Solvent Effect on the Formation of Photoactive Thin Films for the Polymeric Solar Cells

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Abstract. This work investigates the influence of the solvent used on the morphology of polymer photoactive layer for solar cells. The photoactive layer consists a mixture of poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl-C61-butyric acid methyl ester (PCBM), to produce P3HT:PCBM (1:1 ratio) blend thin films, deposited by spin-coating technique of the materials solution. Two types of the solvents used namely; 100% dichlorobenzene (DCB) and 50%:50% cosolvent of DCB and chloroform. The morphological characterizations of P3HT:PCBM blend thin films have been carried out by UV-Visible absorption spectroscopy, X-ray diffraction (XRD) spectroscopy, and Atomic Force Microscopy (AFM). The results reveal that the mixtures of solvent give a better solubility than the pure single solvent. And thus, the choice of solvent used during the fabrication process can significantly affect the optical and morphological properties of the films.

Keywords: organic solar cell, photovoltaic, P3HT, PCBM, solvent effect.
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INTRODUCTION

Nowadays, the research for a renewable energy has been tremendously increases as the crisis of conventional energy is deteriorated. Various natural sources can be exploited and harvested to generate energy. Converting solar energy into electrical energy is one of such utilization of the natural sources. Silicon-based solar energy converter has been leading the solar cells technology for the past few decades. However, the high production cost and onerously fabrication process of silicon wafers made researcher to venture for easier process able nature and low-cost polymer materials. The researches in the polymeric based solar cells that have been carried out for the past decade shown promising results, but the power conversion efficiency (PCE) is still low for it to be fully commercialize [1-5].

Many approaches have been taken to improve the efficiencies of the polymeric-based solar cell. By thermal annealing process, the morphology and optical properties of the device can be improved [1,2]. In this study, we examine the effect of solvent used during fabrication of the pristine and thermal treatment process on P3HT:PCBM blend film. We investigate the optical, structural and morphological properties of the blend thin film as a function of the solvent used for the film preparation. If the polymer materials used to form thin film solar cells are dissolved in a solvent with

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high-volatility temperature, phase separation occurs during the solvent evaporation process. Thus, the interface area increases, leading to an enhancement of exciton dissociation [6-8]. Furthermore, the solvent evaporation rate has a significant effect on the surface morphology of polymer films [9].

EXPERIMENTAL METHOD

The photoactive layer consist a mixture of regioregular poly(3-hexylthiophene) (P3HT), purchased from Sigma-Aldrich and [6,6]-phenyl-C61-butyric acid methyl ester (PCBM), purchased from American Dye Source, Inc. The chemical structures of P3HT and PCBM molecules are shown in Figure 1. The solution of P3HT:PCBM was prepared by mixing both materials and dissolved in two types of solvent; (1) 100% 1,2-dichlorobenzene (denoted as DCB) and (2) cosolvent consist 50% chloroform and 50% 1,2-dichlorobenzene (denoted as DCB:CH) and stirred for 24 hour to maximize mixing. The concentration of P3HT:PCBM was set to 60mg/ml with 1:1 weight ratio.

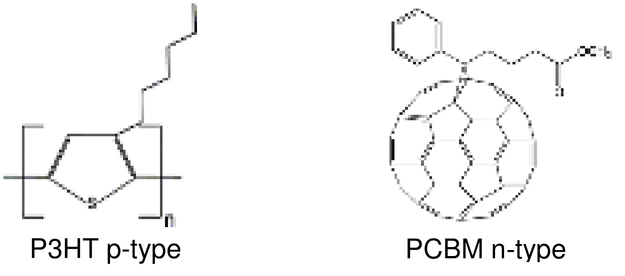


FIGURE 1. (a) The chemical structures of P3HT and PCBM molecules.

The photoactive layers were prepared using two different methods. Firstly, the pristine sample was prepared by spin-coated the mixed P3HT:PCBM solution onto the substrate using at 1500rpm for 60s, and no other further treatment was applied to the sample. The second sample was prepared similar to the first sample, but further thermal treatment was used by quickly annealed the sample after deposition. For thermal treatment process, the sample is thermally treated inside an oven for 10 min at 150ºC and then cooled slowly to room temperature. This second sample is labeled as thermal treated sample.

Absorption spectra measurements were carried out using Jasco V-570 UV/VIS/NIR spectrophotometer. A Siemens D5000 X-ray diffractometer was used to record the X-ray diffraction (XRD) patterns. The surface morphology was visualized via a Veeco D300 Atomic force microscope.

RESULTS AND DISCUSSION

The effect of the solvent used on the photoactive layer is shown in Figure 2. It can be clearly seen that the absorption of blend film prepared from DCB:CH cosolvent is higher compared to that of pure DCB. Besides, the absorption peak is red shifted for the film prepared in the cosolvent compared to that of pure DCB which is due to the increase in conjugation length of the polymer chains. The formation of the photoactive film by using DCB:CH cosolvent is strongly influenced by the solubility of the blend component of P3HT:PCBM. The mixture of solvent of DCB and CH produces better solubility of the blend component than the single solvent of DCB. Results in Figure 2 also reveal that thermal annealing process influences the absorption. The absorption of the thermal treated sample is higher than the untreated sample. The ordering of the P3HT phase in the sample is improved by applying heat to the sample. This effect is visible at the wavelength range between 400nm to 650nm. This optical change will improve the efficiency of the solar cell (will be published elsewhere).

