (BHJ) organic solar cells (OSCs). The core of these cells relies on four key mechanisms: a) light absorption, b) charge creation, c) charge segregation, and d) charge collection. A BHJ solar device must contain an anode, a photo-active layer, a hole transport layer (HTL), an electron transport layer (ETL) and a cathode.

This research intricately chronicles the meticulous process involved in creating a BHJ OSC, meticulously outlining the fabrication steps and the subsequent device characterization. Delving into the role and selection criteria of each constituent material, alongside the rigorous assessments conducted to evaluate their suitability, it reveals the comprehensive electrical performance of the finalized device.

Becquerel [4] was the first to find photovoltaic effect. In 1873 and 1876, the initial discoveries regarding the photoconductivity of selenium were reported by Smith [5]. In 1906 and 1913, the initial discoveries regarding the photoconductivity in anthracene were reported by Pochettino, Spanggaard and Krebs [6], [7]. Tang [8] and Sun [9], proposed the first OSC with the two-layer donor-acceptor idea in 1986 at Kodak research laboratories and reported efficiency of 1%. A dispersed BHJ of MEH-PPV polymer and phenyl-C60-butyric acid methyl ester (C60) and later soluble derivatives of C60 (methanofullerene, C61) increased the efficiency to 2.5% [10]. Due to the nanoscale morphological control and post-production annealing procedure, devices with active layers of P3HT:PCBM that permitted efficiencies of approximately 5% were achieved in 2005 [11]. Peet *et al.* [12] increased near-infrared light harvesting by incorporating a low band gap polymer, such as PCPDTBT, leading to a 5.5% increase in efficiency. Power conversion efficiency (PCE) of around 6% has been reported for devices based on PTB4:PC61BM sheets produced from mixed solvents [13]. Chu *et al.* [14] obtained 7.3% PCE utilizing thieno [3,4-c]pyrrole-4,6-dione and Dithieno [3,2-b:20,30-d] silole copolymer as active layers in 2011. All of these accomplishments demonstrated that polymeric-based OSCs have a promising future. Despite these accomplishments, the present figures still fall below practical usability. Table 1 depicts several significant turning points in the progress of OSCs [14]-[28].

Table 1. Several significant turning points in the progress of OSCs

Year	Event
1839	Becquerrel was the first to find photovoltaic effect.
1906	Pochettino discovered photoconductivity in anthracene.
1958	In their investigation into magnesium phthalocyanines (MgPh), Kearns and Calvin [15] measured a photovoltage of 200 mV.
1964	When magnesium phthalocyanines were sandwiched between two distinct metal electrodes, Delacote *et al.* [16] noticed a rectifying action.
1986	Tang [8] reported the first heterojunction PV device.
1991	By co-sublimation, Hiramoto created the first dye/dye BHJ PV cell.
1993	Sariciftci created the first polymer/C60 heterojunction device.
1994	Yu *et al.* [17] created the first bulk polymer/C60 heterojunction PV.
1995	Yu *et al.* [17] created the first bulk polymer/polymer heterojunction PV.
2000	Peeters *et al.* [18] created PV cells using oligomer-C60 dyads/triads.
2001	Mende *et al.* [19] created hexabenzocoronene and perylene based liquid crystalline PV cells. Ramos created PV cells with double-cable polymers.
2001	Shaheen *et al*. [20] created an OSC and reported PCE of 2.5%.
2005	Li *et al*. [23] created P3HT/PC61BM based OSC with PCE of 4.4%.
2005	Ma *et al*. [11] made P3HT/PC61BM based OSC with PCE of 5%.
2007	Peet *et al*. [12] created an PCPDTBT:PC71BM based OSC with PCE of 5.5%.
2007	Kim *et al*. [24] created an P3HT:PC61BM based OSC with PCE of 6%.
2009	Liang *et al*. [13] created an PTB4:PC61BM based OSC with PCE of over 6%.
2011	Chu *et al*. [14] used “Thieno[3,4-c]pyrrole-4,6-dione and Dithieno[3,2-*b*:20,30-*d*]silole Copolymer” with PCE of 7.3%
2017	Zhao *et al*. [21] used Molecular optimization approach to get 13%.
2019	Yuan *et al*. [26] created an OSC with PCE of 15.7%.
2020	Tran *et al*. [22] reported an OSC with PCE of 17%.
2021	Liu *et al*. [27] reported 18% efficiency OSC.
2023	NREL reported OSC with PCE of 18.2%.

