Crystallography

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Phase Observation of Crystal Structure Factor by using Rocking-curves

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According to the resonant X-ray dynamical theory of diffraction, the crystal structure factor for a crystal with centre of symmetry is given by

$$F_h = F_{hr} + iF_{hi} = |F_{hr}|(1+k^2)^{1/2} \cdot \exp[i\{\arg(F_{hr}) + \theta\}].$$

Here F_{hr} and F_{hi} are the crystal structure factor due to the real and imaginary parts of the atomic scattering factor. For the crystal, $\arg(F_{hr})$ is either 0 or π,

$\theta = \tan^{-1}[k \cdot \cos\{\arg(F_{hi}) - \arg(F_{hr})\}]$ and

$k = |F_{hi}| / |F_{hr}|$.

In the two-beam approximation, the crystal structure factor must satisfy the condition:

$$F_h F_{-h} / (|F_{hr}|^2 + |F_{hi}|^2) = e^{i2\theta}.$$

This condition is expressed as a point on the unit circumference in Fig.1 [1]. If the phase difference $\Delta\varphi$ between interference fringes in the diffracted and transmitted rocking curves is measured, the angle of 2θ can be determined.

The diffraction experiments of GaAs 200 in Laue case were carried out at BL-15C of KEK-PF. The X-rays from synchrotron radiation were monochromated by a Si 111 double-crystal monochromator and by an asymmetric GaAs 200 monochromator. The energy resolution was ±0.5eV. X-rays with σ-polarization were used. The sample thickness was 45μm and the EPD value of the sample was less than 500cm^{-2}.

Fig. 2 shows the diffracted (I_h) and transmitted intensities (I_t) measured by changing the incident X-ray energy ω as (a) 10360.5 eV, (b) 10501.0eV, (c) 11403.0 eV, (d) 11805.0eV and (e) 11861.5 eV [2]. The phase difference $\Delta\varphi$ is π (anti-phase) in Fig.2 (a), 0 (in-phase) in (c) and $-\pi$ in (d).

If the origin of the coordinate is chosen at a Ga site, $\arg(F_{hi})$ is 0, because ω is changed between Ga-K and As-K edges in this experiment. At point B in Fig.1, as the measured $\Delta\varphi$ is -0.4π from Fig. 2 (b), 2θ is -0.41π and $\arg(F_{hr})$ is determined to be π. This result is reasonable, as $(f^0 + f')_{Ga} < (f^0 + f')_{AS}$ near Ga K-edge. At point D, as the measured $\Delta\varphi$ is 0.4π from Fig. 2 (d), 2θ is 0.41π and $\arg(F_{hr})$ is determined to be 0. This is also reasonable, as $(f^0 + f')_{Ga} > (f^0 + f')_{AS}$ near As K-edge.

It is noted that the measurement of 2θ is quite useful for the phase determination of the structure factor.

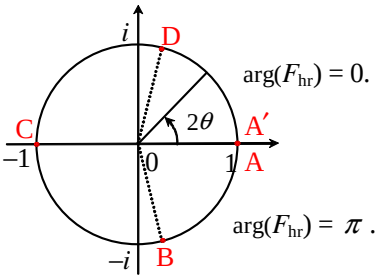

Fig.1 A unit circle representing scattering conditions. $\arg(F_{hi})$ is 0.

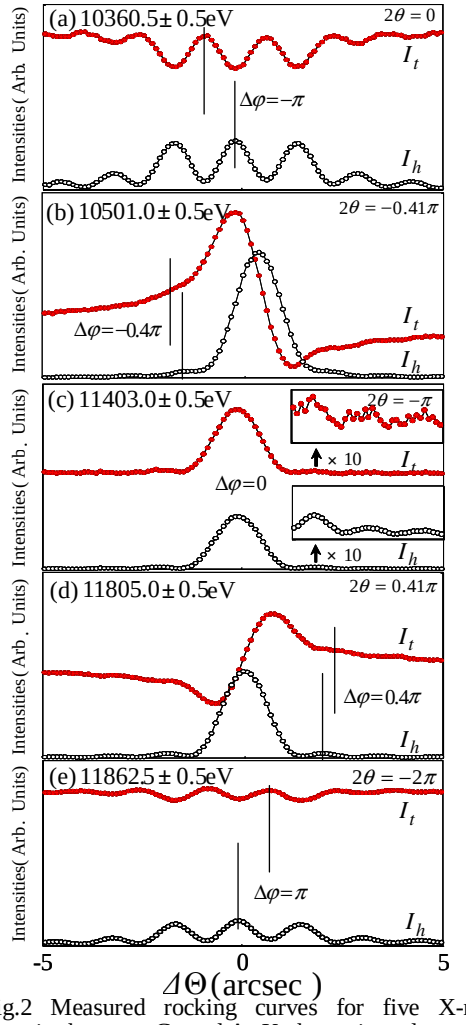

Fig.2 Measured rocking curves for five X-ray energies between Ga and As K-absorption edges.

Reference

[1] Negishi, R., *et al., J. Synchrotron Rad.*, **11**,266-271(2004).
[2] Negishi, R., *et al., J. Phys. Soc. Jpn.*, **77**, 23709_1-3(2008),.