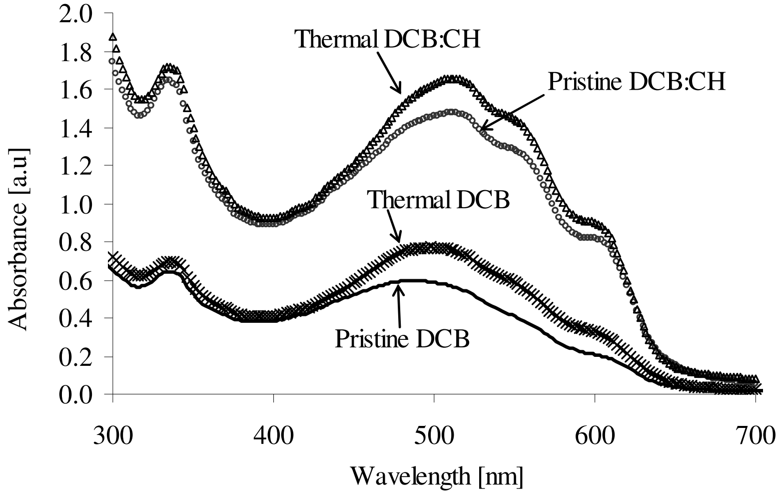


Figure 2: UV-vis absorption spectra of P3HT:PCBM blend film.

Figure 3 shows the XRD spectra of P3HT:PCBM blend films of DCB:CH cosolvent and pure DCB. The XRD peak at approximately 2θ of 5.4° appears in the diffractogram attributed to the partial crystallinity of the P3HT crystallites which are dispersed in amorphous PCBM matrix. The results of XRD are in agreement with the absorption spectra; the crystallinity and the ordering of the polymer can be improved using DCB:CH cosolvent rather than using single DCB solvent.

Figure 4(a) and 4(b) show the atomic force microscopy (AFM) images of two dimensional (2D) as well as three dimensional (3D) for P3HT:PCBM blend films made using DCB solvent and DCB:CH cosolvent respectively. The root-mean-square (rms) roughnesses of these layers were 12.623 nm and 14.2777 nm respectively.

Highest rms roughness is a signature of self-segregation [3]. In other words, the film prepared from cosolvent produced a better interpenetrating polymer chains.

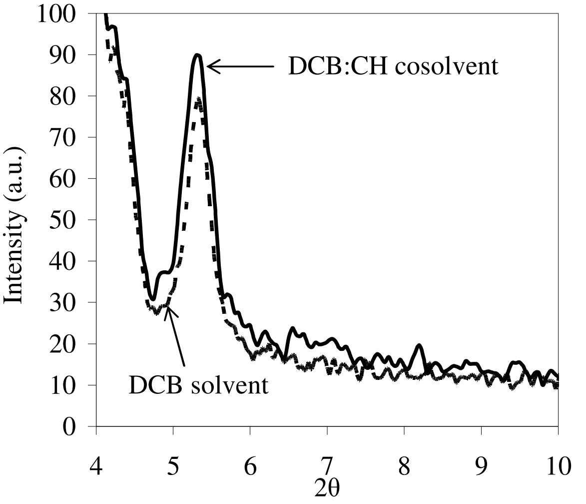
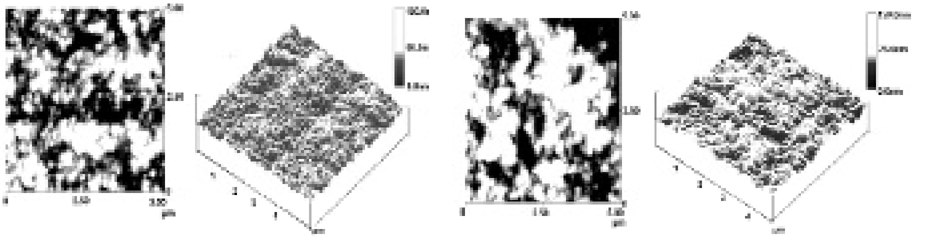


Figure 3: X-ray Diffraction of P3HT:PCBM blend film.



(a) (b)

Figure 4: 2D and 3D atomic force microscopy images of (a) DCB solvent, (b) DCB:CH cosolvent

CONCLUSION

The choice of the solvent used during fabrication affects the morphology of the film. Mixtures of solvent give a better solubility than single solvent. Moreover, the study shows that the morphology and optical properties of P3HT:PCBM blend film are improved by thermal annealing. We also noted that the optical density of the P3HT:PCBM thin film is strongly influenced by the solubility of the blend components.

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