

Structural study of P3HT and P3HT:PCBM thin films by synchrotron X-ray diffraction

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Introduction

The significant progress in the development on the polymeric photovoltaic cells has been made in this decade, and the energy conversion efficiency of polymer-based bulk-heterojunction cell, which is composed of a mixture of polyhexylthiophene (P3HT) and 6,6-Phenyl-C₆₁ butyric acid methyl ester (PCBM), got over 5%. However, the structural properties of the P3HT:PCBM mixture film, which strongly affect the performance of the photovoltaic cells, have not been clearly understood yet because the structure of the inside of the film is much complicated. In this work, we report on the structural characterization of the pristine P3HT film and P3HT:PCBM mixture film by using the synchrotron X-ray diffraction (XRD) techniques.

Experiment

P3HT and P3HT:PCBM blending solutions (P3HT:PCBM = 1:0:7 by weight ratio) were prepared by dissolving the compounds in chlorobenzene. Subsequently, these solutions were spin-coated onto the glass substrates. The film thicknesses of the active layers were approximately 100 nm. The synchrotron XRD measurements ($\lambda=0.154$ nm) were carried out at the beam line 4C in KEK photon factory.

Results and discussion

Figure 1 shows the out-of-plane XRD profile (θ - 2θ mode) of (a) P3HT and (b) P3HT:PCBM. We observed the P3HT (100) and (200) diffraction peaks corresponding to the spacing of the main chain layers of 1.64 nm for both P3HT and P3HT:PCBM films, while we did not find noticeable difference between the XRD profiles of these samples even though these samples were annealed. These results suggest that the crystallization between the main chains of P3HT occurred smoothly nevertheless PCBM was blended in P3HT.

Figure 2 shows the in-plane XRD profile (ϕ - $2\theta_{\chi}$ mode) of (a) P3HT and (b) P3HT:PCBM. A large difference between the profiles of P3HT and P3HT:PCBM was observed. For the pristine P3HT film, we observed the P3HT (010) peak caused by π - π stacking of the thiophene rings in both profiles of as-deposited and annealed samples. For the P3HT:PCBM mixed film, there was no P3HT(010) peak in the profile of as-deposited sample, while this peak was

gradually appeared with increasing the annealing temperature. These results suggest that P3HT was prevented from forming the π - π stacking structure when PCBM was blended in P3HT, although such stacked structures were formed after annealing due to the mass transport of P3HT, which is caused by its glass transition [1]. It is well known that π - π stacking of the thiophene rings is important for the carrier transport, further, the anneal treatment of the P3HT:PCBM cell is required for improving its efficiency [1]. Therefore, the formation of the π - π stacking structure of P3HT may induce the improvement of the electrical properties in P3HT:PCBM photovoltaic cells.

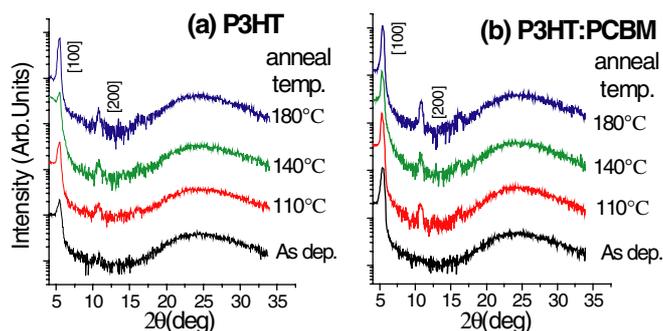


Fig.1 Out-of-plane XRD profile of (a) P3HT and (b) P3HT:PCBM.

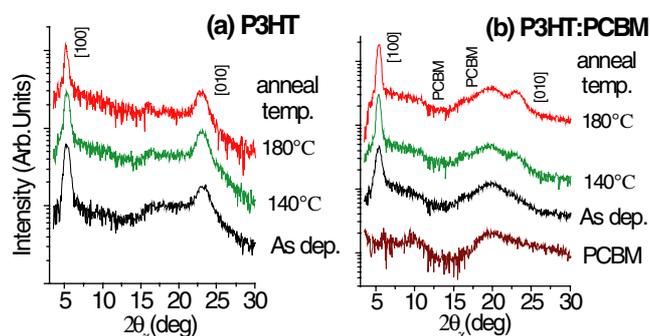


Fig.2 In-plane XRD profile of (a) P3HT and (b) P3HT:PCBM

References

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