Molecular Orientation of Pentacene Films on HOPG

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Organic semiconductors have attracted interest in recent years because they are cheaper, lighter, and more flexible than conventional Si semiconductors. Controlling molecular orientation is necessary for improving the performance of organic semiconductor devices. Pentacene is one of the most representative organic molecules used in many devices due to its high carrier mobility among organic semiconductors. It is known that pentacene on HOPG with clean surface conditions is oriented at a tilt angle of 30° - 41°. On the other hand, it is reported that pentacene does not show polarization dependence on the sputtered HOPG with a rough surface [1]. In this study, we have investigated the molecular orientation of pentacene on HOPG with artificial surface defects in order to clarify the effect of substrate surface conditions on molecular orientation. X-ray absorption fine structure (XAFS) measurements were used to evaluate the molecular orientation in this study.

The experiments were performed at BL-8 of SR Center, Ritsumeikan University. HOPG substrate was cleaved in the atmosphere before loading into ultrahigh vacuum chamber. After that, HOPG was annealed at 400 °C for 30 minutes to remove contamination from surfaces. Ar^+ ion sputtering was performed on annealed HOPG at 0.75 keV for 10 minutes to form artificial defects on the HOPG surface. The HOPG was again annealed at 400 °C for 30 minutes. Pentacene was deposited by vacuum deposition at deposition rate of 0.1 Å/s at room temperature. Pentacene films were deposited at thicknesses of 0.1 Å, 0.5 Å, 2.0 Å, 10.0 Å, and 10 nm. XAFS measurements were performed at room temperature with SR incident angle of 0°, -30°, and -60°. The measurement mode was the partial electron yield.

Figure 1 shows XAFS spectra of a 0.1 Å pentacene film on HOPG with artificial surface defects. There is not much difference in the shape of the spectra at all incident angles. Therefore, the HOPG spectrum was subtracted to obtain the pentacene spectrum. As a result, the tilt angle of a 0.1 Å pentacene film was obtained to be about 28°. Figure 2 shows XAFS spectra of a 10 nm pentacene film on HOPG with artificial surface defects. At a film thickness of 10 nm, the peak is split into two. This is characteristic of the pentacene peak. Indicating that the pentacene derived peak is dominate. The tilt angle was about 71° at a film thickness of 10 nm. Similarly, for film thicknesses of 0.5 Å and above (not shown), the tilt angle ranged from 71° to 78°. On artificially defective HOPG, the pentacene was found to be oriented in the way that initially lies flat and then upright as the film thickness increases. This may be due to the size and number of defects on the substrate surface.

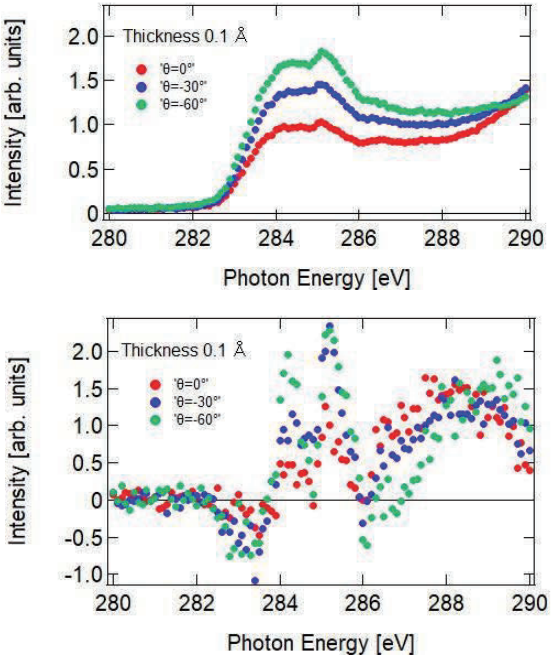

Fig. 1 Polarization dependent XAFS C *K*-edge spectra of pentacene thin film (0.1 Å) on HOPG with artificial surface defects. The subtracted spectra are also shown.

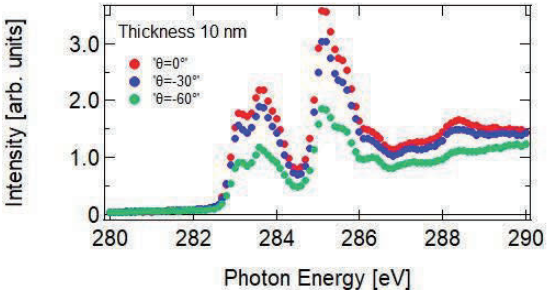

Fig. 2 Polarization dependent XAFS C *K*-edge spectra of pentacene thin film (10 nm) on HOPG with artificial surface defects.

Reference

[1] J. Götzen, D. Käfer, C. Wöll, and G. Witte, Phys. Rev. B, **2010**, *81*, 085440.