

Analysis of bonding structure of ultrathin films of oligothiophene molecules grown on passivated silicon surfaces

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1 Introduction

The knowledge of the interaction between organic molecules and semiconductor surfaces is important to adapt organic semiconductors into the semiconductor technology [1]. In this study, the processes of α -sexithiophene (α -6T) thin layer formation on passivated Si surfaces have been investigated in situ by means of PES, NEXAFS, surface differential reflectance spectroscopy (SDRS) and reflectance difference spectroscopy (RDS).

2 Experiment

Si(001)-(2x1) surface was exposed independently to H₂O, O₂, atomic H, and C₂H₄ gas in an ultrahigh vacuum chamber. α -6T molecules were deposited on these passivated surfaces at room temperature to the nominal thickness of 5 nm at most.

3 Results and Discussion

Figure 1 shows normalized S-2p photoelectron spectra of α -6T thin films on water-adsorbed Si(001). A feature related to the interface is found only in the film with a thickness of 1 nm, which means sulfur atoms are combined with the substrate atoms. On the other hand, The C-1s photoelectron spectra indicate that carbon atoms are also combined with the substrate atoms.

Figure 2 shows S-1s NEXAFS spectra of α -6T film on water-adsorbed Si(001) measured at three incident angles. The thickness was 0.6 nm. The spectrum is dominated by an electronic transition to π^* states at normal incidence,

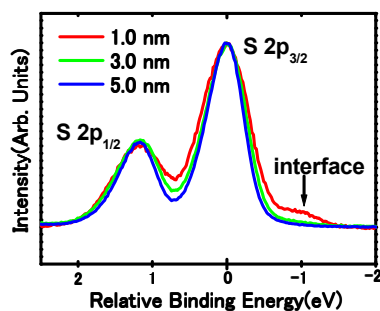


Fig. 1. Normalized S-2p PES spectra of α -6T thin films on water-adsorbed Si(001).

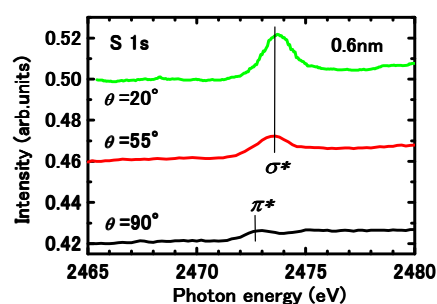


Fig. 2. S-1s NEXAFS spectra of a α -6T thin film on water-adsorbed Si(001).

while it is dominated by that to σ^* states at grazing incidence. This means that majority of α -6T molecules are standing on the substrate.

The main findings obtained from the experimental results including SDRS and RDS as well as PES and NEXAFS are as follows. α -6T molecules are upright-standing to form bulk-like islands or films from the first layer on oxidized Si(001) and monohydride Si(001). Carbon atoms of the standing molecules are combined with the substrate atoms. On water-adsorbed Si(001), isolated α -6T molecules are flat-lying and align parallel to the dimer row until the thickness becomes 3 nm. Sulfur atoms of the lying molecules are combined with -OH of the surface. Above 3 nm, most of molecules are standing and constitute well ordered islands or films. On ethylene-adsorbed Si(001), the majority of α -6T molecules are flat-lying, and isolated molecules and those in the islands or films tend to align parallel and perpendicular to the dimer row, respectively. Thus, the orientation and electronic states of the molecules depend on the method of passivation, which raises the possibility of controlling the molecular orientation by the surface modification.

References

[1] R.J. Hamers, Annu. Rev. Anal. Chem. **1**, 707 (2008).

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