

Mechanism and control of structural evolution of polymer solar cell from bulk heterojunction to thermally unstable hierarchical structure

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Supporting Information

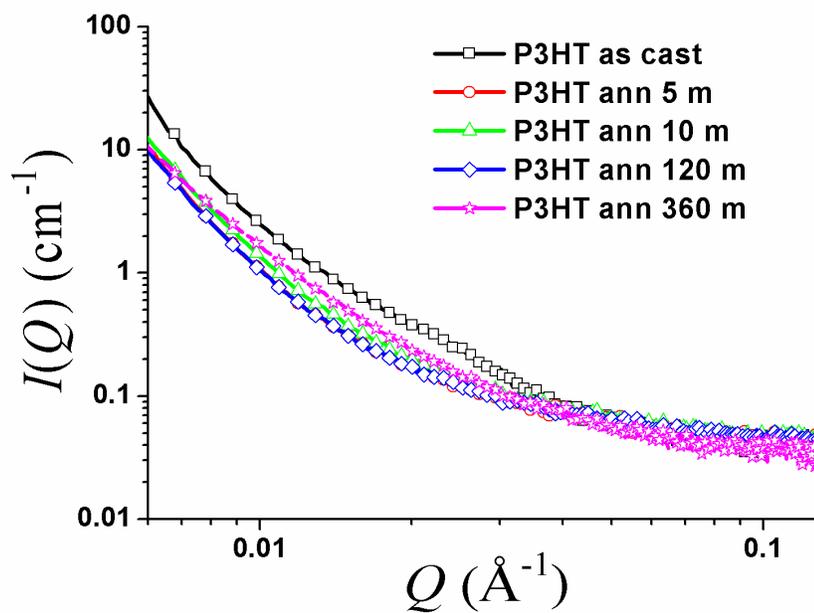


Figure S1. GISAXS profiles of pristine P3HT films annealed at 150 °C for 0, 5, 10, 120 and 360 min.

Using the parameters obtained from the in-plane GISAXS analysis (shown in Table 1) of the P3HT/PCBM blend film annealed at 150 °C for 360 min as the grazing-incidence scattering geometry (considering the hard-sphere structure factor and spherical form factor for the PCBM clusters), we performed the simulation for 2D GISAXS pattern, using the FitGISAXS simulation package (D. Babonneau *et al.*, *J. Appl. Cryst.* (2010), 43, 929–936; U. Jeng, C. H. Su, C.-J. Su, K.-F. Liao, W.-T. Chuang, Y.-H. Lai, J.-W. Chang, Y.-J. Chen, *et al.*, *J. Appl. Cryst.*, **2010**, 43, 110-121.).

As shown below, the 2D simulation resembles that measured with 2D area detector for a same set of data. Moreover, the in-plane GISAXS profile taken from the simulated 2D pattern can also fit the data well. The 2D simulation result supports the conventional GISAXS analysis used.

