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.

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 $\alpha$ 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$\rightarrow$π* 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 $\alpha$ 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 $\alpha$ 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.

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