Molecular orientation of pentacene films on $SrTiO_3$ substrates

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1. Introduction

Pentacene ($C_{22}H_{14}$) has attracted much attention because of its possible application to organic electronic devices. A vertical alignment (*c*-axis alignment) of pentacene molecules is necessary for the transistor performance. Although the pentacene thin films showed the similar "thin film phase" (*c*-axis alignment), the transistor performance such as a mobility was depend on the dielectric substrates [1]. In the present study, we have chosen an amorphous $SrTiO_3$ as a dielectric substrate and investigated the molecular orientation of pentacene on it by near edge x-ray absorption fine structure (NEXAFS) measurements.

2. Experimental

The pentacene films were deposited on amorphous $SrTiO_3$ substrates at room temperature using a thermal evaporation system. The deposition rate was set to 0.4 Å/s. The total film thickness was 30 nm or 100 nm.

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 [2]. 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

Figures 1 and 2 show C K-edge NEXAFS spectra of the samples. These peaks are attributed to the C 1*s* $\rightarrow \pi^*$ transitions. The intensity of these peaks decreased with incident angle, indicating that the pnetacene molecules are aligned vertically on the amorphous $SrTiO_3$ substrate as in the case of the Si substrate. However, the intensity

ratio for the thin film with 30 nm thickness (Fig. 1) was larger than that for the thick film with 100 nm thickness (Fig. 2). This angle dependent intensity ratio can be expressed as

$$\frac{I(\theta)}{I(0°)} = \frac{P \sin^2\theta + (1/2 - 3/2\ P \sin^2\theta) \sin^2\alpha}{1/2 \sin^2\alpha},$$

where P is the polarization factor and α is the polar angle of π^* orbital with azimuthally averaged [3]. Assuming that P = 1, the tilt angles of pentacene molecules are estimated to be 18° ± 7° for the 30 nm film and 28° ± 8° for the 100 nm film.

4. Conclusions

We have investigated the molecular orientation of pentancene films on amorphous $SrTiO_3$ substrates by NEXAFS. We have found that the pentacene molecules are aligned vertically on amorphous $SrTiO_3$ substrates and their tilt angle for a thick film is larger than that for a thin film.

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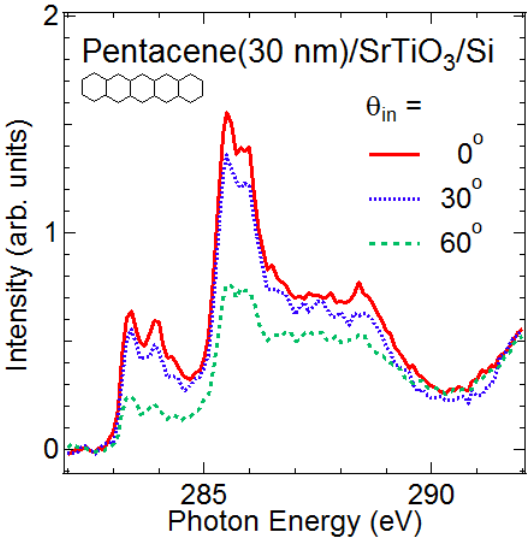

Fig. 1: Incident angle dependence of NEXAFS spectra for the pentacene films (30 nm) on the amorphous $SrTiO_3$ substrate.

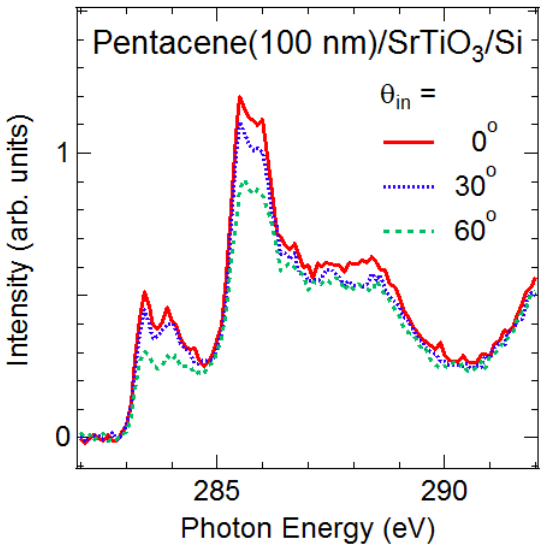

Fig. 2: Incident angle dependence of NEXAFS spectra for the pentacene films (100 nm) on the amorphous $SrTiO_3$ substrate.

References

[1] D. Knipp *et al.*, J. Appl. Phys. **93**, 347 (2003).

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

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