2. EXPERIMENTAL SECTION

2.1. Safety measures

It was critical to undergo safety and chemical handling training before beginning the experiment. Throughout the experiment, appropriate protective gear was required to assure safety. A lab uniform, strong gloves, safety eyewear, and a gas mask were all required. Because of their flammability and potential health concerns if breathed or exposed to skin and eyes, some compounds, such as acetone and IPA, required additional attention when handling. Chlorobenzene (CB), another solvent utilized, required special caution, therefore those parts were performed within a glove box to avoid any contact or fumes. Even while working with non-hazardous compounds such as CU2O, P3HT, PTB7, and PCDTBT, safety precautions were essential. PCBM, in contrast, requires even greater caution due to its high toxicity, necessitating the use of gas masks in addition to standard protective gear. Finally, dealing with hotplates and ovens need careful handling to avoid burns. It was important to be aware of these hazards and follow safety protocols before entering the lab for the experiment.

2.2. Experimental procedure

The illustrated design (Figure 1) depicts an OSC structure that includes a glass substrate covered with an HTL layer made of CU2O. This design was used to create OSCs with three distinct active layers: P3HT:PCBM, PTB7:PCBM, and PCDTBT:PCBM, each followed by an aluminum (Al) cathode deposition.

2.2.1. Cleaning

The device fabrication process initiates with a four-step cleaning procedure. To verify that the glass-ITO substrates were clear of any pesky dust particles or contaminated organic matter (e.g., fingerprints) that could mess with the device-making process. The substrates were handled using metal tweezers. Figure 2 depicts the proper positioning of the tweezers to avoid contact with the device active area [29].

- Step 1: The process commenced with a digital multimeter to assess the conductivity of glass substrates, specifically the ITO-coated areas. Identified as the conductive surfaces, these ITO-coated portions were meticulously cleaned by gently rubbing them with cotton soaked in a soap solution for approximately 15-20 minutes, all while wearing clean gloves. Following this, a holder containing these substrates was immersed in a beaker filled with deionized water supplemented with one to two drops of liquid detergent. This assembly underwent an ultrasonic cleaning process, effectively dislodging and removing any contaminants adhering to the ITO surface. After the ultrasonic treatment, the substrates underwent a thorough rinsing with deionized water to ensure complete elimination of any detergent residues, leaving them pristine and ready for subsequent procedures.
- Step 2: Following that, the holder with the substrates was placed in another beaker of acetone for an extra round of cleaning to remove any leftover organic residue. This beaker was put in an ultrasonic bath at room temperature for 10 minutes to complete the cleaning procedure.
- Step 3: After being removed from the acetone, the holder was submerged in isopropanol (IPA) in a beaker and subjected to a ten-minute ultrasonic bath at room temperature. This process is intended to remove any remnants of acetone that, if left to dry, may produce markings on the ITO surface. Following that, the substrates were carefully transferred from the holder to a Petri dish, with the ITO side facing up. These substrates were dried and kept at room temperature in a sealed Petri dish, ready for use in coating.

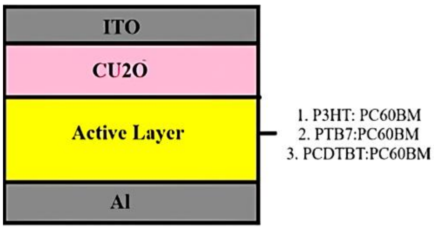


Figure 1. OSC structure

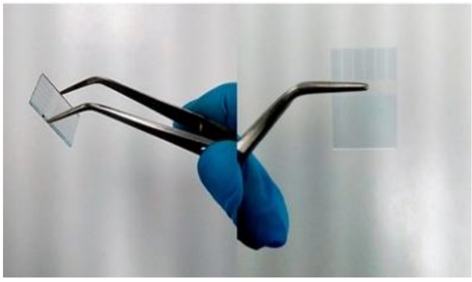


Figure 2. The correct handling of substrates with tweezers [29]

2.2.2. HTL preparation and coating

In OSCs, the layer between the anode and the active layer, known as the HTL, plays a vital role. It does two things: it transports the holes formed when excitons split, transporting them to the anode, and it inhibits electrons, lowering the possibility of carrier recombination. Picking the right material for the HTL is crucial, it needs high conductivity and hole mobility to swiftly deliver as many holes as feasible to the anode. Furthermore, because light passing through, adds to both optical and electrical losses, this layer must absorb as little light as possible. The thickness of the film is also important: too thin and it will not efficiently block electrons; too thick and it will absorb more light than necessary.

