

Orientation analysis of silicon phthalocyanine dichloride thin films using angle-dependent NEXAFS

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Introduction

The orientation of organic semiconductor molecules on surfaces is not only an intriguing phenomenon in molecular science, but also crucial for the properties of optical and electronic devices [1]. Silicon phthalocyanines represent one of the promising candidates for such organic devices because these systems form electronic conductor if the molecules are stacked face-to-face and provide a co-axially contiguous pathway for carrier delocalization [2].

We prepared thin films of silicon phthalocyanine dichloride (SiPcCl₂) on graphite and metals by several methods, including a casting, powder dispersion, CVD, and spin-coating. We investigated the orientation and electronic structure of those films using polarization-dependent near-edge x-ray absorption fine-structure (NEXAFS) spectroscopy. Here we report on the films prepared by dispersion of SiPcCl₂ on highly oriented pyrolytic graphite (HOPG).

Experimental

The experiments were performed at the BL-27A station. The Si and Cl K-edge NEXAFS spectra were measured by the total electron yield method. Thin films were prepared by pressing a slight amount of SiPcCl₂ (Sigma-Aldrich Co.) powder onto HOPG. After heating at ~345 °C in air (1 atm.), excess molecules were removed, leaving products binding to the substrate. The thickness was estimated to be ~4.0 nm using XPS measurements.

Results and Discussion

Figure 1(b) shows the Si K-edge NEXAFS spectra taken with various polarization angles (θ) for the SiPcCl₂ film heated at 345°C. For comparison, the NEXAFS spectra for thin powder before heating is also shown in Fig. 1(a).

It is noteworthy that new peak C appears for the heated film and the intensities of the peak depend remarkably on polarization angles. Considering that the films were heated in air, we hypothesized that Si-Cl bond was replaced with Si-O by oxidation; this was confirmed by XPS measurements. Moreover, the energy position of peak C agrees with that of SiPc(OH)₂. Thus, we attribute the origin of peak C to out-of-plane $\sigma_{\text{Si-O}}^*$ transition.

The intensities of peak C decrease with the increase of incident angles. We thus conclude that polymer chains

like [-PcSiO-]_n structure were formed at high temperature and Si-O chain axis tends to be perpendicular to the graphite plane.

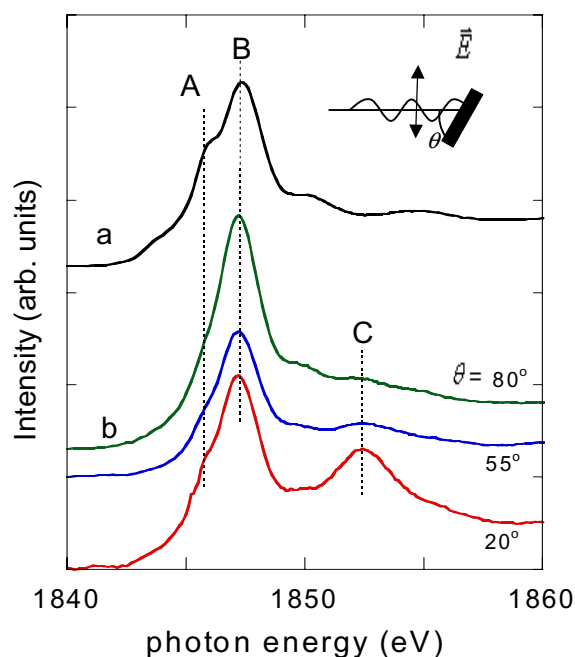


Fig.1 Si K-edge NEXAFS spectra for SiPcCl₂ thin powder (a) before and (b) after heating. The incident angle, θ , is defined as angles between sample surface and synchrotron beam.

Reference

- [1] C.W. Dirk, et al. J.Am.Chem.Soc.105(1983)1539.
- [2] J.R. Ostrick, et al. J.Appl.Phys.81(1997)6804.

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