

# Gelation Mechanism and Hierarchical Structure of P3HT/PCBM in Xylene Solution

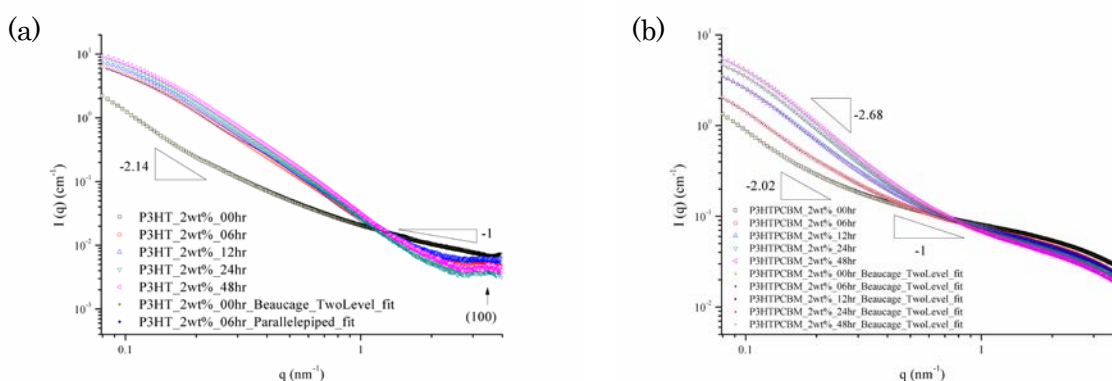
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Poly(3-hexylthiophene) (P3HT) is one of the most widely used electron donor materials in polymer solar cells. The structure of the polymer formed in the solution may have a drastic impact on the morphology of the subsequently cast film; therefore, investigating the solution structure of conjugated polymers is of great importance for optimizing the performance of the optoelectronic devices. It has been shown that the solutions of P3HT with relatively poor solvents undergo gelation upon prolonged aging at room temperature or under subambient condition. Here we investigate the mechanism of such a gelation process for P3HT/xylene solution and also for the solutions of xylene with P3HT and [6,6]-phenyl-C61-butyric acidmethyl ester (PCBM). A macrophase separation generating P3HT-enriched phase and solvent-rich phase of  $\mu\text{m}$  in length scale occurred during the aging. The phase separation took place via the nucleation and growth (NG) mechanism and was followed by the formation of nanowhiskers in the P3HT-enriched domain.<sup>1</sup> The jamming of the P3HT-enriched macrodomains which were mechanically stabilized by the networking of the nanowhiskers led to the gel property of the system. Here we investigate the mechanism of such a gelation process for P3HT/xylene solution and also for the solutions of xylene with P3HT and PCBM (a common acceptor material for polymer solar cell) by means of time-resolved SAXS conducted at beamline BL23A1 in NSRRC.



**Figure 1** Time-resolved SAXS profile of the P3HT and P3HT/PCBM in xylene solution for monitoring the developments of nanowhiskers and crystallinity of P3HT during the room-temperature aging: (a) P3HT (b) P3HT/PCBM

[1] Chen, C. Y.; Chan, S. H.; Li, J. Y.; Wu, K. H.; Chen, H. L.; Chen, J. H.; Huang, W. Y.; Chen, S. A. *Macromolecules* 2010, 43, 7305–7311