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Annealing Effects on the Optical and Structural Properties of Spin Coated Poly (3-hexylthiophene) (P3HT) and Poly (3-hexylthiophene) (P3HT): (6, 6)-Phenyl C61 Butyric Acid Methyl Ester (PCBM) Thin Films

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ABSTRACT

Poly (3-hexylthiophene) (P3HT) and (6, 6)-phenyl C61 butyric acid methyl ester (PCBM) are promising materials for use as solar cells and other optoelectronic applications. P3HT is a semiconducting polymer and PCBM is a fullerene molecule with alkyl side chains. In this work, P3HT: PCBM thin films were deposited using spin coating technique onto clean glass substrates. Annealing effects on optical and structural properties of these materials were studied. Optical studies were done using uv-vis radiation and structural by X ray diffraction. Variation of optical properties such as amount of absorption, %transmission, band gap etc. and also the change in structural properties due to annealing were studied in this paper.

Keywords *- Organic semiconductor, P3HT: PCBM, Thin films, Annealing, Optical properties.*

1. INTRODUCTION

Organic photovoltaic cells (OPV) consisting of polymer fullerene bulk heterojunction, have seen a rapid progress due to their great advantages, such as low cost fabrication, light weight and large area devices [1, 2]. Till date, the polymer Poly (3-hexylthiophene) (P3HT) and its blend with (6, 6)-phenyl C61 butyric acid methyl ester (PCBM) has been the most successful system [3, 4]. P3HT is a semiconducting polymer which has been used in the fabrication of organic field effect transistors (OFETs) [5, 6]. It has useful optoelectronic properties such as high mobility, good chemical stability and low optical band gap [7, 8]. The high whole mobility of P3HT is useful in realizing high efficiency bulk hetero junction photo voltaic cells [9, 10]. The excellent mobility is thought due to the lamella stacking and the stacking of thiophene rings, giving rise to strong interchain reactions [5, 11]. The significance of the increase in optical absorption on photocurrent of P3HT: PCBM solar cells upon annealing have been investigated earlier [12]. Due to the strong impact of annealing on the optical and morphological properties, these parameters are of current research interest. In this work, the structural properties of P3HT: PCBM thin films were studied by XRD. In addition, annealing effects on the optical properties of these thin films by using UV VIS radiation have been studied.

2. EXPERIMENT

For this study, P3HT and PCBM were purchased from Sigma Aldrich and used without further purification. The glass substrates were cleaned with detergent, deionized water, acetone and further with sonification process. P3HT solution was prepared by dissolving the 5mg of sample in 0.25ml of chlorobenzene. A solution for the blend, P3HT: PCBM (1:0.8) was prepared by dissolving the required amount of the material in chlorobenzene. P3HT and P3HT: PCBM thin films were prepared by spin coating the respective solutions onto the cleaned glass substrates. The spin coater was operated at 1000rpm for 60s. After coating, all these thin films were dried in an oven. To study the annealing effects, P3HT and P3HT: PCBM thin films were vacuum annealed at different temperatures ranging from 80^0C to 120^0C in a vacuum 2x10-6Torr. The structures of P3HT and PCBM are as shown in Fig 1.

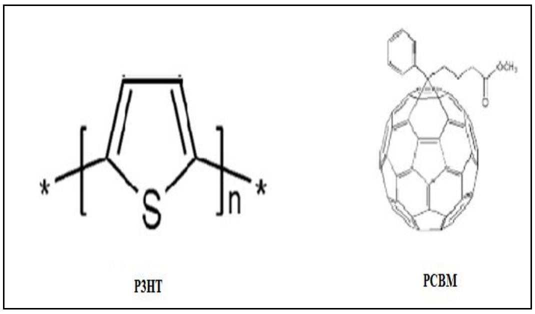

Fig 1: Structure of P3HT and PCBM

3. RESULTS AND DISCUSSIONS

3.1 Structural Studies

X ray diffraction studies were done to study the structure of the deposited of annealed and non-annealed thin films and are as shown in Fig 2.

