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Tuning the Morphological and Optical Characteristics of PCDTBT:PC71BM Blends via Fullerene Ratio Adjustment

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Abstract

Morphological and optical features of the PCDTBT:PC71BM combination of varying concentrations of PC71BM are the subject of this paper in the pursuit of optimizing their use in the organic photovoltaic (OPV) devices. It was deposited as thin films in different ratios of (1:0, 1:1, 1:2, 1:3 and 1:4 w/w) of PCDTBT:PC71BM onto pre-cleaned glass bases using spin-coating technique. The XRD shapes of all the prepared thin films at multiple PC71BM concentrations have a broad peak at about 23° , which suggests that they are amorphous. To examine the surface morphology of the thin films, FESEM was employed. The findings indicated that an increase in PC71BM concentrations resulted in formation of visible clusters on the outer layer. The UV-visible absorption spectra were taken, and two major peaks of pure PCDTBT were observed at about 394 nm and 557 nm. When varying PC71BM concentrations were introduced, there were slight changes in the absorption peaks, blue shift. This conveys morphological and optical changes. These results indicate that the fullerene ratio can be tuned to have a strong effect on the blend characteristics, and this will be a viable way of improving the working characteristics of PCDTBT:PC71BM-based OPV devices.

Keywords: PCDTBT, PC71BM, blend, donor, acceptor.

1. Introduction

The increase demand of global energy is causing an urgent demand of energy sources that are free of carbon. Organic photovoltaic (OPV) solar cells could be a promising technology providing potential benefits in cost-efficiency, manufacturing their lightweight cells, and reduced embodied energy flows as compared to conventional solar cells [1-3]. As a rule, the key component of an organic solar cell system is a conjugated polymer (CP) used as the donor and fullerene[6,6]-Phenyl-C71- butyric acid methyl ester (PCBM) as the acceptor.

The principal determiners of V_{oc} and J_{sc} in bulk heterojunction (BHJ) polymer PV panel are the band gap, HOMO level and hole mobility of the conjugated polymer. The design of the ideal photovoltaic polymer has specifically been geared towards the realization of a narrow bandgap, 1.5 eV, and a low HOMO level, 5.4 eV, to attain the highest possible values of the V_{oc} and J_{sc} [6-8]. Polymers with top occupied energy level (HOMO) energy levels (~ 5.4 eV) with low energy band gap ($E_g \sim 1.5$ eV) are suitable for providing significant short-circuit current (I_{sc}) and high open-circuit voltage (V_{oc}) [4, 5].

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The copolymer poly[N-9'-heptadecanyl-2',7'-carbazole-alt-5',5'-(4',7'-di-2-thienyl-2',1',3'-benzothiadiazole)] (PCDTBT), illustrated in Fig.1, offers an optical bandgap of 1.88 eV, with HOMO and smallest Unoccupied Molecular Orbital (LUMO) energy states of -5.45 eV and -3.60 eV, respectively. These properties align well with the requirements for enhanced absorption of the solar spectrum. Owing to its relatively narrow bandgap and deep HOMO level, PCDTBT has been identified as an optimal electron donor layer in BHJ architectures [9]. Using PCDTBT as the electron donor material can improve both light absorption and open circuit voltage (V_{oc}) [9]. Its extended absorption in the red region enables it to capture a bigger part of solar energy, thereby improving device performance.

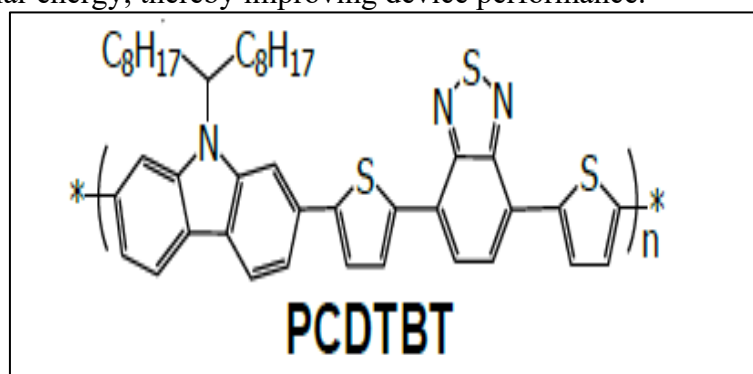


Figure 1: The chemical structure of the parent PCDTBT[9]

