

Structure and Device Performance in Bulk Heterojunction Polymer Solar Cells

This report features the works of Wei-Fang Su, Cheng-Si Tsao, and their co-workers published in *ACS Nano* **6**, 1657 (2012) and *J. Phys. Chem. C* **116**, 10238 (2012).

Bulk heterojunction (BHJ) polymer solar cells feature a great promise as mechanically flexible devices for energy conversion, in addition to light weight and fabrica-

tion less expensive than of silicon-based solar cells. In solar cells of this type, the electron donor and acceptor are mixed together, forming a thin film of conjugated

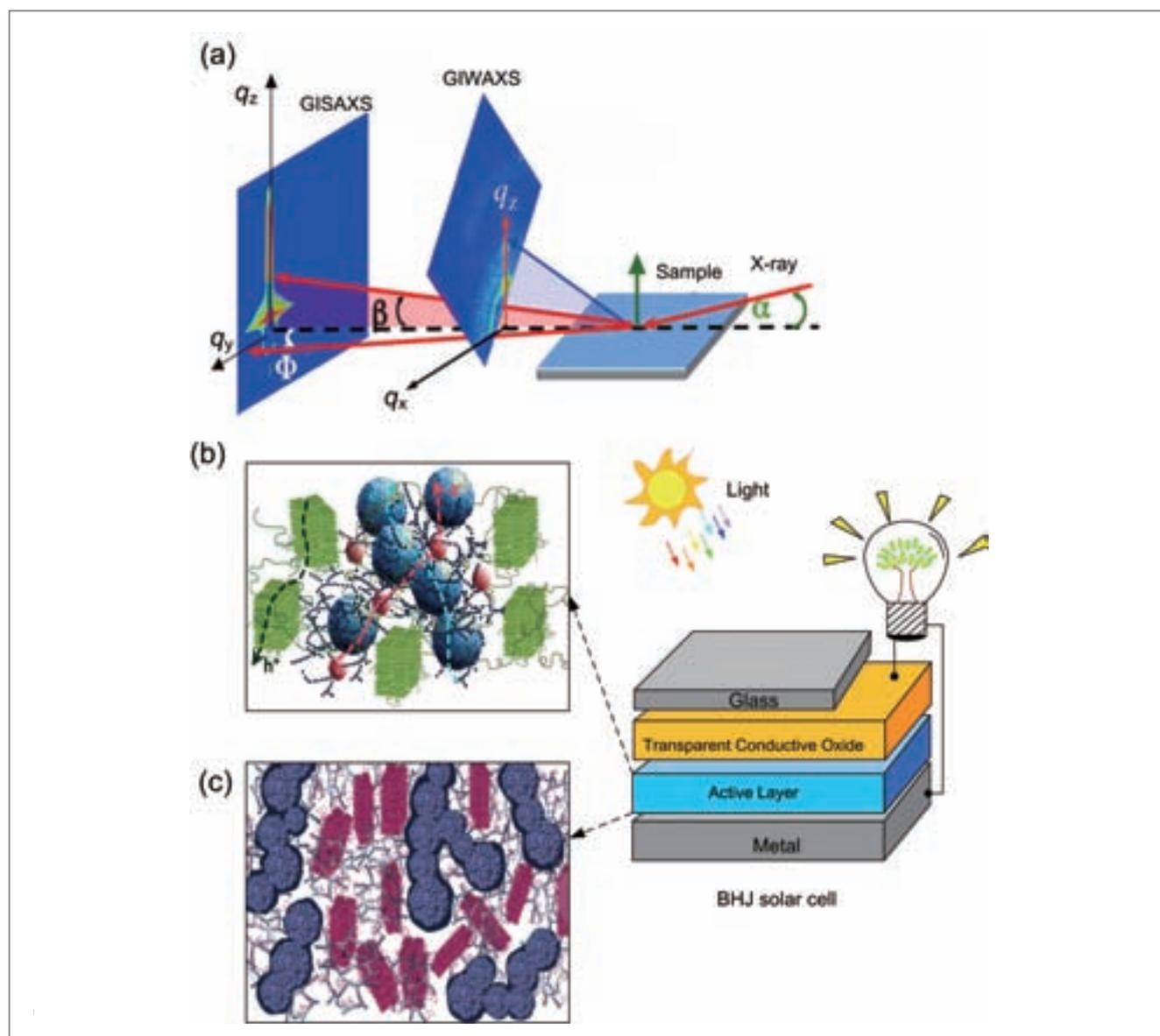


Fig. 1: (a) Schematic setup for synchronized GISAXS/GIWAXS, with incident angle α of the beam and scattering angles β and Φ in the out-of-plane (q_z) and in-plane directions (q_x); (b) structure of the active layer in a P3HT/PCBM/Cu₂S INP hybrid film, in which the nanoparticle-tuned nanostructure provides a much more effective transport path through the conventional interconnected PCBM clusters or INP-containing network in the PCBM/P3HT amorphous domain coupled with interconnected PCBM clusters; and (c) structure of an active layer in P3HT/PCBM domains in a P3HT/PCBM film. Figures (b) and (c) are adapted from Ref. 1 and 2, respectively.

