Crystal Structures Studied by Stereo Atomscope

Stereo atomscope, which is realized by the combination of display-type spherical mirror analyzer (DIANA) and circularly polarized X-ray, opens a way to study three-dimensional crystal structures directly [1]. In this paper, the atomic stereo-photograph of Cu (001) single crystal, one of the typical studies of stereo atomscope, will be introduced.

The basic principle of stereo atomscope is circular dichroism in photoelectron angular distribution (PEAD), where forward focusing peak positions rotate in the same direction as that of circularly polarized X-ray electric vector (Fig. 1). The rotation is caused by the angular momentum transfer from circularly polarized X-ray to emitted photoelectrons. The azimuthal shifts of the forward focusing peaks at clockwise (cw) and counterclockwise (ccw) circularly polarized X-rays are utilized as parallax. Here, the cw and ccw circularly polarized lights are defined according to the rotation direction of the electric vector at the sample observed from behind. From the azimuthal shift formula ($\Delta = m/kR \sin^2\theta$) [2], the atomic distance (R) or the magnetic quantum number (m) can be obtained.

The schematic image of DIANA is shown in Fig. 2. The emitted photoelectrons of a particular kinetic energy converge to an exact focal point, and the two-dimensional angular distribution of the photoelectrons can be measured simultaneously without rotating the sample. The wide acceptance angle (±60°) and the distortion free angular distribution of the photoelectrons make DIANA the best analyzer for taking atomic stereo-photographs. Circularly polarized X-rays are produced at beamline **BL25SU**.

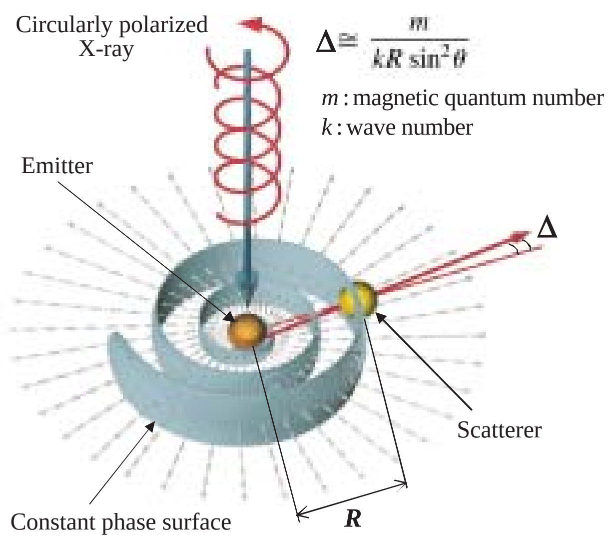

Fig. 1. Image of circularly polarized X-ray and forward focusing peak rotation. The blue strip describes the constant phase surface on which photoelectrons propagate perpendicularly.

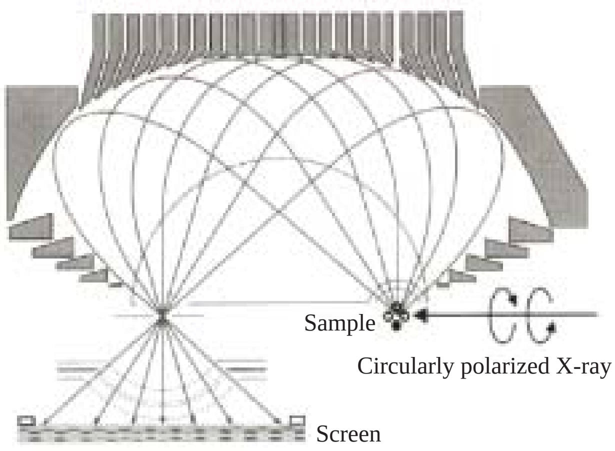

Fig. 2. Schematic image of DIANA. The emitted photoelectrons of a particular kinetic energy converge to an exact focal point.