Fullerene [6,6]-Phenyl-C71- butyric acid methyl ester (PCBM) can be used as the acceptor in conjugated polymers. In recent decades, fullerene derivatives like [6',6']-vinyl C61 butyric acid methyl ester (PC61BM) and [6',6']-vinyl C71 butyric acid methyl ester (PC71BM) have seen a sharp increase in their applications as electron acceptors because of their advantageous electron affinity [15]. These ball-shaped fully conjugated networks boost electron delocalization due to their pronounced electron affinity and solely electron-driven transport. However, because of their purification-intensive processing procedures, these fullerene derivatives have been described as having a comparatively small absorption band in the visible wavelength, and high production costs. Electron-accepting and electron-donating polymers in bulk heterojunction (BHJ) polymer solar cells show similar effects [16]. As an n-type organic semiconductor, the fullerene derivative of [6',6']-vinyl C71 butyric acid methyl ester (PC71BM) has been widely exploited because its excellent electron transfers capabilities [17-19].

In bulk-heterojunction (BHJ) polymer solar cells, a composite of PCDTBT: PCBM active layer can be constructed where the active layer of an organic conjugated polymer (CP), such as PCDTBT is utilized as the donor and a fullerene- depend derivative (PCBM) is used as the p-type acceptor. The process of photovoltaics, photon absorption generates electron-hole pairs (excitons) that diffuse through the PCDTBT layer. Charge separation occurs at the PCDTBT:PCBM interface due to inherent interfacial voltage, with subsequent carrier collection through PCDTBT (holes) and PCBM(electrons) [9,10]. Solar cells that use the PCDTBT:PC71BM combination have demonstrated a high (PCE) of 5.6% [11-14].

In this research, the possibility of improving the morphological and optical features of the prepared films was studied using different ratios of PCDTBT:PC71BM was studied to improve the efficiency of manufactured photovoltaic systems. To streamline the film manufacturing process and improve device performance, it is essential to understand the role of the donor PC71BM in the acceptor PCDTBT. In this research, a thorough analysis was presented of how PC71BM concentration affects the active layer's morphological and optical characteristics.

2. Materials and Methods

2.1 Materials

Sigma-Aldrich provided the materials considered in this investigation. These included [6,6]-phenyl C71 butyric acid methyl ester (PC71BM), poly [N-9-heptadecanyl-2,7-carbazole-alt-5,5-(4,7'-di-2-thienyl-2,1',3'- benzothiadiazole)] (PCDTBT), chloroform and chlorobenzene.

2.2 Sample Preparation

To create a homogeneous solution, the PCDTBT:PC71BM mixture was dissolved in different ratios (1:0, 1:1, 1:2, 1:3, 1:4) in chloroform and chlorobenzene (CF:CB) solvents and mixed with a magnetic stirrer for 7 hours at 50°C. The spin coating method (2000 rpm spinning speed for 30 seconds; altering the spin speed, the thickness of the blended films can be altered) was used to deposit the PCDTBT:PC71BM on glass substrates. The glass layers were mechanically scrubbed with a detergent in deionized water after being ultrasonically agitated in ethanol and then acetone. The same detergent solution was then used to clean the glass substrates in an ultrasonic bath, and they were rinsed multiple times using ultrasonic agitation in water. The films were cured on a heated surface at 100°C for 10 seconds to form solid films.

3. Characterizations

To study the structural characteristics of the prepared films, an X-ray diffractometer (Philips-PW1730- Netherlands) was used. The 2θ angular scanning range was between 3° and 60° at a speed of 5,0000°/min. The surface morphology of the prepared films was determined using a Field Emission Scanning Electron Microscope (FESEM) (TESCAN-Mira III). For optical properties, a UV-Vis spectrophotometer (made by Shimadzu, Japan) was used.

4. Results and Discussion

Figure 2 illustrates the XRD structures of the prepared PCDTBT:PC71BM films, from which the effect of the various PC71BM concentrations can be noted. The XRD pattern for PCDTBT showed an amorphous nature, consistent with previous reports [9,20]. The XRD patterns of PCDTBT and PCDTBT:PC71BM blends with different blends ratios showed broad peaks around 23°. These patterns revealed the amorphous nature of PCDTBT:PC71BM for all the PC71BM concentrations. The amorphous framework contributes to broadband optical absorption; this enhances the solar photon uptake capability [16].

