7A/2001S2-003

Development of X-ray Standing Wave Method using ultra-soft X-rays

Reona YOKOTA¹, Hiroshi KONDOH¹, Ikuyo NAKAI¹, Toru SHIMADA¹, Masanari NAGASAKA¹,Toshiaki OHTA^{*1}, Hisataka TAKENAKA², Tohru NAKAMURA³ ¹Univ. of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan ²NTT-AT, 162 Shirakata, Tokai, Naka, Ibaraki 319-1193, Japan ³AIST, 1-1-1 Higashi, Tsukuba, Ibaraki 305-8565, Japan

Introduction

The X-ray standing wave (XSW) method is a powerful tool for determination of specific atom locations relative to the lattice plane. So far, a number of XSW experiments have been conducted mainly using soft X-rays whose wavelength are comparable to crystal lattice constants. In this paper, we report a new approach of the XSW method by combining ultra-soft X-rays with periodic multilayers. We used a W/C multilayer as *Standing Wave Generator* and obtained SW profiles via. photoelectron detection, which enables us to determine vertical locations of specific atoms in an organic monolayer with a high sensitivity.

Experimental

Monolayer Preparation

4-octyl-4'-(5-carboxypentamethy-lene-oxy)- azobenzene (referred to Az) was synthesized and used for the monolayer. The chemical structure of Az molecule is shown in Fig. 1. $_{ca.29\text{\AA}}$



Fig. 1 Chemical structure of Az

Az was dissolved in chloroform at a concentration of 1 mmol / \emptyset . The solution was spread on ultrapure water containing Cd²⁺ ions. The monolayer was compressed at a speed of 300 mm²min⁻¹, and the surface pressure was monitored. The single-layer deposition of the monolayer was undertaken in the upstroke onto a W/C multilayer (80 periods of W/C layer pairs with 30.9Å interval). Transfer was performed at 15 mN m⁻¹ by standard vertical deposition with the dipping speed of 3 mm min⁻¹. The monolayer deposited on the multilayer is schematically illustrated in Fig. 2.

XSW measurement

The XSW experiments were carried out at the beam line 7A in the Photon Factory. The end station at this beam line is equipped with a hemispherical analyser for collection of photoelectron spectra. All SW profiles were taken for photon energies ranging from 610 to 700 eV by monitoring photoelectron intensities of N1s and Cd3d peaks.



Fig. 2

Result and discussion

Fig. 3 shows the SW profiles of N1s and Cd3d. We performed curve-fitting analyses for the profiles with two structural parameters, coherent factor (f_{co}) and vertical location from the center of the W layer (Δz). The resultant parameters are listed in Table 1. Carbon K-edge NEXAFS spectra were also measured to get information on the molecular orientation. The orientation angle of Az molecules was ca. 50° from the surface normal.

Fairly high f_{co} values indicate narrow distribution in height both for N and Cd atoms. It is clear from the Δz value for Cd that the Cd atoms are segregated at the molecule-substrate interface. Assuming the orientation angle of ca. 50°, the Δz value for the N atoms should be approximately 15 Å, which is in good agreement with the observed value (14.5±0.2 Å) as shown in Fig. 4.

In conclusion, the XSW technique using ultra-soft Xrays and W/C multilayer can provide information on vertical locations of specific atoms involved in rather thick monolayers like organic thin films.



Fig. 3 Fit of N1s (a) and Cd3d (b) XSW profiles



Fig. 4 Result of XSW experiment

*ohta@chem.s.u-tokyo.ac.jp