Correlation between Nanostructures and Efficiency in Polymer Solar Cell

The present work systematically and thoroughly describes the characterization of a bulk heterojunction polymer solar cell, consisting of thin films of a conducting polymer/fullerence derivative blend, using by grazing incidence small-angle and wide-angle X-ray scattering techniques. The quantitative nanostructural parameters of the polymer solar cell, including (1) the mean radius of aggregated fullerence clusters, (2) the specific surface area, (3) the local connection between fullerence clusters and (4) the correlation length of network formed by fullerence molecules, were determined to be well correlated to the device's performance. The detailed interpretation considerably extends the current knowledge and provides a guide for achieving high efficiency of the polymer solar cell.

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Bulk heterojunction (BHJ) polymer solar cell based on poly (3-hexylthiophere)/[6,6]-phenyl-C61-butyric acid methylester (P3HT/PCBM) has attracted a great deal of attention over last decade.[1, 2] The improvement in device performance of this system critically depends on the three-dimensional self-organized nanostructure of the active layer (morphology of BHJ film). The usual microscopy tools such as transmission electron microscopy or atomic force microscopy applied for characterizing the morphology of P3HT/PCBM thin film only provide the local observation and have the limitations in sampling and sample preparation. Compared to the conventional microscopic tools, grazing-incidence small-angle and wide-angle X-ray scattering (GISAXS and GIWAXS) technique are powerful tools to characterize the full structures at different scales for a bulk sample.[3, 4] In the present study, we employed the improved GISAXS analysis to thoroughly resolve the self-assembly nanostructure of BHJ film. The combined measurement of GISAXS and grazing-incidence X-ray diffraction (GIXRD) was used to concurrently study (1) the spatially aggregated structure and molecular dispersion of PCBM phase and (2) dimensions of P3HT crystallites oriented along the vertical direction of the film.

The obtained GISAXS profiles agree with the observation of the other GISAXS study.[5] However, there is a slight upturn of the intensity in the low-Q region (0.005 Å^{-1} ~ 0.02 Å^{-1}) for the pristine P3HT film, which was rarely mentioned. Apparently, relative to the well-known structures of PCBM clusters and P3HT crystallites, there exists a larger scale of structures consisting of (1) the P3HT crystallites, (2) amorphous P3HT region, and (3) the PCBM molecules dispersed or intercalated within P3HT molecular chains. An improved model of combining Debye-Anderson-Brumberger equation (DAB model) and polydispersed spheres having Schultz size distribution were used to describe nanostructure of bulk heterojunction. According to the fitting results, the 3D self-organized structure of a P3HT/PCBM film (annealed at 150 °C

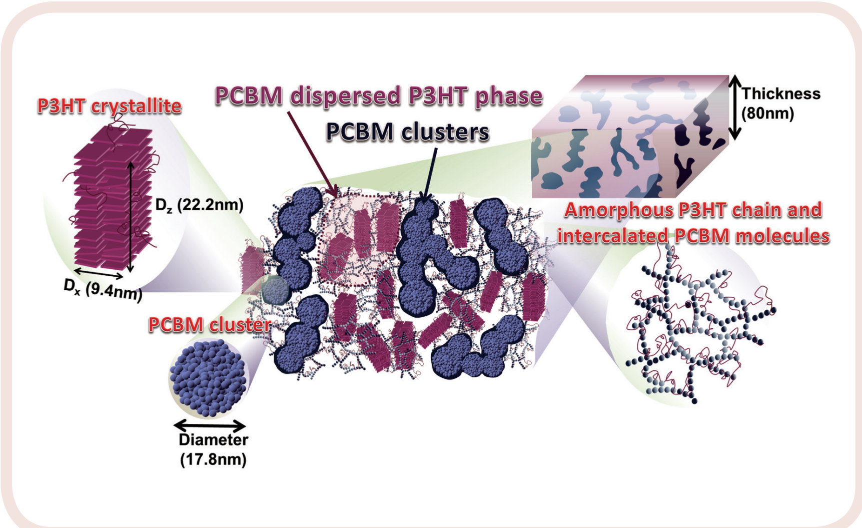

Fig. 1: Schematic of the 3D phase-separated structure of a P3HT/PCBM film comprising PCBM-dispersed P3HT phase (including the P3HT crystallites, the amorphous P3HT chain region and the network of intercalated PCBM molecules) and PCBM clusters shown with different length scales (from upper left to lower left clockwise).

for 15 min and cooled down to room temperature and annealed at 150 °C for 5 min) comprising the PCBM clusters and PCBM-dispersed P3HT phase (including the P3HT crystallites, the amorphous P3HT chain region and the network of intercalated PCBM molecules with different length scales) is illustrated in Fig. 1. The established quantitative indexes (1) the size of PCBM cluster, (2) the specific interface area between PCBM and P3HT phases, *Sv* and (3) the index of quantitatively measuring the agglomeration formed by the partial attachment of some neighboring PCBM clusters into a continuous pathway can be served as a guide to evaluate the device performance and rationally design of annealing conditions. The roles of these structural characteristics in improving the power conversion efficiency are identified. The structural parameters and indexes can be quantitatively evaluated and well correlated to the device performance.

Beamline 23A1
SWAXS end station

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