Single crystal Cu(001) was cleaned by repeated cycles of Ar bombardment and annealing. The clean surface was checked by reflective high-energy electron diffraction (RHEED). Experimental results are shown in Fig. 3. The photographs (a) and (b) show the Cu2*p* PEAD patterns taken by DIANA with a pass energy of 500 eV using the cw and ccw circularly polarized X-rays, respectively. The forward focusing peaks distribute regularly. They shift right at cw and left at ccw circularly polarized X-rays. The shift angles become smaller and the peak intensities become weaker for inner peaks, which indicates that the forward focusing peaks are caused by atoms lying in different layers. In order to understand the distribution easily, we marked the forward focusing peaks by circles with different colors. The PEAD patterns show good agreement with the simple projection (d) from the fcc crystal structure model (c) of Cu(001), where the atoms lying in different layers are distinguished by different colors.

The two PEAD patterns form the atomic stereo-photograph viewed from specific atoms. It displays the three-dimensional atomic arrangements of four nearest layer atoms in single crystal Cu(001) along the [001] direction with a magnification of approximately 1 billion. The distorted peaks in the PEAD patterns are caused by the low transmission and inhomogeneity of retarding grids. The forward focusing peak, which should appear at the right-down position, cannot be observed because of the shadow caused by the electron gun of DIANA. The forward focusing peaks should be sharper under higher kinetic energies; however, the kinetic energies of more than 500 eV are unavailable at present due to the discharge of the analyzer.

Using atomic stereo-photography, not only the atomic stereo-photographs of one-element single crystals, but also those of compounds and intercalation compounds were obtained successfully [3,4]. The direct atomic stereo-photographs obtained by stereo atomscope without any conversion process make it possible to realize real-time observation, which will be used in understanding the dynamics of atoms. The improvements of the stereo atomscope are currently in progress for the construction of an ultimate microscope.

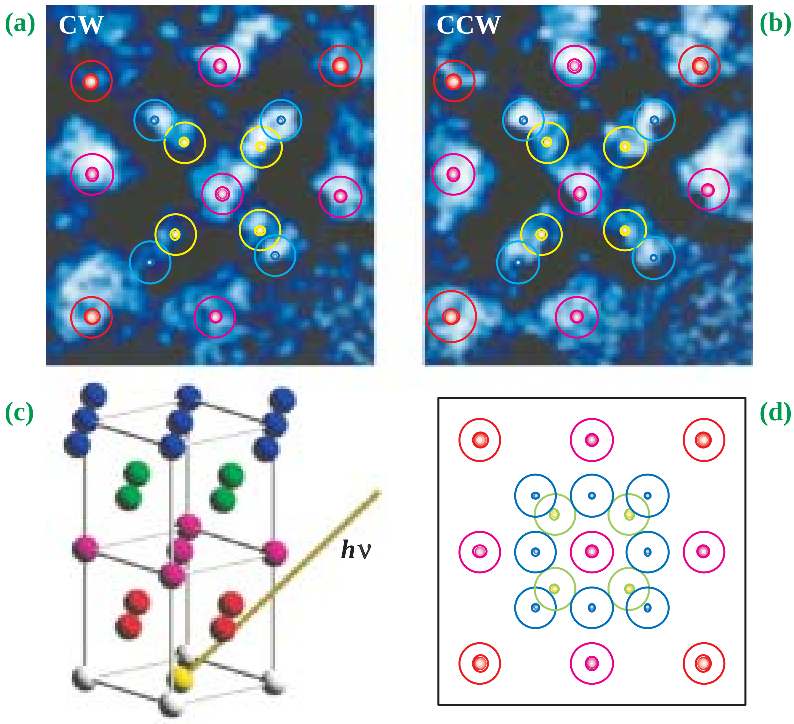

Fig. 3. **(a), (b)** Cu2*p* PEAD patterns taken by DIANA with a pass energy of 500 eV using the cw and ccw circularly polarized X-rays. **(c), (d)** fcc crystal model of Cu(001) and atomic arrangement simple projection.

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