polymer/fullerene derivative blend. The device performance of these BHJ solar cells depends strongly on the morphology of the active layer of the BHJ thin films, which is formed by separation of the nanodomains of the conjugated polymer and fullerene phases. In general, an ideal morphology for the BHJ thin films features phase-separated nanodomains of size ca. 10 nm, corresponding to an exciton diffusion length, to assist the dissociation of the exciton and charge transport in organic electronic materials. Understanding the kinetics of fullerene aggregation and polymer crystallization and their correlation in the morphological development of conjugated polymer/fullerene composite films would hence provide notions about the optimal processing of future BHJ solar cells with varied components of fullerene derivatives or other conjugated polymers. The commonly used tool X-ray diffraction reveals limited structural information about fullerene aggregates, because the proposed fullerene aggregate size for optimized BHJ thin-film solar cells scatters in a wide range 5 - 60 nm. Simultaneous two-dimensional grazing-incidence small-angle and wide-angle X-ray scattering (GISAXS and GIWAXS) at beamline **BL23A1** of NSRRC provides a scattering angle over a wide range ($q = 0.3\sim 10\text{ nm}^{-1}$) to capture the kinetics of fullerene aggregation and conjugated polymer crystallization in the corresponding BHJ thin films (Fig. 1(a)).

Prof. Wei-Fang Su (National Taiwan University, Taiwan) and Dr. Cheng-Si Tsao (Institute of Nuclear Energy Research, Taiwan) cooperatively studied the BHJ polymer solar cell, consisting of poly(3-hexylthiophene)/[6,6]-phenyl-C₆₁-butanoic acid methyl ester, P3HT/PCBM. They focused on the effects of various PC_xBM-type (PC₆₀BM and PC₇₀BM)¹ and inorganic nanoparticles (INP)² on various morphological structures, and the efficiency of power conversion (PCE) in the BHJ P3HT/PCBM solar cells. The detailed morphologies of the spatially aggregated PCBM phase and the organization of P3HT-related phases in the P3HT/PCBM derivative and P3HT/PCBM/INP hybrid film were quantitatively characterized with simultaneous GISAXS and GIWAXS techniques. The structural characteristics correlate well with the device performance and the photovoltaic properties.

In a P3HT/PCBM/INP hybrid system,¹ these authors found that significant PCE improvements 55 % (from 1.1 to 1.7 %) for the sample as cast and 23 % (from 3.5 to 4.3 %) for the thermally annealed sample were obtained because the network of the dispersed INP, forming an additional interpenetrating network, provides a more efficient path for the transport of charge carriers, and thus significantly enhances the PCE value and photovoltaic properties (Fig. 1(b)). This approach is demonstrated to be an effective method that is beneficial for the design and fabrication of highly efficient BHJ solar cells.

In the P3HT/PC_xBM derivative system,² the GISAXS/GIWAXS results revealed nanostructures of two types observed in the BHJ thin films: (1) intercalated PC_xBM molecules around the boundary of the P3HT crystalline domain and within the amorphous domain, and (2) aggregated PC_xBM clusters in PC_xBM domains. The lamellar spacing of P3HT crystalline domains in P3HT/PC₇₀BM, larger than for P3HT/PC₆₀BM, indicated that greater interfacial areas are generated between PC₇₀BM and P3HT on a molecular scale for increased efficiency of charge separation (Fig. 1(c)). The size, volume fraction, partial attachment, and spatial distribution of PC₆₀BM clusters are, however, larger than those properties of PC₇₀BM clusters, exhibiting more efficient electron transport in P3HT/PC₆₀BM. A correlation is observed between nanostructures and PCE (3.25 % and 2.64 %, respectively, for P3HT/PC₇₀BM and P3HT/PC₆₀BM). These authors proposed that the structure of fullerene intercalated with P3HT, rather than the size of the fullerene cluster, plays a major role in the PCE performance of a BHJ solar cell without thermal annealing.

References

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