Molecular orientation of copper phthalocyanine on pentacene in organic solar cells by NEXAFS spectroscopy

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1. Introduction

Organic solar cells (OSCs) have been considered to be a promising alternative to inorganic solar cells because of many desirable properties such as low cost, lightweight, and flexibility. Copper phthalocyanine (CuPc) is a planar small-molecule, which is widely used as a stable and efficient donor material in OSCs. The molecular orientation of CuPc plays an important role on the OSC performance, since the π−π stacking direction of the orbital largely contributes to the carrier transport. A thin organic material is sometimes additionally placed between the donor and the anode to control the orientation of overlaid donor molecule [1]. In this short report, the effect of the thin pentacene layer on the molecular orientation of CuPc is investigated as a function of the pentacene thickness by near edge x-ray absorption fine structure (NEXAFS) spectroscopy.

2. Experimental

Figure 1 shows the cross-sectional view of the sample with the structure of indium-tin oxide (ITO)/ pentacene (0, 2, 3, 4, 6, 8, 10 nm)/ CuPc (20 nm). Organic materials were evaporated on the ITO substrate at a rate of 0.5 Å/s under a pressure of approximately 1.0×10^{-3} Pa.

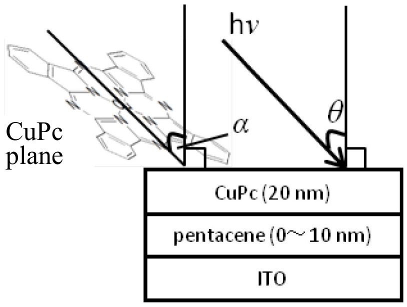

Fig. 1 Schematic structure of the sample for NEXAFS.

NEXAFS spectra were measured using the beam-line BL-8 of the SR Center at Ritsumeikan University. The attention was paid to the π^* peaks of the nitrogen K-edge spectra approximately at 398 eV of photon energy. The incident angle θ of synchrotron radiation was adopted at three cases of 0° and ±60° in order to assess the molecular tilt angle α of CuPc.

3. Results and Discussion

Figure 2 shows the N K-edge spectra of the samples with seven kinds of thickness *d* of pentacene. The spectra provide the information of the molecular orientation of CuPc with nitrogen atoms. The peak at 398 eV is attributed to the N $1s \rightarrow \pi^*$ transition. The intensity of the peak at 0° is much larger than that at ±60° for the sample without pentacene (*d* =0 nm). As the thickness *d* is increased, the intensity at ±60° is increased compared with that at 0°. The intensity at ±60° is larger than that at 0° for the sample with *d* =10 nm.

Figure 3 shows the dependence of the tilt angle α on the pentacene thickness *d*. This is calculated from the intensity ratios of the peak at 0° and that at ±60° in Fig. 2 [2]. Here, average value and standard deviation are depicted among four sample data for each *d*. The molecular plane of CuPc is standing-up, that is, almost perpendicular to the ITO substrate surface for small *d*. As *d* is increased, the orientation changes from standing-up to lying-down configuration. The tilt angle α is, however, saturated at 40° for larger *d*.

The molecular orientation can be successfully evaluated for thin CuPc film with its thickness of only 20 nm.

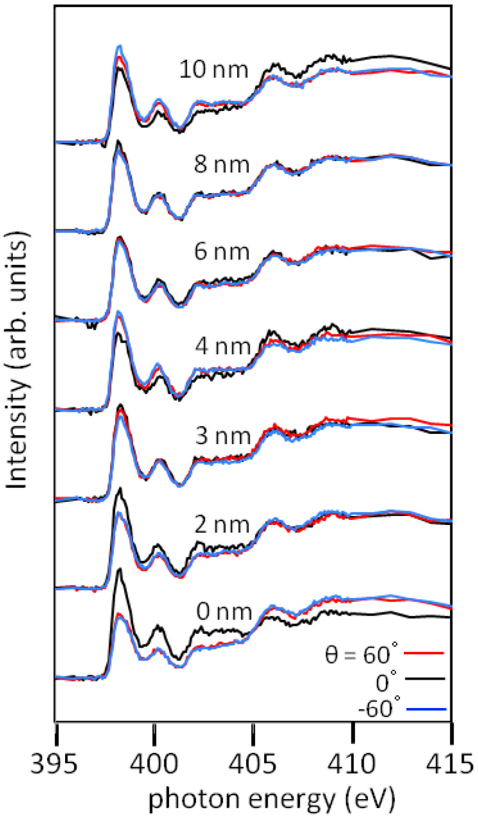

Fig. 2 N K-edge spectra of CuPc on pentacene with various thickness *d*.

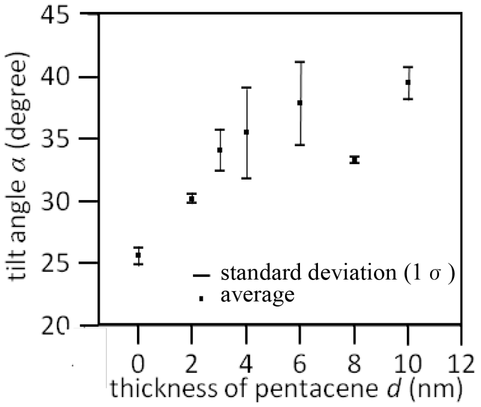

Fig. 3 Tilt angle of CuPc vs pentacene thickness *d*.

4. Conclusions

Molecular orientation of CuPc on pentacene has been studied by NEXAFS spectroscopy. The orientation changes from standing-up to lying-down configuration as the thickness of pentacene is increased.

References

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[2] J. Stöhr: ”NEXAFS Spectroscopy”, Second Printing, Springer, Berlin, 2003, chap.9.