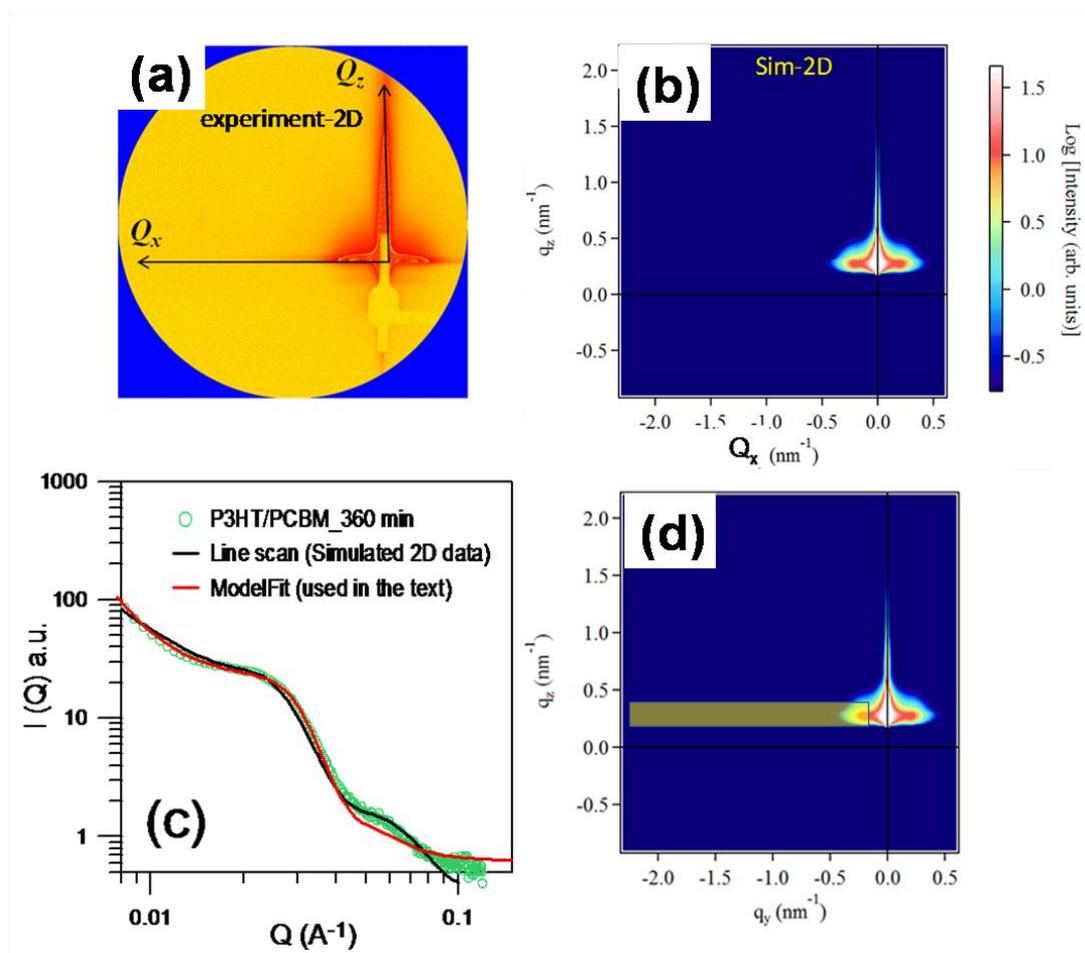


Figure S2.1 Measured 2D GISAXS pattern for the P3HT/PCBM blend film annealed for 360 min (a) (data are also shown in Fig 1 (e)) is compared to a simulated 2D pattern (b) using the parameter obtained from the GISAXS line profiles analysis (Table 1). Compared in (c) are the GISAXS in-plane profiles extracted from the measured and simulated 2D patterns as that marked in (d).

We assume that the several PCBM clusters (mean radius = 7 nm) aggregate into a larger domain with a fractal-like structure (as shown in the below). The details of fitting model (fractal aggregation comprised of the polydispersed PCBM clusters as the primary particles) are shown in the literature (Teixeira, J. J. Appl. Cryst. 1988, 21, 781-785). The correlation length of fractal domain is 194 nm. This model cannot give the best fit to the data compared to the model used in the text. Nevertheless, it is the most appropriate model which gives the good fitting among the other possible models.

