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Structure determination of self-assembled monolayer on oxide surface by soft-X-ray standing wave

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Introduction

Determination of geometrical location of adsorbed atoms and molecules on a surface is one of the key factors to be elucidated in surface science. A normal incidence X-ray standing wave (NIXSW) using soft X-rays has excellent characteristic, in which the distance between adsorbed atoms and surface can be precisely determined [1]. In this work, we present the first results for the geometrical determination of atoms and molecules adsorbed on a surface of insulating oxide with wide band-gap. The system investigated is decyl-phosphonic acid (DPA, C_{10}-alkyl phosphonic acid) adsorbed on a sapphire surface, which is one of the candidate systems for self-assembled monolayers (SAM) of organic molecules on oxide surface.

Experimental

The experiments were performed at the BL-27A station. A C(0001) face of a sapphire plate was used as a substrate. The substrate was immersed in 0.01 Mol/dm^3 of DPA-ethanol liquid for 20 hours, and then rinsed by supersonic waves in ethanol. For the NIXSW measurements, the sample surface was irradiated by soft X-rays from the surface normal. The intensities of the total electrons, P 1s and C 1s photoelectrons were plotted as a function of the photon energy.

Results and discussion

Fig.1 shows the total electron yield for clean surface of sapphire as a function of the photon energy. The most intense peak was observed around 3050 eV, which is due to the standing wave originating from the sapphire substrate. This energy nearly corresponds to one of the Bragg diffraction peaks from α-Al_2O_3 with corundum structure.

Fig.2 displays the intensities of the P 1s photoelectrons, as a function of the photon energy around 3050 eV. The normalized intensity of the photoelectron ($I(E)/I_0$) being concerned is described as

$$I(E)/I_0=1+R(E)+2F[R(E)]^{1/2}\cdot\cos[2\pi d_H-\delta(E)] \qquad (1)$$

where $R(E)$ is the reflectivity of the substrate, $\delta(E)$ is the energy-dependent phase modulation caused by the X-ray standing wave, F is the structure factor, and d_H is the coherent position of the atoms measured from the surface [2]. The photon energy, E, is normalized by the "W parameter" that stands for the deviation from the Bragg

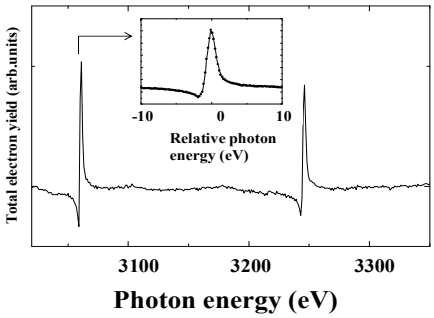

Fig.1 Total electron yield for clean sapphire substrate as a function of photon energy. The incidence angle of X-rays was surface normal.

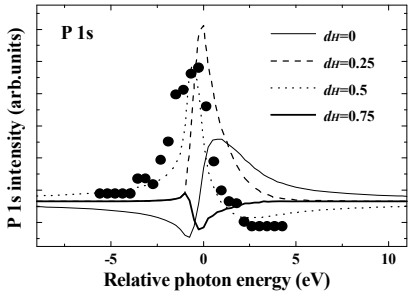

Fig.2 Intensity of P 1s for DPA/Sapphire as a function of photon energy. The theoretical curves calculated by eq.(1) for four different locations of phosphorus atoms are also shown.

diffraction condition [3]. The intensity of the P 1s follows the theoretical curve for d_H=0.5. This means that the phosphorus atoms in DPA molecules are located at the half of the coherent position, i.e., d=0.21 nm, deduced from the Bragg energy. Therefore, it is concluded that phosphorus atoms are located at 0.11 nm from the surface and DPA molecules form SAM through phosphonic acids. The results shed light on the further applications of NIXSW to the structure analysis of atoms and molecules on insulating materials like oxides.

References

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