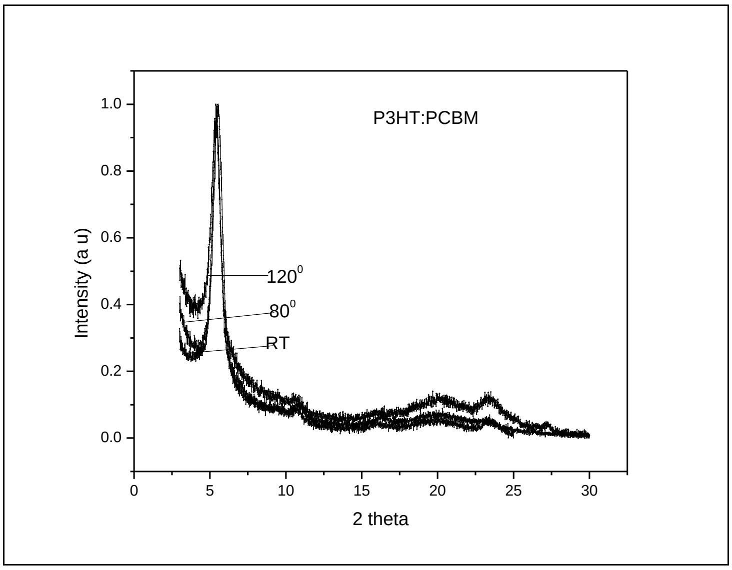

Fig 2: XRD Pattern of P3HT PCBM Thin Films.

Peaks corresponding to P3HT and PCBM were obtained for the films by X-ray diffraction technique. Miller indices of the corresponding peaks were indexed and parameters like diffraction angle 2θ and interplanar distance were calculated as tabulated in table 1.

2θ(degrees)	80^0C	100^0C	120^0C
P3HT	5.53	5.45	5.39
PCBM	9.44	9.42	9.36
Inter planar distance (Å)			
P3HT	15.95	16.20	16.38
PCBM	9.35	9.37	9.43

Table 1: XRD Parameters of P3HT, PCBM Thin Films.

The value of d (the interplanar spacing between the atoms) was calculated using Bragg's Law, $2d\sin\theta = n\lambda$ and hence inter planar spacing, $d=\lambda/2\sin\theta$ for (n=1) and wavelength λ = 1.5418 Å. In P3HT, as the annealing temperature is increased, the peak is more pronounced indicating more crystalline nature of the material. The values of diffraction angle 2θ decreased from 5.53^0 to 5.39^0 and the interplanar distance increased from 15.95 Å to 16.38 Å as the annealing temperature is increased. Increased interplanar spacing indicates that the material is more orderly in nature. Similar behavior was observed in PCBM, as the annealing temperature increased from 30 to 120 degree, the interplanar distance increased from 9.35 Å to 9.43 Å and the angle varied from 9.44^0 to 9.36^0.

3.2. Optical Studies

The absorption characteristics of the films were studied in the wavelength region 300-700 nm. Fig 3, shows the absorption spectra of P3HT thin films before and after annealing.

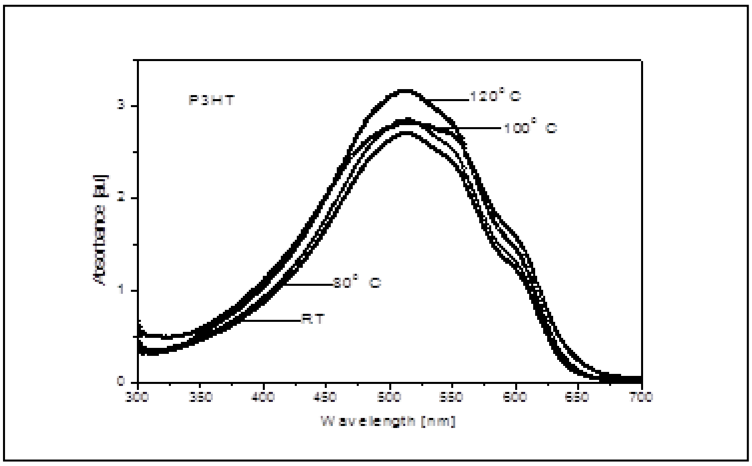

Fig 3: UV-Vis Absorption Curves of P3HT Before and After Annealing.

P3HT has characteristic absorption peak at around 516nm which is in accordance with the literature. The characteristic absorption band of P3HT is due to the Π- Π* transition of the P3HT backbone [5]. For the P3HT film, slight increase in the absorption band was observed with annealing. The increase in the absorption strength after annealing can be attributed to increased packing of the P3HT domains.

