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Molecular orientation of the pentacene ultrathin films grown on SiO_2 substrates

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Introduction

Pentacene has been attracting much attention recently because it shows the highest FET mobility. The orientation of pentacene molecules in the first few monolayers has large influence on the mobility. There were some *ex situ* measurements of the orientation of pentacene grown on SiO_2 substrates and showed the Standing-mode growth (Fig. 1). The atmosphere would, however, have influence on the orientation or morphology of pentacene films as shown in the previous study [1]. Accordingly, we carried out all experimental processes from deposition of pentacene to characterization of films under vacuum condition without exposure to the atmosphere in order to reveal whether the observed structure is truly as-grown one or changed by the influence of the atmosphere.

Experiment

Three types of SiO_2 substrates were used; prepared by oxidation of a Si wafer with Shiraki method, Shiraki method and following anneal in dry O_2, and a commercially obtained Si wafer with thermally oxidized amorphous SiO_2 layer. Pentacene was evaporated from a Knudsen cell in a custom-designed all-in-vacuum system with a base pressure of 10^{-7} Pa. C K-edge NEXAFS and AFM measurements were carried out under vacuum condition without exposing the specimens to the atmosphere.

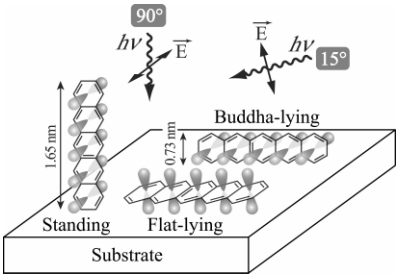

Figure 1: Schematic illustrations of the possible configurations of pentacene molecules on a substrate with each π* orbitals. The incident directions of X-ray with its electric vector are also shown.

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Results and Discussion

Figure 2 shows the NEXAFS spectra of pentacene films deposited on the SiO_2 substrate prepared by Shiraki-method. Pentacene films deposited on SiO_2 substrates prepared by other methods also showed similar NEXAFS spectra. Clear polarization dependence was observed in all films with different thickness, that is, π*-peak was most enhanced at normal X-ray incidence (90°), while almost no peak was observed at grazing incidence (15°), indicating that pentacene molecules grew with Standing-mode. Detailed curve fitting analysis of π*-peaks revealed that the inclination angle of π* orbital to the substrates was almost 0° in the sub-monolayer film, and less than 10° ± 5° even in the film with 10 nm thick (shown as 'multi layer' in Fig. 2). We also measured AFM and the height of each islands showed about 1.6 nm, indicating the Standing-mode growth. The results of NEXAFS and AFM revealed that pentacene grows in Standing-mode from the initial stage of the growth in vacuum condition irrespective of the type of SiO_2 substrates prepared by different procedures. Thus, our study elucidated that the pentacene islands with standing molecules were not formed by the effect of exposure to the atmosphere but by the nature of the pentacene on SiO_2. The growth mechanism could be explained by the interaction between the molecules and the substrates, and the thermodynamic behavior of growing molecules [2,3].

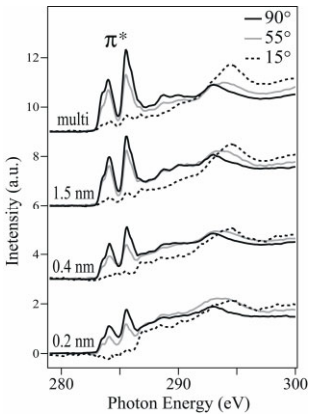

Figure 2: C K-edge NEXAFS spectra of pentacene films grown on SiO_2 prepared by Shiraki-method. Peaks observed around 283-288 eV correspond to the transition from C 1s to π* orbital of pentacene.

References

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