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Anchoring of organic molecules with silicon alkoxide on oxide surface

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Introduction

For application of organic thin films, it is important to immobilize organic molecules on inorganic surfaces. However, lattice constants of organic crystals are generally fairly larger than those of inorganic substrates. So it is difficult to immobilize organic molecules on inorganic surfaces such as metals and oxides. In order to solve this problem, many studies have been reported about anchoring of organic molecules on metal surfaces. For example, it is well known that alkyl molecules are immobilized on gold surface using strong Au-S bond [1]. On the other hand, in spite of important properties of oxides such as transparency and insulating (or semiconducting) nature, there have been few reports about the immobilization of organic molecules. In this report, we have investigated the immobilization of alkyl chain molecules with silicon alkoxide on oxide surfaces.

Experimental

The experiments were performed at the BL-27A station. Mercapto-propyl-trimethoxy-silane (MPTS) molecules [$SH(CH_2)_3Si(OCH_3)_3$] were adsorbed on Al_2O_3 thin films. The Al_2O_3 surface was made by oxidation of aluminum films. The MPTS molecule was adsorbed in the vacuum chamber using gas line with a stop valve. The chemical state of the interface between the Al_2O_3 surface and the MPTS molecule was measured by X-ray photoelectron spectroscopy (XPS). The molecular orientation was estimated by polarization dependencies of near edge X-ray absorption fine structure (NEXAFS) spectra. The sample was rotated around the vertical axis.

Results and discussion

Fig.1 shows the Si 1s X-ray photoelectron (XP) spectra for MPTS molecules on the Al_2O_3 surface. The thickness was precisely calibrated by the XPS peak intensities of Al 1s and Si 1s, the inelastic mean free paths of the photoelectrons, and the photoionization cross sections. For 3 layers (Fig.1(a)), single peak is observed at 1844.3eV (marked A). Considering the thickness, this peak originates from condensed MPTS molecules. On the other hand, for monolayer, another peak appeared at lower binding energy side (marked B) at 1839.6 eV, while peak A is still observed. Assuming that some part of the monolayer forms island structure, the peak B originates from not molecular MPTS but the interface between MPTS molecules and the Al_2O_3 surface. The results indicate that the MPTS molecules and the surface form chemical bonds through silicon alkoxide.

Fig.2 shows the Si *K*-edge NEXAFS spectra for monolayered MPTS film on the Al_2O_3 surface for two different angles. The peaks A and B correspond to the resonances from Si 1s to σ* orbitals localized in the Si-C and Si-O bonds, respectively [2]. The peak A is enhanced at 15 degree, while the intensity decreases at 45 degree. On the other hand, the incident angle dependencies of the intensity of the peak B is reverse to that of the peak A. These results suggest that the Si-C bond is perpendicular to the surface, and the alkyl chain of a MPTS molecule locates the vertical direction on the surface. In summary, it was elucidated that the silicon alkoxide is a good anchor that combines alkane molecules and oxide surfaces.

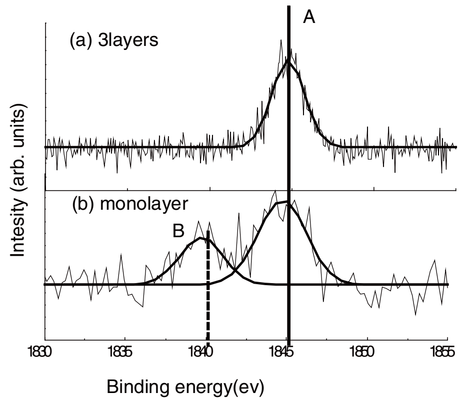

Fig.1 Si 1s XP spectra of 3 layer(a) and monolayer(b) MPTS film on the Al_2O_3 thin film.

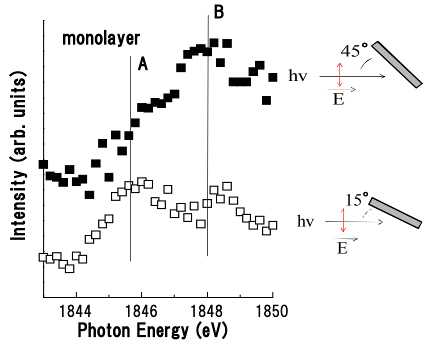

Fig.2 Si *K*-edge NEXAFS spectra of monolayered MPTS on Al_2O_3 film for two different X-ray incident angles.

References

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