

## Adsorption behavior of L-cysteine molecule with ITO substrates using angle-dependent NEXAFS and XPS techniques

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### Introduction

Near Edge X-ray Adsorption Fine Structure (NEXAFS) is a suitable method for the study of chemical state of metal molecular interface, since it provides information about the electronic structures of both core levels and valence unoccupied states that are localized at the sulfur atom. Especially, NEXAFS at the S K-edge has advantages over that at the S L-edge because the core-to-valence resonance peak directly probes the valence unoccupied  $3p^*$  states due to the dipole selection rule [1-3]. In this study, we describe angle-dependent NEXAFS and XPS studies of L-cysteine [ $\text{HSCH}_2\text{CH}(\text{NH}_2)\text{COOH}$ ] adsorbed on Indium-Tin-Oxide (ITO) substrates, which show that highly oriented L-cysteine molecules are formed in the surfaces.

### Experimental

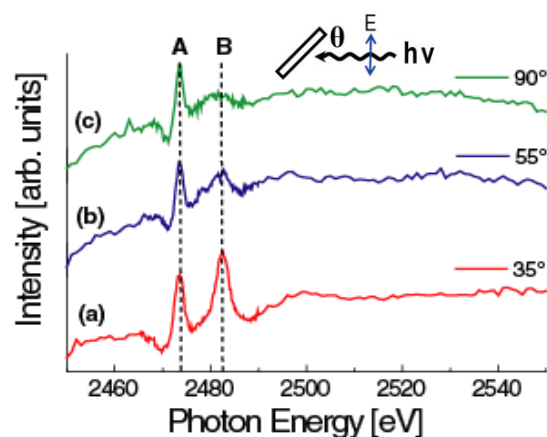
All experiments were carried out at the BL 27A soft X-ray station in the Photon Factory of the High Energy Accelerator Research Organization (KEK-PF), Japan. The chemical bonding states at the metal-molecular interface were measured by near edge X-ray adsorption fine structure (NEXAFS) at the S K-edge, and S  $1s$  X-ray photoelectron spectroscopy (XPS). The NEXAFS spectra were measured by a total electron yield (TEY) for a variety of x-ray incident angles. The samples were prepared by vacuum-deposition method using Knudsen-cell evaporator. The ITO substrates were cleaned with ultra-supersonic in 2-propanol. The thickness was determined by the XPS measurements.

### Result and Discussion

Figure 1(a), (b), and (c) show the S K-edge NEXAFS spectra for vacuum-deposited L-cysteine thin layers on ITO substrates taken with  $35^\circ$ ,  $55^\circ$ , and  $90^\circ$  polarization angles ( $\theta$ ). Two resonance peaks are observed at 2475.0 eV (marked A) and 2484.0 eV (marked B). Two peaks are similar in widths, but are shifted in energy with each other. The lower energy one (peak A) is close to that for multilayer L-cysteine, while the higher one (peak B) is most likely for molecules strongly interacted with the substrate. Thus, we here tentatively consider that the both peaks originate from resonant excitation from S  $1s$  to valence unoccupied  $\sigma^*$  orbitals that are localized at the S-C bond [4]; hereinafter, this resonance is referred to as

S  $1s \rightarrow \sigma^*(\text{S-C})$ . It is noteworthy that the intensities of peak B depend remarkably on polarization angles, while those of peak A depend scarcely. The intensities of peak B decrease with the increase of incident angles, indicating that S-C bonds tend to be pointing upward from the surfaces. The results of orientation are in good agreement with the fact that molecules interacted with surfaces exhibit oriented configuration.

In summary, we consider that two adsorption states exist in this L-cysteine thin layer on ITO substrate. One state is highly oriented layer at first layer on ITO substrate and the other is molecular state L-cysteine which is not oriented on top of this layer.



**Fig.1** Polarization dependence of S K-edge NEXAFS spectra for vacuum-deposited L-cysteine thin layers on ITO substrates.

### References

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