

Study of Surface Modification of TiO₂ Nanorods in Poly(3-hexylthiophene)/TiO₂ Hybrid System

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X-ray was used to investigate the crystallinity of poly(3-hexylthiophene) in the P3HT/TiO₂ hybrid films. The procedures for XRD sample preparation were as follows: P3HT/IM/TiO₂ (the IMs were: pyridine, Cudye, oligomer 3HT-COOH) hybrid solution (chlorobenzene was chosen as the solvent) was dropped on the indium tin oxide glass substrates and allowed to dry slowly. The polymer chains in the slowly drying films had abundant time for self-arrangement before the solvent was all evaporated, so the polymer chains in these drop-casted films were highly ordered such that the XRD diffraction peaks can be revealed. Subsequently, the samples were thermal annealed at 140°C for 60 minutes in inert atmosphere to derive more highly-crystallized films. The thickness of all films was controlled with care to be the same (all about 4.1 μm as measured by alpha stepper). The XRD results of P3HT/IM/TiO₂ hybrid films are shown in Fig. 1(a). The diffraction peak at 5.3°, which corresponds to the (100) crystal plane of P3HT, along with the weak diffraction signals at 10.7° ((200) plane of P3HT), 16° ((300) plane of P3HT) and 25.3° ((010) plane of P3HT) can be revealed¹. The small signals at 30.4° and 35.3° were found to be originated from the ITO substrates. From Fig. 2 we can see that the intensity of the prominent (100) diffraction peak for different samples was in an increasing order of P3HT/TiO₂-pyr, P3HT/TiO₂-Cudye and P3HT/TiO₂-(oligomer 3HT-COOH), being higher in IM-contained films. This fact indicates that IM, as the organic molecule existed on the interface of P3HT and TiO₂, can serve as the intermediate to enhance the crystallinity of P3HT, especially when a driving force for ordering of polymer chains is applied. Together with the results of contact angle measurement, it can be inferred that the compatibility between P3HT and TiO₂ after surface modification can be enhanced by showing more similar contact angles and higher crystallinity in the hybrid films.

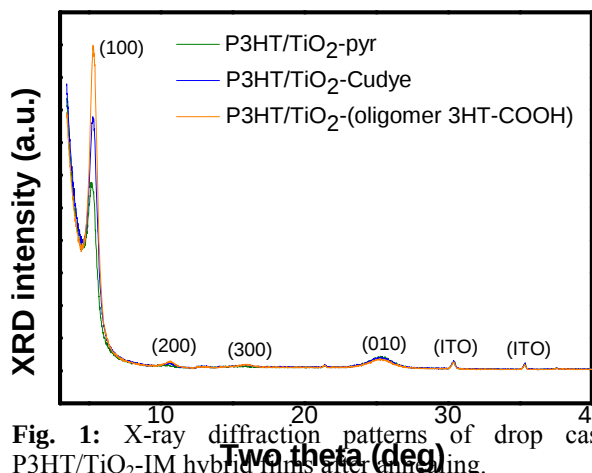


Fig. 1: X-ray diffraction patterns of drop casted P3HT/TiO₂-IM hybrid films after annealing.

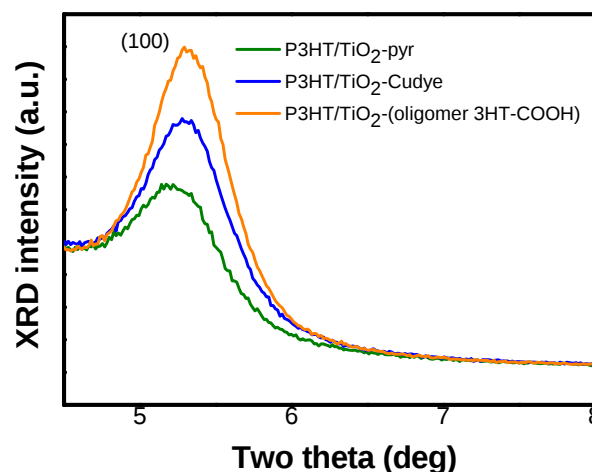


Fig. 2: The (100) peak of P3HT X-ray diffraction patterns.

Reference

- [1] R. J. Kline, M. D. McGehee, E. N. Kadnikova, J. Liu, J. M. J. Fre'chet, and M. F. Toney, *Macromolecule* **38**, No. 8 (2005).