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One-dimensional ordered structure of α-sexithienyl on Ag and Cu(110)

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Introduction

The orientation of α-sexithienyl (6T) on various substrates have been studied mainly in the out-of-plane direction, and there are few studies focused on the in-plane molecular orientation. If one-dimensional structure of 6T molecules is fabricated, various applications can be expected, such as nano-scaled molecular devices or polarized light emitting devices. In the present study, we have tried to prepare a 1D structure of 6T on Ag(110) and Cu(110), clarified its formation process and obtained the orientation distribution function of 6T by means of continuously measuring azimuthal dependent NEXAFS.

Experiment

Mechanically and electrochemically polished Ag(110) and Cu(110) were cleaned by repeated cycles of Ar^+ sputtering and annealing. 6T was evaporated from a Knudsen cell in a custom-designed ultrahigh-vacuum system with a base pressure of 4×10^{-8} Pa. S K-edge NEXAFS was carried out at the station BL-11B of the Photon Factory in the Institute of Materials Structure Science.

Results and Discussion

First, we studied the out-of-plane orientation. From the intensity of two intense peaks (π*-peak; S 1s to π* orbital, which is perpendicular to 6T molecular long axis, and σ*-peak; parallel to long axis), it is revealed that 6T molecules on the Ag(110) grew with their molecular long axes parallel to the surface (flat-lying mode). Next, we investigated the in-plane orientation. In RHEED measurement, sharp streak patterns of 6T were observed only in the [001] direction for 6T/Ag(110). Figure 1 shows a plot of σ*-peak obtained by continuously measuring azimuthal dependent NEXAFS of 6T grown on Ag(110). These results suggested one-dimensional ordered structures of 6T molecules grown on Ag(110) surface as depicted in Fig. 1. 6T molecules grown on Cu(110) at 300 K and subsequent annealing at 360 K also showed the similar one-dimensional ordered structure. These peculiar structures could be explained by the lattice commensurability of 6T and Ag, Cu(110) surface.

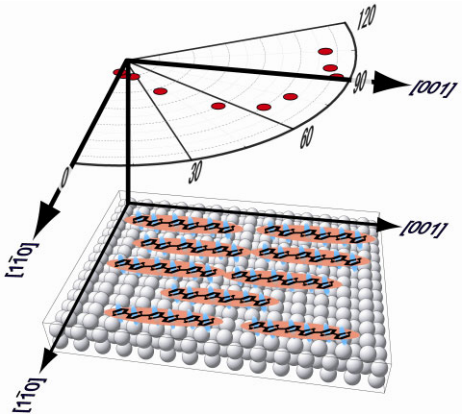

Figure 1: Polar plot of σ*-peak intensity as a function of the in-plane polarization azimuth of x-ray normally incident on 6T/Ag(110) and corresponding orientation of 6T molecules.

Here, we propose a new method to obtain the orientation distribution function of molecules with twofold symmetry, supposing the orientation distribution function could be represented as $f(\alpha)=\frac{1}{\sqrt{2\pi\sigma}}e^{-\frac{1}{2\sigma^2}\alpha^2}$, where α and σ^2 are the azimuthal angle between the molecular long axis and the Ag, Cu[001] direction and its dispersion, respectively. The intensity of the NEXAFS peak is proportional to $\cos^2\theta$, where θis the angle between the electric vector of the x-ray and the transition moment of the peak. The intensity of σ* peak observed by NEXAFS is, thus, represented as $I(\varphi)=\int_0^{2\pi} f(\alpha)\cos^2(\varphi-\alpha)d\alpha$, where φ is the azimuthal angle between the electric vector of incident x-ray and Cu$[1\bar{1}0]$ direction. By fitting the experimental result with the fitting function, σ was determined to be 18°, 29° for 6T/Ag(110), 6T/Cu(110), respectively. We could obtain the orientation distribution function of the molecules for the sample with twofold symmetry.

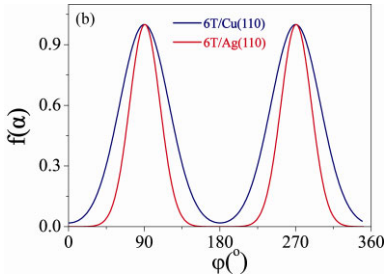

Figure 2: The orientation distribution functions of 6T molecules in the grown film.

References

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