In (2), t is the path length of the rays in the crystal.

For a sphere, considering the usual spherical coordinates r, α, φ (the polar axis z is normal to the diffraction plane), t is calculated as follows:

$$t(r,\alpha,\varphi) = -2r\sin\theta\sin\alpha\sin\varphi + [R^2 - r^2\cos^2\alpha - r^2\sin^2\alpha\sin^2(\theta-\varphi)]^{1/2} + [R^2 - r^2\cos^2\alpha - r^2\sin^2\alpha\sin^2(\theta+\varphi)]^{1/2}, \quad (4)$$

with θ = Bragg angle, R = radius of the sphere.

From the symmetries of t in α and φ, the integration of (2) can be reduced to a quarter of the sphere:

$$\int_{\text{sphere}} dv = 4\int_0^R dr \int_0^{\pi/2} d\alpha \int_{-\pi/2}^{\pi/2} d\varphi\, r^2\sin^2\alpha. \quad (5)$$

This three-dimensional integration cannot be performed exactly in the general case, but can be accurately carried out by the numerical Gauss method. This calculation was done on an IRIS 80 (CII H-B) computer with 10^3 to 32^3 grid points of integration for the range 0·1–4·0 of μR, which is that over which the Becker–Coppens extinction theory is valid and covers most practical situations with accurate data. The results of this computation are given in Table 1.

For $\theta = 0$ and 90°, $\bar{T}_{\mu R}$ can be exactly known from (1) and the exact values of A for these angles (*International Tables for X-ray Crystallography*, 1959):

$$\theta = 0°,\quad \bar{T}_{\mu R} = 3 - 2(\mu R)^3/[1/2\exp(2\mu R) - 1/2 - \mu R - (\mu R)^2];$$

$$\theta = 90°,\quad \bar{T}_{\mu R} = 1 + \{2[1 + 4\mu R + 8(\mu R)^2] \times \exp(-4\mu R) - 2\}/[(1 + 4\mu R)\exp(-4\mu R) - 1 + 8(\mu R)^2].$$

These functions provide a good check of the accuracy of the previous computation and we found that the root-mean-square error based on them is less than 0·0005 for all of Table 1 (these exact values are given in Table 1 instead of the computed ones). The accuracy of this table is therefore better than 0·1%.

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Polarization states of dynamically diffracted X-ray beams.

By S. ANNAKA, *Tokyo University of Mercantile Marine, Etchujima, Koto-ku, Tokyo, Japan* and T. SUZUKI and K. ONOUE, *Faculty of Science and Technology, Sophia University, Kioicho, Chiyoda-ku, Tokyo, Japan*

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Abstract

A phase difference between the coherent σ and π components of dynamically diffracted X-rays was observed in the Laue case. The incident X-ray beam was linearly polarized Cu $K\alpha$ radiation. A Si single crystal was used to produce the phase difference. The Ge 333 reflexion was used to polarize the incident beam and also to examine the polarization state of the diffracted beam in the 220 Laue-case reflexion from a Si crystal. For comparison, the polarization state in the Bragg case was also analysed.

Polarization phenomena of X-rays are one of the basic problems in X-ray scattering. Recently, changes in the polarization states of X-ray beams were reported for Laue-case diffraction (Skalicky & Malgrange, 1972; Sauvage, Petroff & Skalicky, 1977) and for simple transmission through a (110) Si crystal (Cohen & Kuriyama, 1978). In the former case it was shown that the phase difference between the σ and π components was produced in a similar way to linearly polarized visible light.

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According to the dynamical theory of X-ray diffraction for the two-beam case (Kohra, 1961; Batterman & Cole, 1964), two diffracted waves with different wave vectors are produced which correspond to the two branches (I, II) of the dispersion surfaces and thus in the Laue case the *Pendellösung* fringes can be observed. Furthermore, for the same branch, *e.g.* branch I with wave vector $\mathbf{k}_{h1}$, there are two different wave vectors, $\mathbf{k}^{\sigma}_{h1}$ and $\mathbf{k}^{\pi}_{h1}$ corresponding to the σ and π dispersion surfaces. At the exact Bragg condition and for the symmetrical Laue case the phase difference φ between the σ and π components for the branch I is given by

$$\varphi = 2\pi(\mathbf{k}^{\sigma}_{h1} - \mathbf{k}^{\pi}_{h1}).\mathbf{r}, \quad (1)$$

where $\mathbf{r}$ denotes the position vector. Equation (1) can be rewritten using the real part of the Fourier coefficient of the susceptibility of the crystal ψ'_H

$$\varphi = \pi|\mathbf{k}||\psi'_H|(1 - |\cos 2\theta|)\, t_0/\cos\theta, \quad (2)$$

where $\mathbf{k}$, t_0 and θ are the wave vector of the incident X-ray beam, the thickness of the specimen and the Bragg angle, respectively. In this communication we report some experimental results for the change of the polarization state in the symmetrical Laue case, and gave a comparison with the symmetrical Bragg case.

