Molecular orientation of pentacene on polyimide substrate of TCA-DDM studied by NEXAFS

Yuuki Kanekiyo[1], Masaru Takizawa[2], Hidetoshi Namba[1], and Tetsuo Tominaga[3]

1) Department of Physical Sciences, Faculty of Science and Engineering, Ritsumeikan University, Kusatsu, Shiga 525-8577, Japan

2) Research Organization of Science & Engineering, Ritsumeikan University, Kusatsu, Shiga 525-8577, Japan

3) JSR Corporation, Yokkaichi, Mie 510-8552, Japan

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, 2,3,5-tricarboxycyclopentyl acetic dianhydride - diamino diphenyl methane (TCA-DDM) film is chosen as a substrate, which can control orientation of pentacene molecules. TCA-DDM films rubbed by pile impression give a zig-zag surface, because TCA-DDM has bridge bonds in a molecule as shown in the inset of Fig. 1. So we can expect molecular alignment perpendicular to the substrate.

2. Experimental

First, TCA-DDM was dissolved in an organic solvent and spin-coated onto an indium-tin-oxide-coated glass plate. After heating to 80 °C to evaporate the solvent, the polymers were baked at 230 °C for 20 min. The polyimide films were rubbed using a rayon-cloth rubbing machine at 400 rpm rotation speed, 30 mm/sec plate speed, and the 0.4 mm depth of the pile impression. Then, pentacene was evaporated on the polyimide substrates at room temperature. The 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 using 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 rubbing direction.

3. Results and Discussion

Figures 1 and 2 show C K-edge NEXAFS spectra of the samples in the parallel and the perpendicular geometries, respectively. These peaks are attributed to the C 1*s* → π^* transitions. With depositing pentacene, the peak intensities around 284 eV and 286 eV increase. These peaks decrease with the incident angle, indicating that the pnetacene molecules are aligned vertically on the substrate. Figure 3 shows the polarization dependence of those peak intensities in the direction of parallel and perpendicular to the substrate as a function of the incident angle of SR. The polarization dependences in both directions are almost the same, indicating that the rubbing at the present experiments is not effective to align pentacene molecules. The present results suggest that strong interaction of π-electrons in pentacene with the substrate is disturbed by the zig-zag shape of TCA-DDM molecule. Hence inter-molecular interaction of pentacenes is strong enough to coalesce, which is independent of the rubbing direction of the substrate.

4. Conclusions

We have performed the NEXAFS measurements on pentacene thin films on TCA-DDM in order to investigate the molecular orientation of pentacene. Orientation of pentacene molecules is vertical to the substrate and insensitive to the rubbing direction.

Reference

[1] H. Namba *et al*., J. Synchrotron Rad. **5**, 557 (1998).

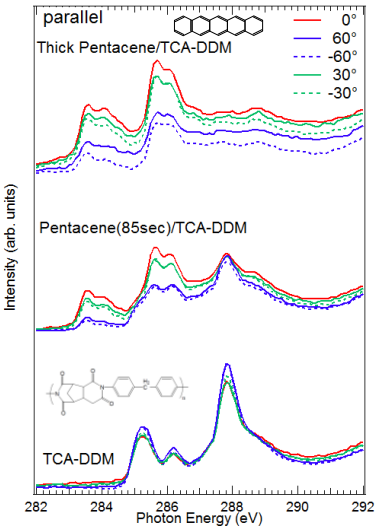

Fig. 1 Incident angle dependent NEXAFS spectra of the pentacene films on TCA-DDM for the parallel geometry.

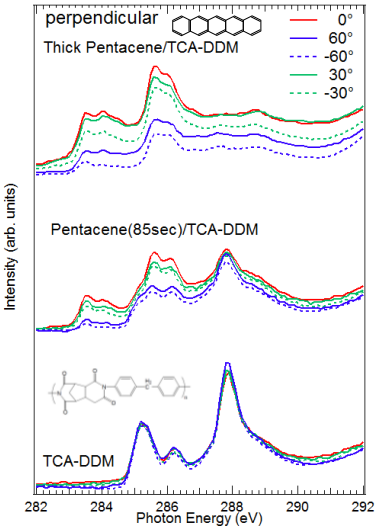

Fig. 2 Incident angle dependent NEXAFS spectra of the pentacene films on TCA-DDM for the perpendicular geometry.

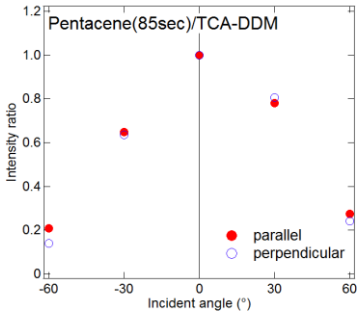

Fig. 3 Polarization dependence of the absorption peaks around 284 eV for the parallel and the perpendicular geometries.