HTL in this case is CU2O. Copper iodide (CUI) concentration was originally optimized. CUI is a powder that has been combined with acetonitrile. The substrate was then spin-coated at 4000 rpm for 60s before being immersed into a NaOH solution. The concentration of NaOH solution was also optimized. Then kept in oven for 15 minutes at 150 degrees Celsius. Figure 3 depicts the procedure for making CU2O on an ITO substrate. The substrate was then subjected to ultraviolet spectroscopy and FTIR spectroscopy. Information about the aforementioned spectroscopies is available in the referenced papers [30]-[32].

2.2.3. Preparation of active layer material and deposition

The BHJ layer, which serves as the active layer, is made up of two materials: one that absorbs and one that throws them away. In OSCs, they are often organic polymers and fullerene derivatives. When producing the mixture, these two ingredients must readily blend together in the same liquid. To absorb more sunlight and form excitons, the material that absorbs light (donor) requires a low-energy band gap. It is critical that this material absorbs a wide range of solar wavelengths. An extended exciton diffusion length is a desirable property because it means the exciton can move farther through the donor material to reach its interface with the acceptor before breaking apart (dissociation). This prevents exciton recombination losses. Furthermore, the donor should let holes to flow quickly towards the active layer without recombining with electrons. Similarly, the acceptor material must route electrons quickly to its interface without combining with holes. To avoid charge accumulation, it is critical that the mobility of holes and electrons in both the donor and acceptor materials be as balanced as feasible.

Choosing the correct donor and acceptor materials is critical when creating blends for the active layer in solar cells. They must match in terms of energy levels, particularly at their interfaces. This pairing aids in the separation of excitons into free carriers. The energy difference between their lowest unoccupied molecular orbitals (LUMO) should be exactly right: not too tiny (causing no splitting) and not too high (causing losses and lowering the voltage). Finding this balance is critical, it is like balancing a tiny energy gap while producing a high-voltage output. The voltage output is proportional to the difference between the donor's highest occupied molecular orbital (HOMO) and the acceptors LUMO.

P3HT:PCBM, PTB7:PCBM, and PCDTBT:PCBM were employed as active layer materials in this study. These were made and stirred overnight before being used for spin coating. It was then spin-coated for 60 seconds at 1000 rpm. The oven was then set at 100 ℃ for 10 minutes. The substrate was then kept in the oven. This is followed by the deposition of cathode. Aluminium was employed as the cathode material in this case. Thermal vapour deposition was used to deposit it.

Figure 3. Schematic representation of preparation process of CU2O on ITO substrate [33]

3. DEVICE CHARACTERIZATION

3.1. J-V characteristics

The schematic representation of a solar cell's current density-voltage (J-V) curve under light is presented in Figure 4. The short-circuit current density (J_{SC}), open-circuit voltage (V_{OC}), fill factor (FF), and power conversion efficiency (PCE) are the general characteristics of OSC devices. These four values define a solar cell's performance and are hence its essential distinctive parameters.

All cells must be examined under a standard lighting environment with the intention of evaluating device performance. The Air Mass 1.5 spectrum (AM 1.5G, depicts sunlight with the Sun at an oblique angle of 48.2o above the earth's atmosphere), with an incidence power density of 1000 $W.m^{-2}$ (100 $mW.cm^{-2}$) is the standard test condition (STC) for solar cells, independent of their design or active material. This is also known as the typical 1 sun value at a temperature of 25 degrees Celsius.