The experimental arrangement is shown in Fig. 1. The linearly polarized and horizontal X-ray beam of Cu $K\alpha$ was obtained by the 333 reflexion from a grooved Ge crystal (Post, 1975). The beam from the crystal was polarized at 45° with respect to the horizontal plane (*cf.* insert in Fig. 2) and diffracted by the vertical (220) plane of a perfect Si crystal. The polarization state of the 220 reflexion beam was analysed by measuring the integrated intensities of the 333 reflexion from a Ge crystal. The crystal and the scintillation counter (SC) were rotated about an azimuthal axis parallel to the incident beam. The optical path length l of the X-rays in the symmetrical Laue-case diffraction can be expressed as $l = t_0/\cos\theta$. The crystal was etched to give a path length of 52 μm with a phase difference of 180° at the exact Bragg condition for the σ and π components. In Fig. 2 the observed integrated intensities of the 333 reflexion are plotted against the rotation angle ω of the analyser crystal (*cf.* C in Fig. 1). Here, $\omega = 0°$ refers to a horizontal beam. The values of the intensities (open circles) are normalized to the intensity at $\omega = 0°$; maximum reflection intensity is obtained at $\omega = 20°$, approximately.

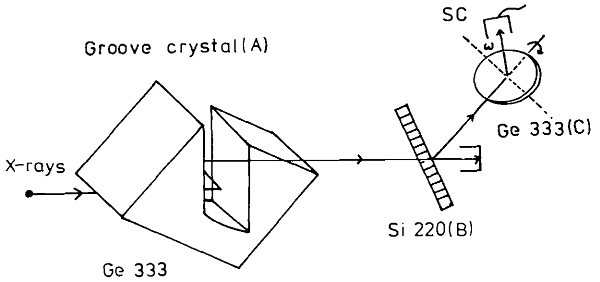

Fig. 1. Schematic view of the experimental arrangement. The plane of polarization of a horizontal X-ray beam from the polarizer (A) is inclined by 45° with respect to the plane of incidence of Si (B). Groove surfaces of the polarizer are cut at 45° with respect to the (111) plane. The polarization state of the 220 reflexion beam from the silicon was analysed with the analyser (C).

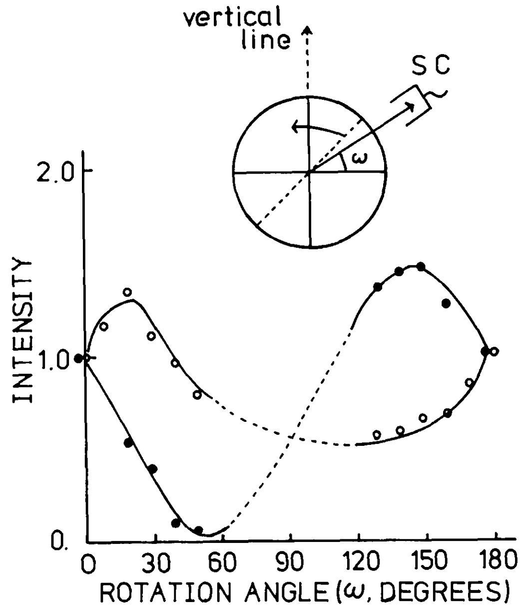

Fig. 2. Relative intensity variations of the 333 reflexion from the analyser against its rotation angle ω about the incident beam. Open circles and full circles correspond to the 220 Laue-case and Bragg-case diffractions, respectively. The plane of polarization of an incident beam is shown as a dotted line in the insert.

In a similar fashion, the polarization state of the reflected 220 beam in the symmetrical Bragg case, which should produce no phase difference, was analysed. The observed integrated intensities of the 333 reflexion are plotted in Fig. 2 (full circles). Assuming an amplitude ratio $1/\cos 2\theta$ for the σ and π components, the calculated intensity variation against ω coincides well with the experimental one. When the experiment of the Laue-case diffraction is compared with that of the Bragg case, it can be easily seen that the plane of polarization of the reflected beam must have rotated from its original position at the right of the vertical (*cf.* insert in Fig. 2) to a position at its left.

One may conclude that for the Laue-case diffraction and for a linearly polarized incident beam the phase difference between the σ and π components is produced. However, it will be difficult to determine the change of the polarization states in the dynamical diffraction, because four diffracted waves with different absorption coefficients are produced in the crystal and the amplitude ratio of the intrinsic rocking curve for the σ and π components depends on the Bragg angle θ.

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