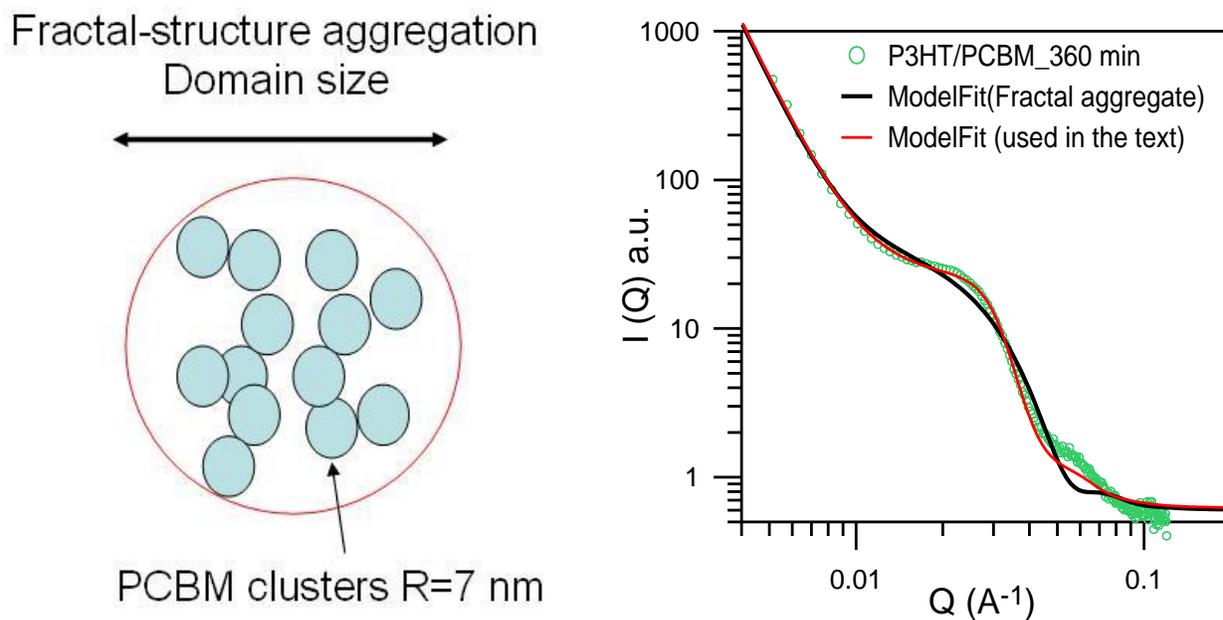


Figure S2.2 GISAXS profile of the P3HT/PCBM film annealed for 360 min in comparison with the model fitting of fractal aggregation.

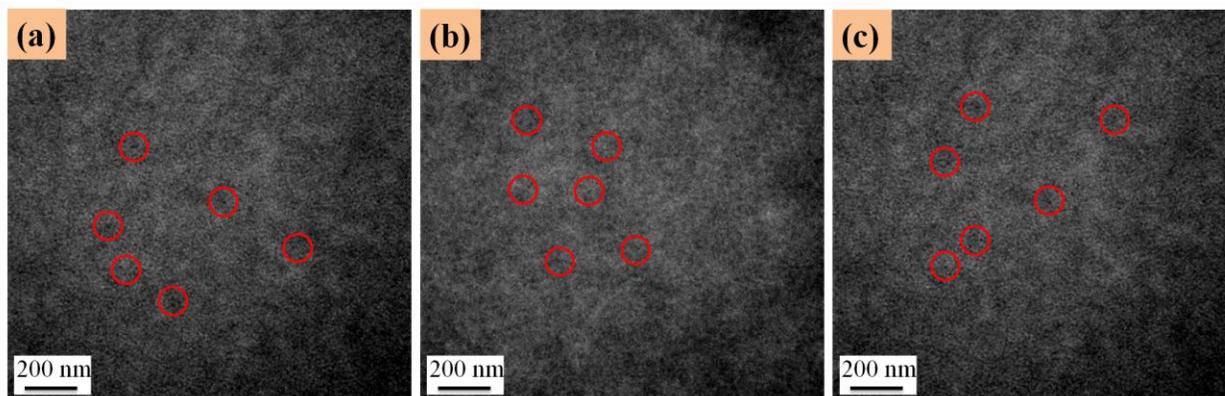


Figure S3. TEM image of the P3HT/PCBM:8%bis-PCBM film annealed at 150 °C for (a) 10, (b) 120 and (c) 360 min shows the nanoscale fullerene cluster.