- VOC: "The open-circuit voltage (VOC) is the difference in energy levels between the potential in the region with the freest electrons and the potential in the region with the freest holes" [34].
- J_{SC}: The number of photogenerated carriers produced in the active layer during illumination and the efficiency with which charges are separated throughout the photoactive layer are the two main factors that define the quantity of J_{SC} [34], [35].
- FF: $\frac{V_m \times I_m\ (maximum\ power\ point)}{Jsc \times Voc}$ [34].
- Finally, "PCE is defined by the product of Jsc, Voc, and the fill factor" [35].

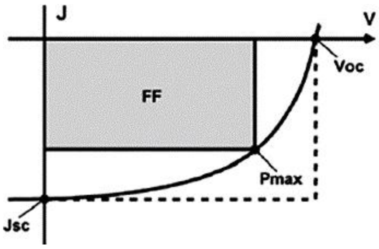


Figure 4. Characteristic J-V curve of an OSC [36]

4. RESULTS AND DISCUSSIONS

4.1. UV and FTIR spectral analysis

UV-visible spectra were obtained for the spin-coated CUI layers before annealing and CU2O after annealing at 150 °C for 10 minutes (Figure 5). The CUI displayed distinct peaks at 407 and 538 nm, closely aligning with the excitonic peaks of CUI and CU2O as documented in prior studies [37]. Both CUI and CU2O were subjected to FTIR analysis; the resultant graph is shown in Figure 6 below. This closely matches the features of CUI and CU2O that have been reported in earlier research.

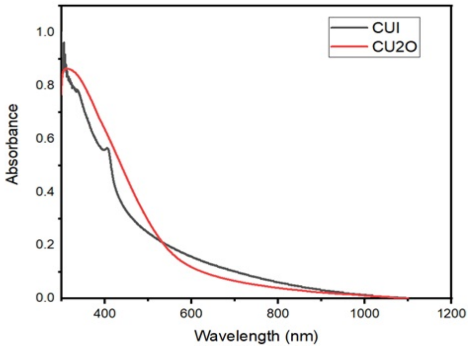
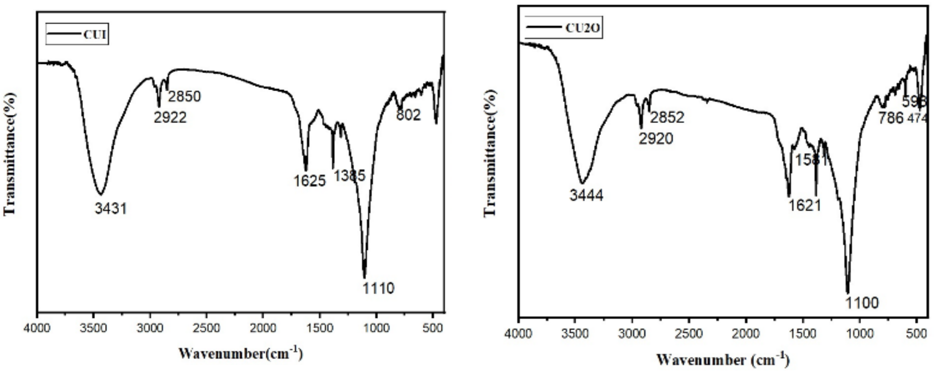


Figure 5. UV-Vis pattern of CUI and CU2O film



(a) (b)

Figure 6. FTIR pattern of CUI and CU2O film: (a) CUI and (b) CU2O film

4.2. J-V characteristics

OSCs fabricated and tested using several active layer materials, including P3HT:PCBM, PTB7:PCBM, and PCDTBT:PCBM, gave comparable outcomes (Figure 7). The results of the experiments and analysis indicated that the PCDTBT:PCBM combination performed better in terms of PCE. The J-V characteristics of PTB7:PCBM and PCDTBT:PCBM were plotted as shown below in Figure 8.

J-V study revealed that the efficiency observed with the P3HT:PCBM configuration was registered at 0%, primarily due to multiple factors. The material available in the laboratory was deemed old, potentially compromising its intrinsic properties crucial for effective photovoltaic performance. Moreover, chemical degradation or impurities in the aging material might have hindered its ability to form an efficient active layer within the solar cell. These circumstances likely impacted the material's capacity to generate a functional interface for efficient charge separation and collection, resulting in the recorded 0% efficiency. This instance underscores the significance of material freshness and quality control in achieving viable OSC performance, highlighting the necessity for optimal material conditions in research and development endeavors within this field.

