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Circular dichroism of forward focusing peaks and diffraction rings in 2π steradian Si 2p photoelectron pattern

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Abstract

2 π steradian Si 2p photoelectron pattern from Si(0 0 1) surface was measured. The circular dichroism of rotational shift around the incident-light axis was observed. Shifts for the forward focusing peaks in {1 1 1} and {0 1 1} directions were inversely proportional to the distance between the emitter atom and neighboring atoms in {1 1 1} and {0 1 1} directions, respectively. These shifts correspond to the parallax in stereograph of the atomic arrangements. On the other hand, such rotational shifts were not observed in {1 1 2} directions due to the first order diffraction rings around {1 1 0} directions. A gross feature of Si 2p photoelectron pattern can be explained by forward focusing peaks and first order diffraction rings around them.

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1. Introduction

The photoelectron from a localized core level is an excellent probe for element-specific atomic structure analysis. Forward focusing peak (FFP) appearing in photoelectron intensity angular distribution (PIAD) pattern indicates the direction of neighboring atom seen from emitter atom. FFP rotational shift caused by circularly polarized light excitation was shown to be inversely proportional to the distance between the emitter and scatterer atoms both experimentally [1] and theoretically [2]. Taking advantage of this circular dichroism, a stereo atomscope was realized [3–5]. Even real-time visualization has been achieved [6].

However, the diffraction patterns formed by the interference between direct photoelectron wave and scattered wave hinder precise determination of atomic distance. Systematic study of diffraction patterns have not been done yet.

We measured 2 π steradian (full hemisphere) Si 2p PIAD pattern from Si(0 0 1) surface. The circular dichroism of rotational shift around the incident-light axis was observed for FFPs in {1 1 1} and {0 1 1} directions. Rotational shifts were in the same direction as the rotation of the electric vector of incident light. On the other hand, the first order diffraction rings around FFPs in {0 1 1} directions appeared at several degrees off from {1 1 2} directions. Rotational shifts in {1 1 2} directions were also expected, however the circular dichroism of diffraction rings were more pronounced in this case. Here we show that the gross feature of Si 2p PIAD pattern can be explained by FFPs and first order diffraction rings around them.

2. Experimental

The experiments were performed at the circularly polarized soft X-ray beamline BL25SU of SPring-8, Japan [7]. The Si(0 0 1) sample was annealed at 1400 K for a few seconds in

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the ultra high vacuum chamber to obtain a clean surface. After the annealing, a sharp 2 × 1 RHEED pattern was observed. Neither the C 1s nor the O KLL peak was detected in the core-level spectra.

PIAD from sample at specific kinetic energy is most efficiently measured by a two dimensional display-type spherical mirror analyzer (DIANA) [8–10] which enables measurement of a two-dimensional angular distribution of specific kinetic energy electron at the same time [3–5,11–13]. Fig. 1 (a) is a schematic diagram of DIANA and measurement set up. Light was incident from the direction 45 ° inclined from the center of the analyzer. Photoelectrons emitted from the sample are energy analyzed and PIAD pattern is projected onto the fluorescent screen with the emission angle preserved. Acceptance angle of the analyzer is ±60°.

Sample was mounted on a five-axis manipulator. Light was incident from the surface normal direction. The emission angle (θ_{out}) dependence from 0° to 90° respective to the surface normal was measured simultaneously. By scanning the sample azimuth for 360°, 2π steradian PIAD was obtained [12]. Helicity ($\sigma_\pm$) of monochromatized circularly polarized soft X-ray was reversed by switching the path of storage ring electron in twin helical undulators at 0.1 Hz [14]. Total acquisition time for a pair of 2 π steradian PIADs excited by σ_+ and σ_- helicity light was 2 h.

3. Results and discussions

Fig. 2 shows a series of PIADs excited with σ_+ and σ_- helicity light together with circular dichroism patterns. Photoelectron kinetic energy was 600 eV. Azimuthal angle was varied from -5 ° to 365° at the interval of 5°. FFPs in the [0 0 1] direction marked with dot matches with rotational axis. FFPs in the {0 1 1} and {1 1 1} directions indicated by open circles move from left to right as the sample rotates. In the case of σ_- excitation, FFP rotational shifts in counterclockwise direction were observed, while in the case of σ_+ excitation, shifts were in clockwise direction. In the circular dichroism patterns shown in Fig. 2(b), such shifts appear as a pair of bright and dark patterns.