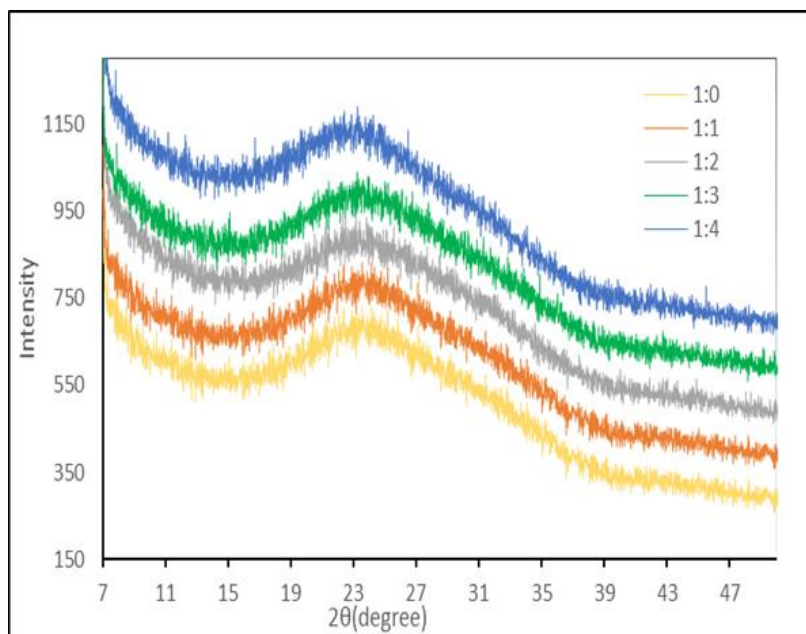


Figure 2: X-ray diffraction spectra of PCDTBT:PC71BM thin films at different blends ratios.

The surface morphology of the PCDTBT thin films using FESEM is shown in Fig.3. The FESEM image shows that the pristine PCDTBT thin film has an amorphous surface with small aggregates and slight roughness. This morphology reflects the disordered nature of the polymer and may affect charge transport and optical properties in devices. Generally, smoother, well-interconnected domains are preferred for efficient charge transport, while excessive roughness can lead to charge trapping.

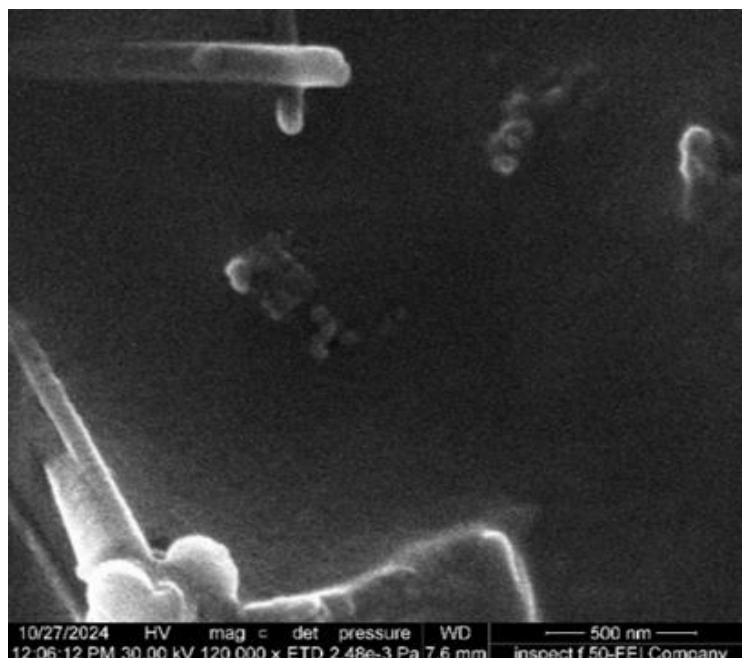


Figure 3: Feld emission scanning electron microscopy image of PCDTBT thin film.

The surface morphologies of the blend PCDTBT:PC71BM with various blend ratios are shown in Fig.4. Images for 1:1, 1:2, and 1:3 blends ratios showed distinct cluster formations, likely representing phase-separated domains of the PCDTBT polymer and PC71BM fullerene. The appearance of these clusters suggests that phase separation has occurred, which is

beneficial up to a certain scale, as it can enhance exciton dissociation at the interfaces between donor (PCDTBT) and acceptor (PC71BM). However, the uniformity and size of these clusters are critical. If they are too large, they may lead to poor charge transport due to limited pathways for electrons and holes to reach the electrodes. The surface of the 1:4 blend ratio appeared rougher and showed larger aggregates. Increased surface roughness and aggregates can affect light absorption and charge collection, as they may introduce sites for charge recombination, thereby reducing the efficiency of the photovoltaic device [21,22]