Also, J-V studies of PCDTBT:PCBM and PTB7:PCBM configurations revealed significant performance differences in OSC fabrication. The PCDTBT:PCBM combination demonstrated a notably higher PCE of 1.68%, coupled with a FF of 34.6%, an V_{OC} of 0.5449V, and a J_{SC} of 8.91 $mAcm^{-2}$. Conversely, the PTB7:PCBM configuration displayed a respectable, albeit lower, efficiency of 0.85%, accompanied by a FF of 30.3%, a V_{OC} of 0.4293V, and a J_{SC} of 6.57 $mAcm^{-2}$. These findings highlight the distinct performance characteristics of each material pairing, emphasizing the superior efficiency and electrical properties exhibited by PCDTBT:PCBM while acknowledging the respectable metrics achieved by PTB7:PCBM. Such comparative analyses offer invaluable insights into material-specific strengths, guiding strategic choices for optimizing organic photovoltaic technologies.

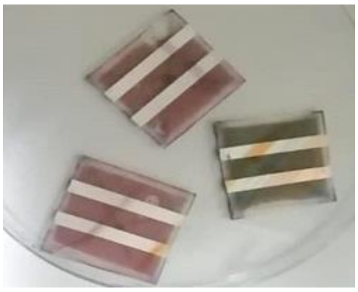
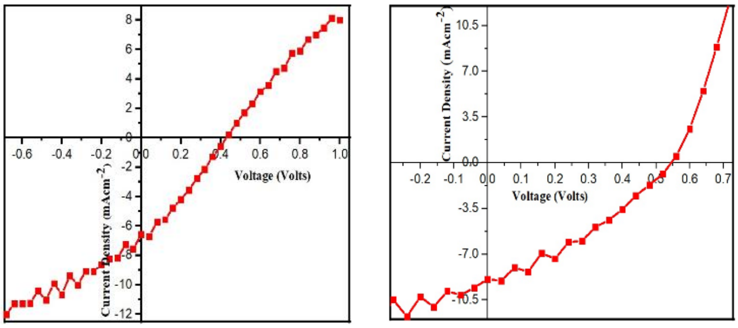


Figure 7. Fabricated OSCs



(a) (b)

Figure 8. The J-V characteristics: (a) J-V Curve of PTB7:PCBM based OSC; and (b) J-V curve of PCDTBT:PCBM based OSC

5. CONCLUSION

In conclusion, in this study, OSCs using three active layer materials: P3HT:PCBM, PCDTBT:PCBM, and PTB7:PCBM were fabricated. The comparative analysis revealed distinct efficiency disparities, with PCDTBT:PCBM showcasing superior performance, followed by PTB7:PCBM, while challenges were encountered with aged P3HT:PCBM materials. This underscores the critical role of material quality and freshness in achieving optimal cell efficiencies, emphasizing the need for well-maintained chemical materials in our research endeavors. Furthermore, the current manuscript delves into the operational principles of a BHJ OSC. It provides a comprehensive account of the fabrication procedure employed in constructing the aforementioned photovoltaic device. Before detailing each step, the manuscript offers explanations regarding their significance and physical implications. The insights gained, both in material selection and machinery utilization, pave the way for further advancements in optimizing organic photovoltaic technologies in achieving efficient solar cell production.

ACKNOWLEDGEMENTS

The authors would like to express their sincere gratitude to CSIR-NPL for their unwavering support and provision of resources throughout the course of this research. The authors would like to express their thanks to Dr. Sushil Kumar, Chief Scientist and Professor (AcSIR), Advanced Materials and Devices Metrology Division, CSIR-NPL, New Delhi, for providing the invaluable opportunity to undergo research at CSIR-NPL. Special thanks to Dr. Neeraj Chaudhary for imparting expertise in fabrication.

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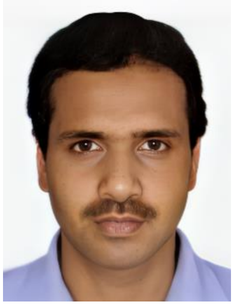

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