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Molecular orientation in polymer/fullerene blend films studied by NEXAFS

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With the increasing demand for renewable energy, organic photovoltaics have attracted much attention due to the low cost, lightweight and flexibility in recent years. Polymer solar cells based on bulk heterojunction (BHJ) consisting of interpenetrating networks of conjugated polymers as electron donors and fullerene derivatives as electron acceptors, are being developed for their potential application [1]. They provide a large interfacial area where efficient exciton dissociation can occur. The morphology of BHJ plays an important role in obtaining high efficiency organic photovoltaic devices. The order and orientation of the polymer backbone in the bulk heterojunction can influence device properties, such as the exciton diffusion, and charge carrier transport.

In this study, the molecular orientation of polymer/fullerene blend film was examined by near edge X-ray absorption fine structure (NEXAFS) spectroscopy. Poly-{bi(dodecyl)thiophene-thieno[3,4-c]pyrrole-4,6-dione} (PBTTPD) was used as electron donor, and (6,6)-phenyl-C_{61}-butyric acid methyl ester (PCBM) is used as electron acceptor. Figure 1 show the molecular structures of PBTTPD and PCBM. The blend of poly-3-hexylthiophene (P3HT) and PCBM has been used as a model system in BHJ solar cells. Compared with P3HT, PBTTPD is co-polymer which has donor and acceptor in the main chain and the higher power conversion efficiency of PBTTPD blend film is reported [2].

Samples for NEXAFS measurement were spin-coated on the gold coated silicon substrate from each solution. Pure PBTTPD PCBM, and blend of PBTTPD:PCBM (1:1.5 by weight) were dissolved in chloroform. NEXAFS measurements were performed at BL6 of Hiroshima Synchrotron Radiation Center.

Oxygen K-edge NEXAFS spectra were measured for PBTTPD, PCBM and PBTTPD: PCBM blend films. Figure 2 shows the NEXAFS spectra of blend films. Red line shows spectrum of normal incidence and black line shows that of grazing incidence. First strong peak come from $\pi^*_{C=O}$ resonant excitations of both PBTTPD and PCBM. NEXAFS spectrum of blend film was well reproduced by the superposition of PBTTPD and PCBM. From the angular dependence of $\pi^*_{C=O}$ excitation, orientation angle of each molecule was obtained. Both PBTTPD of pure and blend films show "edge-on" orientation, which has the plane of polymer backbone perpendicular to the substrate. The effect of the coexistence of PCBM is considered small for polymer orientation which is important for charge transport process.

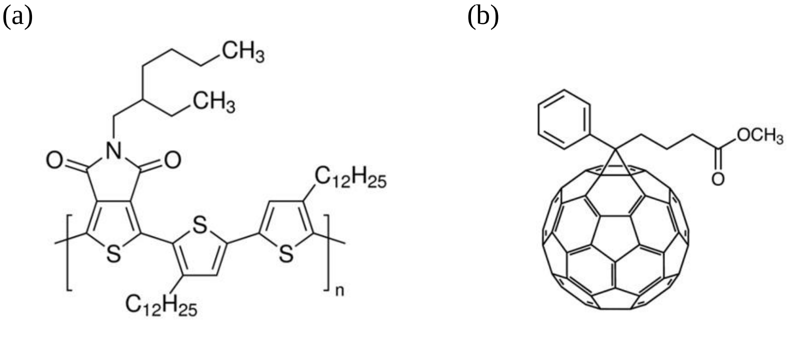

FIGURE 1. Molecular structures of (a) PBTTPD and (b) PCBM.

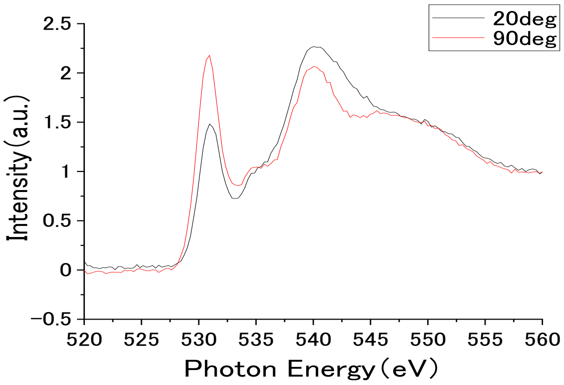

FIGURE 2. Oxygen K-edge NEXAFS spectra of PBTTPD:PCBM blend film measured at different incidence angle.

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