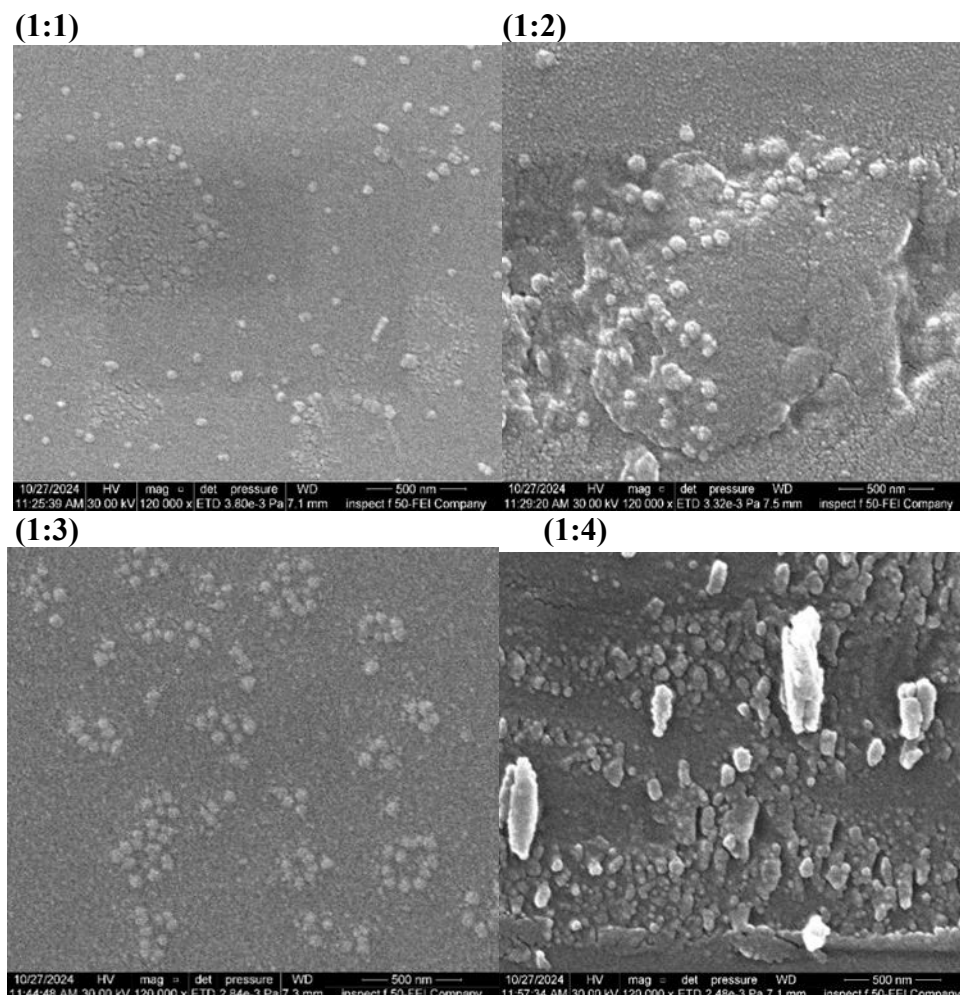


Figure 4: Field emission scanning electron microscope images of PCDTBT: PC71BM with different blend ratios of (1:1,1:2,1:3,1:4).

The UV-visible absorption spectrum of PCDTBT thin film, displayed in Fig.5, shows two separate absorption bands at approximately 394 nm and 557 nm, corresponding to the first and second excited singlet states, respectively. These absorption bands are due to the π^* - π electronic transitions [23-25]. These electronic transitions changes are linked to a charge transfer character, which shows how charge moves inside PCDTBT's molecular structure. The property is significant in the electronic and optical properties of the material that are relevant in applications in organic electronics and photovoltaics. These outcomes are in line with the other research results that have also indicated similar absorption characteristics of PCDTBT-based thin films [25, 26].

