

Effect of pentacene anode buffer layer on small-molecule organic solar cells

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1. Introduction

Anode buffer layer placed between indium-tin oxide (ITO) anode and donor layer has been reported to play several roles in improving the performance of small-molecule organic solar cells (OSCs). One of them is to force the molecular orientation of the overlaid donor to lie flat with respect to the substrate surface, which enhances charge transport in the direction between anode and cathode [1]. In this short report, the effect of the thin pentacene layer as an anode buffer on the molecular orientation of copper phthalocyanine (CuPc) is investigated as a function of the pentacene thickness d by near edge X-ray absorption fine structure (NEXAFS) spectroscopy, where CuPc is widely used as a stable and excellent donor material.

2. Experimental

Figure 1 shows the cross-sectional view of the sample with the structure of ITO/pentacene ($d=0-20$ nm)/CuPc (20 nm). Organic materials were evaporated on the ITO substrate at a rate of 0.5 \AA/s under a pressure of approximately $1.0 \times 10^{-3} \text{ Pa}$.

NEXAFS measurements were performed at BL-8 of 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 $\pm 60^\circ$ 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 four 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 $\pm 60^\circ$ for the sample without pentacene ($d=0$ nm).

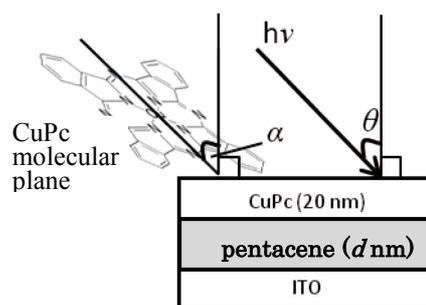


Fig. 1 Schematic structure of the sample for NEXAFS.

As the thickness d is increased, the intensity at $\pm 60^\circ$ is increased compared with that at 0° . The tilt angle α , which is calculated from the intensity ratios of the peak at 0° and that at $\pm 60^\circ$ [2], is also depicted. 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 tilt angle α is increased, but is saturated at 34° for larger d .

Separate AFM measurement shows that the surface roughness of both pentacene and overlaid CuPc layers becomes larger as d is increased. X-ray diffraction measurement also shows that the standing-up CuPc crystal structure without pentacene layer becomes distorted as d is increased. Thus, the pentacene layer does not bring about a lying-down configuration of CuPc film molecules with respect to the substrate surface. The origin of the improvement of OSCs is possibly due to the increase in the area between donor-acceptor interface with enhanced roughness, bringing about the increase in the carrier generation there. Figure 3 shows the schematic cross-sectional view of expected interface roughness of OSCs.

4. Conclusions

Molecular orientation of CuPc on pentacene has been studied by NEXAFS spectroscopy. The pentacene layer does not bring about a lying-down configuration of CuPc film molecules with respect to the substrate surface.

References

- [1] P. Sullivan, T. S. Jones, A. J. Ferguson, S. Heutz, Appl. Phys. Lett. **91**, 233114 (2007).
- [2] J. Stöhr, "NEXAFS Spectroscopy", Second Printing, Springer, Berlin, 2003, chap.9.

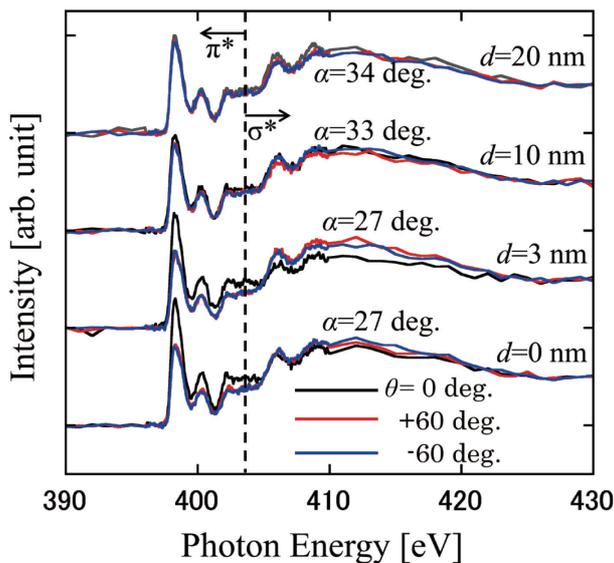


Fig. 2 N K-edge spectra of CuPc on pentacene with various thickness d .

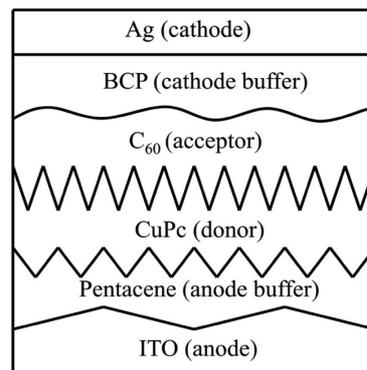


Fig. 3 Schematic cross-sectional view of expected interface roughness of OSCs.