Anomalous Dispersion Effects on X-ray Multiple Diffraction in Silicon

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We have studied the anomalous dispersion effects on the phases of reflections in silicon using three-beam multiple diffraction for photon energies from 4.2 keV to 2.7 keV[1]. From the experiments of X-ray three-beam diffraction with the primary reflection G=(002) and secondary reflection L=(1-11) at different energies, we have observed the shift of triplet phase of about 18 degrees due to the increase of the imaginary part and the decrease of the real part of the atomic scattering factors as the photon energy approaches 2.7 keV. In addition, the triplet structure factors involved can be determined even with the presence of the forbidden (002) reflection.

The Experiment - Renninger Scan

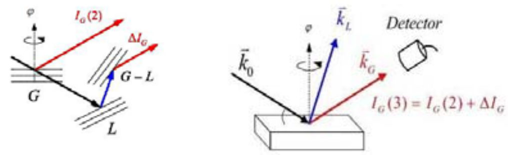

Fig. 1 and Fig. 2: The geomtey relation of incident and reflected beams

The interaction among the diffracted beams inside the crystal results in intensity modification on the primary reflection. We use a photo diode to monitor the intensity-modified diffracted beam. The intensity modification versus φ is recorded, the so-called Renninger scan.

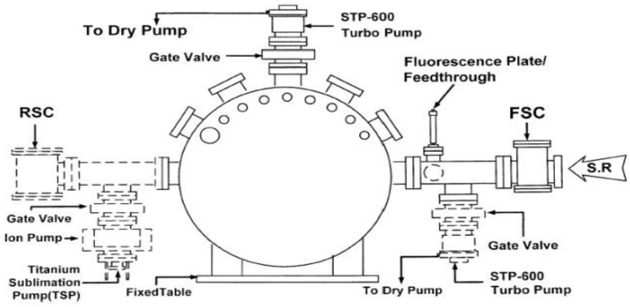

Fig. 3: Soft X-ray diffractometer, in which the vaccum pressure can go down below 10e-6 torr.

The experiment was carried out in vacuum at beamline 16A, NSRRC, because of the air absorption for photon energies below 5 keV.

Quantitative Determination of Phases of X-ray Reflections

The interaction among the diffracted beams inside the crystal leading to phase determination can be described by the dynamical theory of X-ray diffraction. The first-order approximation, polarization of wave fields, and Lorentz factor of rotation are considered. The formula can be derived from the theory, where I_2 is the intensity of two beams diffraction, A and B are in relation to the X-ray wavelength and geometric factors in the reciprocal space.

$$\frac{I_G}{I_2} = 1 + AF_3 \frac{\Delta\varphi\cos\delta_3 - \frac{\eta}{2}\sin\delta_3}{(\Delta\varphi)^2 + (\frac{\eta}{2})^2} + BF_3{}^2 \frac{1}{(\Delta\varphi)^2 + (\frac{\eta}{2})^2} \quad (1)$$

$$F_3 = \left|\frac{F_L F_{G-L}}{F_G}\right| \quad (2) \qquad \delta_3 = \delta_{\mathrm{L}} + \delta_{\mathrm{G\text{-}L}} - \delta_G \quad (3)$$

Result

From the fitting of each peak at different energy of X-ray, the triplet phase of G(002) L(1-11) will shift about 18 degrees from 180°. This is due to the increase of the imaginary part and the decrease of the real part of the atomic scattering factors as the photon energy approaches 2.7 keV.

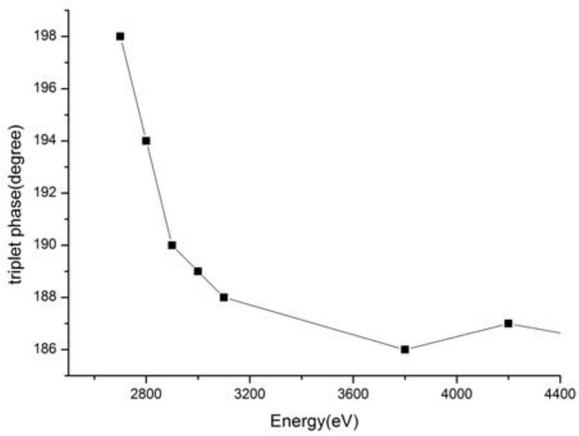

Fig. 4: The shift of triplet phase vs. photo energies.

Reference

[1] S.-L. Chang and M.-T. Tang, Acta Cryst. A **44**, 1065 (1988).