Molecular orientation analysis of C_8-BTBT thin film by X-ray absorption spectroscopy

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An organic molecule 2,7-dioctyl[1]benzothieno[3,2-b]benzothiophene (C8-BTBT) has attracted much attention as an organic semiconductor material with high carrier mobility. Since the molecular orientation can strongly influence on the carrier mobility, it is important to quantitatively determine the molecular orientation of C8-BTBT. X-ray absorption fine structure (XAFS) utilizing linearly polarized synchrotron radiation is a promising tool for such a molecular orientation study. In the previous study, C K-edge XAFS spectra have revealed the surface molecular orientation of the thin films [1]. In order to investigate the entire molecular orientation of C8-BTBT thin films grown under an external temperature gradient [2], S K-edge XAFS spectra have been measured.

XAFS measurements were performed at the BL-13 of SR center, Ritsumeikan University. XAFS spectra were collected by total electron yield through a sample drain current. In order to analyze the molecular orientation of the C8-BTBT thin films, the incidence angle with respect to the substrate normal was varied. Furthermore, in order to see the in-plane anisotropy of the C8-BTBT thin films, the samples were azimuthally rotated around the substrate normal.

Figure 1 shows S K-edge XAFS spectra. The prominent peak around 2473 eV can be seen. For many thiophenic compounds, the π* and σ* transitions overlap and the intensities of σ* transitions are stronger than those of π* transitions [3]. Therefore, the peak around 2473 eV is attributed to the σ* transitions. This peak intensity increases with increasing the incident angle. This result indicates that the C8-BTBT molecules are standing-up on the substrate. From Fig. 2, it was found that C8-BTBT molecules have anisotropy with respect to the temperature gradient direction because the peak intensities respect to the angle between the electric field and temperature gradient direction are different. Thus, the molecular orientation of the C8-BTBT in the bulk has the same tendency as that near the surface.

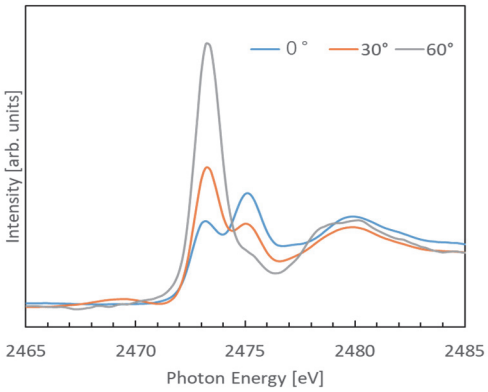

Fig. 1: Polarization-dependent S *K*-edge XAFS spectra of the C_8-BTBT thin film.

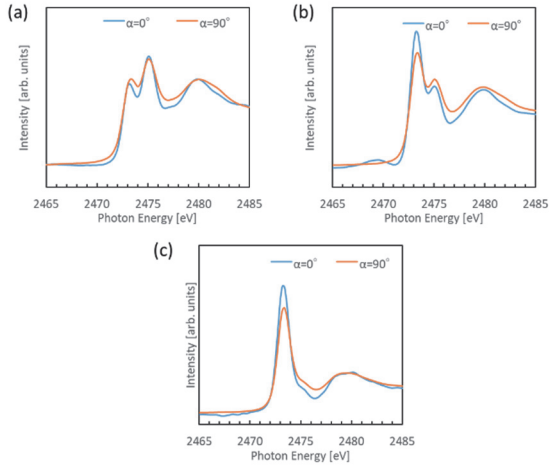

Fig. 2: In-plane polarization-dependent S *K*-edge XAFS spectra of the C_8-BTBT thin film. The incident angle was varied to be 0° (a), 30° (b), and 60° (c). α is the angle between the electric field and the temperature-gradient direction.

Reference

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