Crystallography

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Phase Determination of Crystal Structure Factor by Using Measured Rocking Curves

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In the last year, we observed the phase difference $\Delta\varphi$ between the interference fringes of the diffracted intensities I_h and those in the transmitted intensities I_t for an absorbing crystal and pointed out that the phase difference would be applied to phase determination [1]. In this paper, we report on a novel method of phase determination of the crystal structure factor by using the phase difference.

For a crystal with a center of symmetry, the crystal structure factor is given by

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

Here, F_{hr} and F_{hi} are the Fourier transforms of the real and imaginary components of the structure factors respectively, $k = |F_{hi}|/|F_{hr}|$, $\delta = \alpha_i - \alpha_r$ and $\theta = \tan^{-1}(k\cdot\cos\delta)$.

If we take the site of a resonant atom as the origin of the coordinate in a unit cell of a crystal, α_i is zero as $f'' \geq 0$. Once δ is given, we can determine α_r, i.e., the phase of F_{hr}. According to a dynamical diffraction theory including resonant scattering, the crystal structure factor satisfies the condition [2]

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

Fig.1 shows the measued diffracted intensities I_h and transmitted intensities I_t of GaAs 200 in the Laue case when the X-ray energy is changed across the absorption edge of Ga (10367 eV). The phase 2θ changes as a function of the X-ray energy ω as shown in the left inset of each figure. The phase difference $\Delta\varphi$ is (a) $-\pi$ for $\omega = 10360$eV , (b) -0.4π for 10501eV, (c) -0.1π for 10914eV, and (d) 0 for 11403eV.

We have the relation between $\Delta\varphi$ and 2θ as shown in Fig.2. In the cases of Figs.1 (b) and (c), $2\theta < 0$ and the value $\delta = \pi$ is obtained regardless of the value of *k*. Then α_r is determined to be $-\pi$, which agrees with the calculated value. This approach is quite useful to phase determination, because the phase is to be determined by simply measuring rocking curves. It is also an adavantage that this approach can be easily extended to a crystal with no center of symmetry.

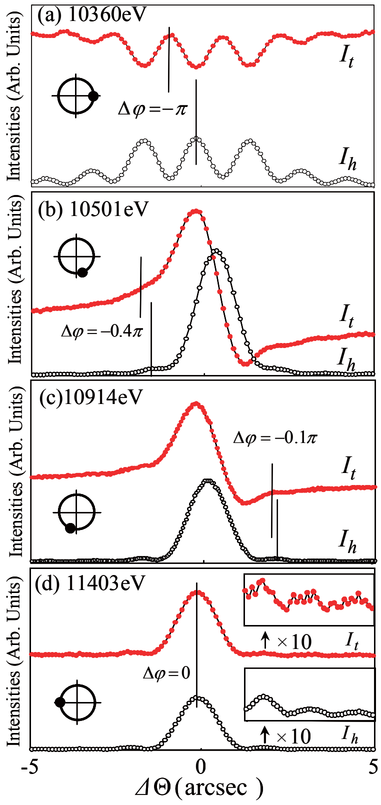

Fig.1 Measured rocking curves. The crystal thickness is 45μm.

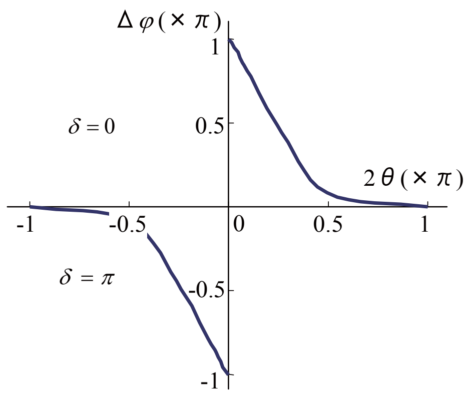

Fig.2 The calculated relation between 2θ and Δφ.

References

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