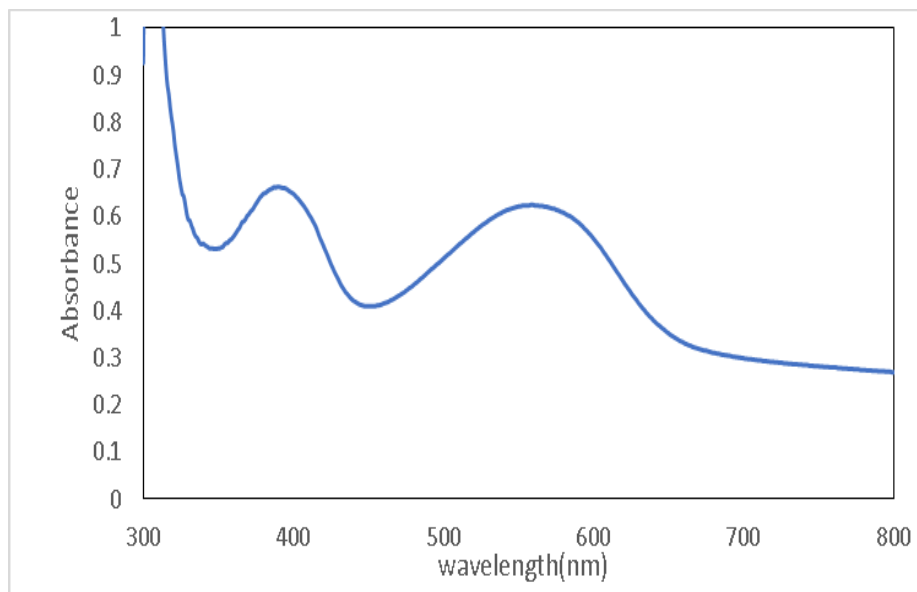


Figure 5: The absorbance spectrum of PCDTBT thin film.

The UV-visible absorption spectrum of PCDTBT:PC71BM blend at different PC71BM concentration is presented in Figure 6, which demonstrates the dependence of the absorption properties of the blend on the PC71BM concentration. The spectra had the same trend but with lower absorption than the pure PCDTBT. Their spectra show a wide and weaker band between 500 and 600 nm with a strong a prominent peak at 400 nm, which is the same as the absorption bands of the PCDTBT thin film. Lower absorbance was observed with the increase in the concentration of PC71BM. The 400 and 600 nm absorption bands give insignificant blue shifts as the concentration of PC71BM rises, which could have been caused by enhanced aggregation of the blend by fullerene.

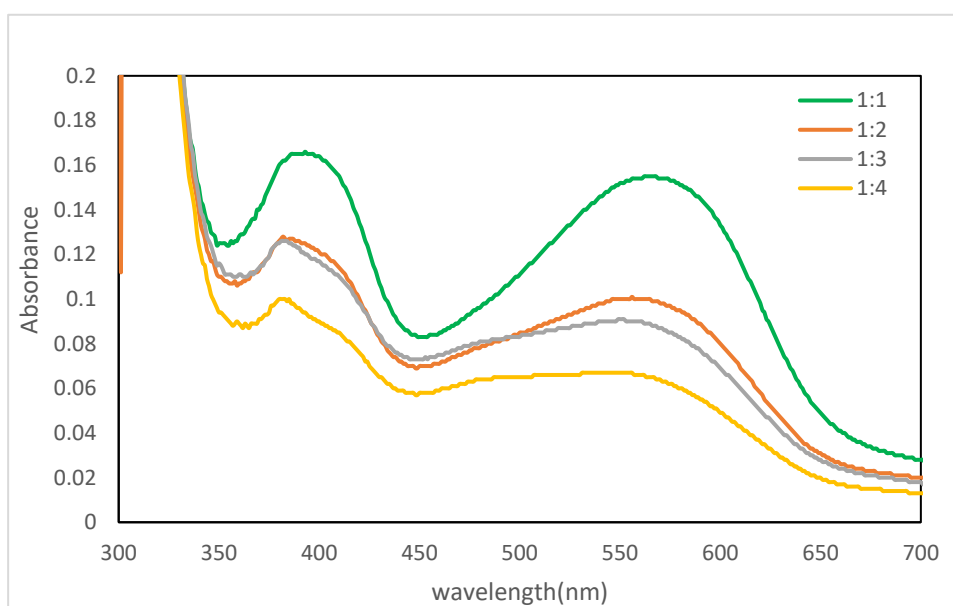


Figure 6: The absorbance spectra of PCDTBT:PC71BM blend thin film.

5. Conclusions

This paper has examined the changes in morphological and optical properties of PCDTBT:PC71BM blend with various concentrations of PC71BM, through XRD, FESEM and UV-visible characterization. The XRD has established the amorphous state of the combined blends of PCDTBT:PC71BM. FESEM data showed that increased concentration of PC71BM results in changes in the morphology of the film causing phase separation and changes in the uniformity of surfaces which are important parameters in charge transport and device efficiency in OPV. The findings show that when the PC71BM concentration is increased, the UV absorption is increased, owing to the high UV absorption properties of fullerene, but it also has an effect on the visible range of absorption, which is used in power photovoltaic devices.

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