

Molecular orientation of pentacene on HOPG studied by NEXAFS

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1. Introduction

Thin films of pentacene ($C_{22}H_{14}$) are attractive molecular materials in organic semiconductors. Molecular orientation in pentacene films is closely related to electronic conduction and anisotropy of the conductivity. Hence determination of molecular orientation in organic and polymer films is very important. Near edge x-ray absorption fine structure (NEXAFS) is a promising tool for such a structural study. In this report, highly ordered pyrolytic graphite (HOPG) is chosen as a substrate because HOPG is a flat substrate surface and can interact attractively with pentacene.

2. Experimental

Pentacene films were deposited on HOPG substrates, which were cleaved in air using adhesive tape before loading into the chamber, at room temperature using a thermal evaporation system. The total film thickness was varied with the deposition time.

NEXAFS 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 [1]. Carbon K-edge NEXAFS 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.

3. Results and Discussion

Figure 1 shows C K-edge NEXAFS spectra measured on bare and pentacene-covered HOPG. The peaks in the spectra are attributed to the C $1s \rightarrow \pi^*$ absorption. With depositing

the pentacene, the peak intensity around 284 eV increases. These peaks increase with the incident angle, indicating that pentacene are aligned horizontally on the substrate. Figure 2 shows the polarization dependence of the peak areas between 282 and 284.9 eV of pentacene and between 284.2 and 286 eV of HOPG as a function of the incident angle of SR, respectively. The polarization dependence of pentacene is symmetric which is similar to that of HOPG. Pentacene molecules are lying on the substrate, which is due to strong π -electron interaction between pentacene and HOPG. As the film thickness increases, the curvature of the polarization dependence decreases. This suggests that tilting pentacene molecules is induced by thickening of the film, which agrees with the previous report [2].

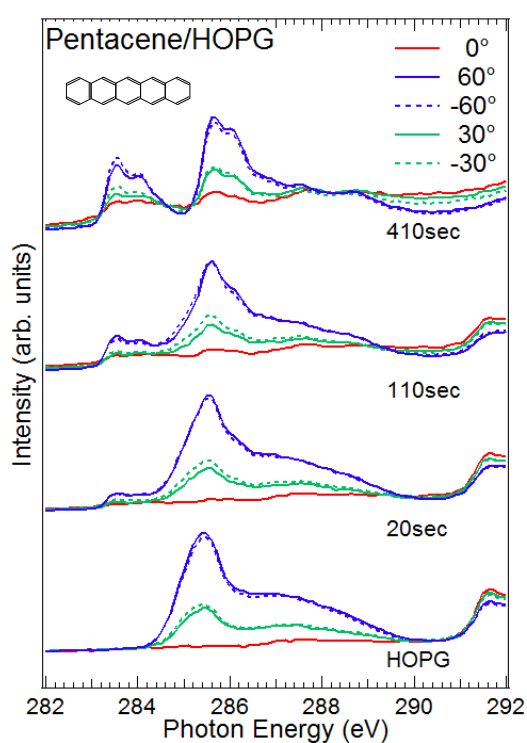


Fig. 1 Incident angle dependent NEXAFS spectra of the pentacene films on HOPG.

4. Conclusions

We have performed the NEXAFS measurements on pentacene thin films on HOPG. It is found that pentacene molecules on HOPG are initially aligned horizontally and then become tilted.

References

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

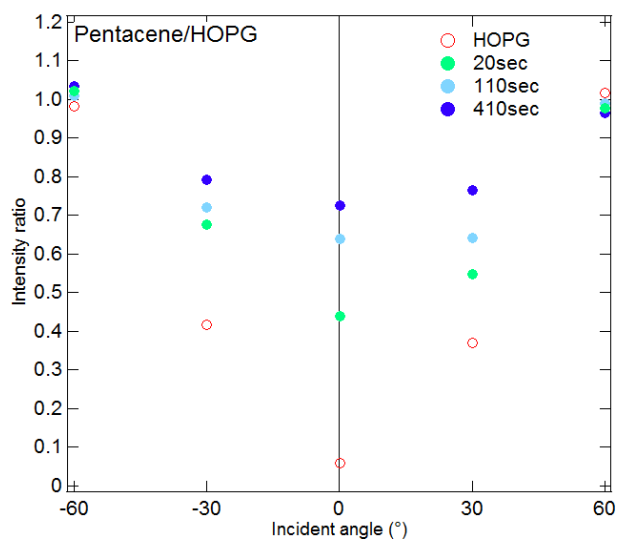


Fig. 2 Polarization dependence of the absorption peaks of pentacene and HOPG.