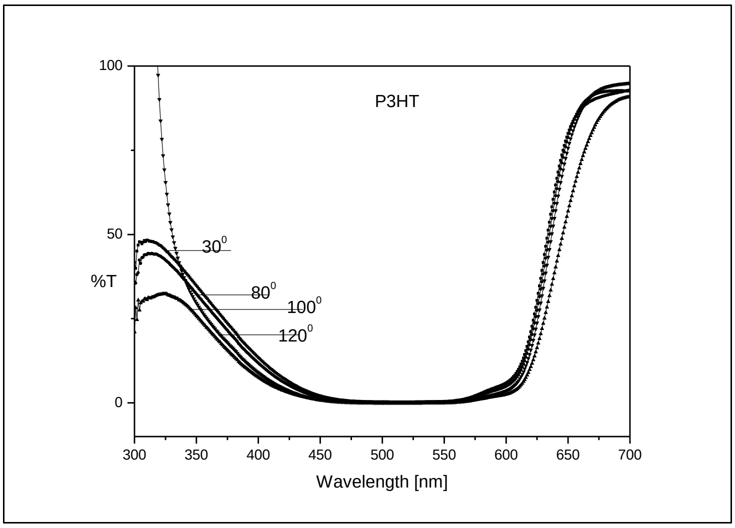

Fig 4: Transmission Curves of P3HT after Annealing at Different Temperatures.

Fig 4, shows the transmission spectra of P3HT thin film. Change in %T was observed due to annealing. Change in band gap due to annealing was observed as shown in table 2. Band gap was found to be minimum at an annealing temperature of 100^0C.

P_3HT	RT	80^0	100^0	120^0
$\%T_{max}$	91	93	90	95
Bandgap (eV)	2.17	2.15	2.10	2.13

Table 2: Optical Parameters of P3HT Annealed Thin Films.

The optical absorption spectra of P3HT: PCBM composite films are represented in Fig 5. The absorption spectrum is combination of two spectra, one of P3HT and the other of PCBM. With annealing, the absorption spectra had changed considerably. It was found that the absorbance of the film increased with thermal annealing. The intensity of the absorption peak increased with increase in the annealing temperature till 120^0C. The annealing enhances the crystallinity due to the diffusion of PCBM molecules into P3HT leading to more π-π^* absorption. Photons can penetrate deeper into the active layer where more P3HT: PCBM interfaces are available for efficient exciton dissociation. Above the glass transition temperature of P3HT, the chains of the polymer become soft and form an interpenetrating network of P3HT and PCBM [13, 14]. These results suggest that different P3HT domains are formed during annealing which results in structural rearrangement between the two components. Annealing could be an efficient method to tune the optical properties of P3HT: PCBM blend, which inturn can be used in optimizing the device performance where these materials are used as active layers.

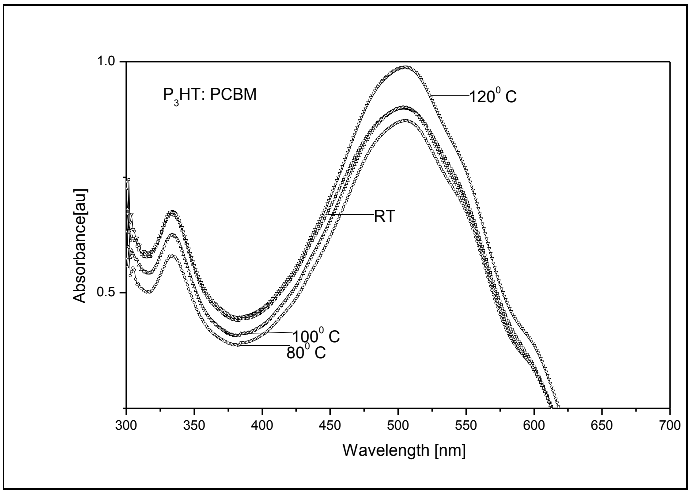

Fig 5: UV-V is Absorption Curves of P3HT: PCBM after Annealing at Different Temperatures.

The improvement of the device performance can be attributed as follows as per previous report [15], upon annealing PCBM diffuses into the polymer matrix in the composite films, which results in the increase in the carrier mobility in the active layer. Another study considered an enhanced contact at the interface due of annealing by forming bonds between the active layer and the electrode [16].

4. CONCLUSION

In conclusion, we have studied the optical and structural properties of spin coated annealed and non-annealed P3HT/PCBM films. We have demonstrated that thermal annealing improves the optical properties of P3HT thin films and also P3HT: PCBM thin films. Increase in the annealing temperature increased the absorption. UV-vis spectrum results showed that efficiency can be improved by annealing. With annealing temperature crystalline nature increased and the films xrd showed a sharp peak and change in 2 theta and interplanar distance indicating more orderly nature of the material. Annealing temperature can be used to optimize the absorption and charge separation of P3HT: PCBM heterojunction to be used in organic photovoltaics.

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