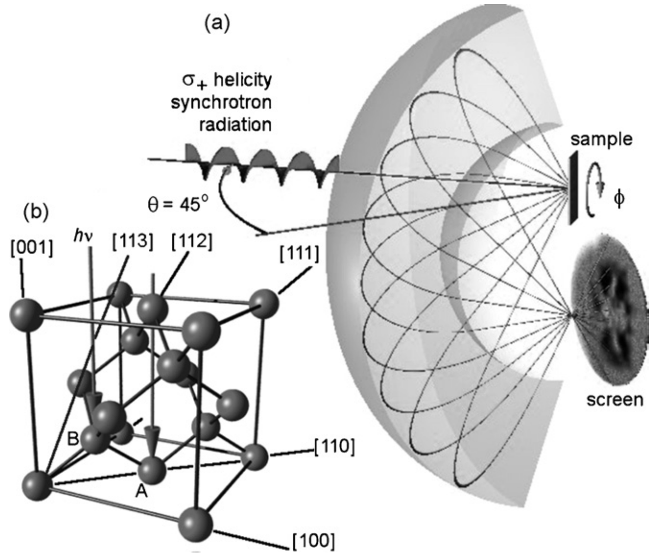

Fig. 1. (a) Schematic drawing of display-type analyzer and Si(0 0 1) sample. (b) Structure model of diamond lattice. Arrows indicate incident light. Two kinds of non-equivalent sites are labeled as A and B.

Fig. 3 is a pair of $\sigma_\pm$-excited PIADs displayed in Mercator projection. 'Gaussian weight coefficients' having a peak at the center of the screen were applied to each PIAD. Then the series of azimuthal angle scanned PIADs were seamlessly combined [12]. Bright spot in the center ($\Theta = 35.6°$, $\Phi = 0°$) corresponds to the FFP of the first nearest atom in the [111] direction. Angle of rotational circular dichroism was ±2.5°. Two features appearing at the left and right sides of panels ($\Theta = 45°$, $\Phi = \pm 45°$) correspond to the FFP of the second nearest atoms in the [0 1 1] and [1 0 1] directions. Angle of rotational circular dichroism was ±1.8°. Finally, [1 1 0] FFP was observed at horizon ($\Theta = 0°$, $\Phi = 0°$). Angle of rotational circular dichroism was ±0.9°. When the left panel seen with the left eye, and the right panel with the right eye, respectively, the three dimensional atomic arrangement of the first and second nearest Si atoms can be recognized. Thus the stereo photographs have been successfully obtained.

Note that the broad structure around [1 1 2] direction ($\Theta = 54.6°$, $\Phi = 0°$) is splitted into two parts. The position of intensity maxima in the feature around [1 1 2] direction shows circular dichroism *in opposite side*. In order to clarify this reason, we combined all the PIADs together and examined 2π steradian PIAD.

Fig. 4 is 2 π steradian PIAD displayed in stereo projection. No symmetry operation was applied. Four-fold rotational symmetry is due to the superimpose of diffraction patterns from two non-equivalent atom sites A and B shown in Fig. 1(b). Diffraction rings [15] were investigated and their radii were determined from the systematic PIAD analysis of photoelectron kinetic energy dependence. Radii of the first order diffraction rings around [1 1 1], [1 1 0], and [0 0 1] FFPs were 38.0 °, 24.0°, and 22.5°, respectively.

The first order diffraction rings around {1 1 1} directions overlaps with FFPs in {0 1 1} directions. They enhance circular dichroism intensity of {0 1 1} FFPs. On the other hand, the first order diffraction rings around {0 1 1} directions appears at about 6° off from FFPs in {1 1 2} and 10° off from FFPs in {1 1 1} directions. FFPs in {1 1 1} directions due to first nearest atoms appear strong compared to the {0 1 1} diffraction rings, however, those in {1 1 2} directions have comparable intensity with that of the {0 1 1} diffraction rings. Two splitted parts in the broad structure around [112] direction is due to the diffraction rings around {0 1 1} directions and rotates in the same direction as {0 1 1} FFP. FFPs in {1 1 2} directions rotate little and rather enhance the circular dichroism of these diffraction patterns. This is the reason of the circular dichroism *in the opposite side*. Rotational shifts in {1 1 2} directions were also expected. However the circular dichroism of diffraction rings were more pronounced in this case.