

Molecular orientation of a C₈-BTBT thin film grown under an external temperature gradient

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A 2,7-dioctyl [1]benzothieno[3,2-b]benzothiophene (C₈-BTBT) has attracted much attention as a transparent organic semiconductor with high charge carrier mobility. Packing structure of the molecules is considered to be important for the high charge carrier mobility. X-ray absorption fine structure (XAFS) utilizing linearly polarized synchrotron radiation (SR) is a promising tool for such a molecular orientation study. In this study, we have investigated the molecular orientation of C₈-BTBT thin films grown under an external temperature gradient.

We have applied an external temperature gradient during drop-casting to control the direction of solvent evaporation. When a solution containing C₈-BTBT was dropped on a Si substrate bridging two heat stages, evaporation started at the hotter side of the droplet and proceeded toward the colder side. After the solution extended toward the colder region, a thin film was formed in a 7mm-long region. The film thickness varied from 20 nm to 50 nm over the distance of 3 mm.

XAFS measurements were performed at the BL-8 of SR Center at Ritsumeikan University, equipped with a grazing incidence monochromator with a varied-line-spacing plane grating. Carbon *K*-edge XAFS spectra of the samples were measured in partial electron yield by a micro-channel plate detector with retarding grids. The retarding voltage was set to -150 V. The incident angle of SR with respect to the surface normal was varied and the electric vector of SR was changed in either parallel or perpendicular to the growth (temperature gradient) direction.

Figures 1 and 2 show C *K*-edge XAFS spectra of the samples in the parallel and the perpendicular geometries, respectively. These peaks are attributed to the C $1s \rightarrow \pi^*$ transitions. The peak intensities around 286 eV and 288 eV decrease with the incident angle, indicating that the C₈-BTBT molecules are standing-up on the substrate.

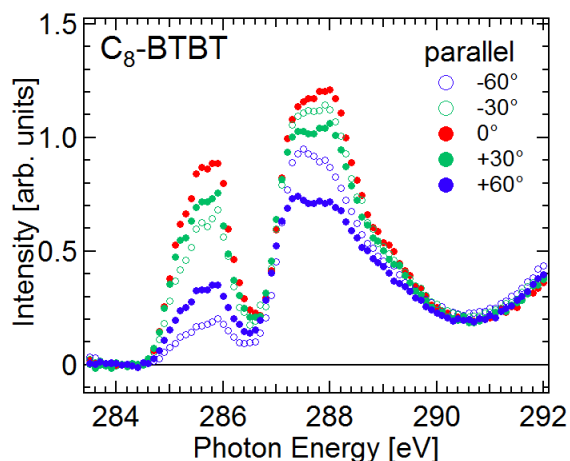


Fig. 1 Incident angle dependence of XAFS spectra of C_8 -BTBT for the parallel geometry.

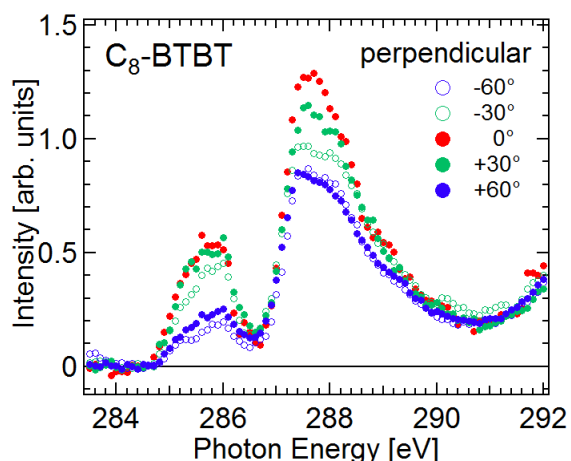


Fig. 2 Incident angle dependence of XAFS spectra of C_8 -BTBT for the perpendicular geometry.

Figure 3 shows the polarization dependence of the integrated areas from 284.6 eV to 286.6 eV in the direction of parallel and perpendicular to the growth direction as a function of the incident angle of SR. The polarization dependences of intensity for parallel geometry is stronger than that for perpendicular geometry. According to the theoretical expression of polarization dependent intensity [1], the molecular orientation of the C_8 -BTBT was evaluated. This analysis shows that the molecular plane is tilted $\sim \pm 20^\circ$ to the normal direction of the substrate and the azimuthal angle is $\sim \pm 50^\circ$ with respect to the growth direction (simulation curves in Fig. 3).

In summary, we have found that the C_8 -BTBT molecules preferentially stack to the temperature gradient direction.

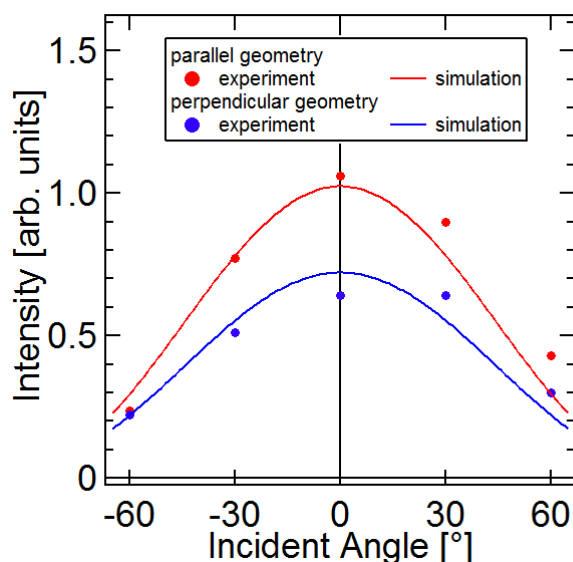


Fig. 3 Polarization dependence of the absorption peaks around 286 eV for the parallel and the perpendicular geometries.

References

- [1] J. Stöhr, *NEXAFS Spectroscopy* (Springer, New York, 1992).