11.7-8 THE FOUR-BEAM CASE: NEUTRON MEASUREMENTS ON α-QUARTZ. By H.Jagodzinski,N.Semioschkina,H.Boysen,F.Frey, Institut für Kristallographie, Universität München, F.R.Germany

Multiple beam diffraction can be applied to determine phase relationships between the waves involved. We are concerned with the 4-beam case where apart from 0* three further reciprocal lattice points $\underline{h}_1,\underline{h}_2,\underline{h}_3$ lie simultaneously on or close to the Ewald-sphere or - with other words- three Kossel cones have a common generator coinciding with the direction of the incoming beam. In practice this may be accomplished by turning the crystal around a basic vector $\underline{h}_1$ and simultaneously adjusting an appropriate wavelength. The active area in reciprocal space is determined by the wavelength band, instrumental parameters and the sample mosaic. Making the observations in the direction of a forbidden reflection (here $\underline{s}_1$) interference effects may be studied between waves which are all due to "Umweganregung",i.e.their intensities are of the same order of magnitude. Compared with the 3-beam case the dominating influence of $\underline{h}_1$ is avoided,i.e. interference effects may be studied over the whole pattern. The resultant wave bears information about phase differences

$$[\phi(h_2) + \phi(h_1 - h_2)] - [\phi(h_3) + \phi(h_1 - h_3)]$$

(and others due to double Umweganregung-effect). Experiments were carried out with neutrons for three reasons:(i) absorption is negligible,(ii) a tunable wavelength band is easily available, (iii) polarization effects do not occur: in an X-ray experiment- in particular a synchrotron storage ring- there is some uncertainty about polarization in a multiple-beam experiment in the transition regime between kinematical and dynamical theory of diffraction.Monochromator: Ge(333),mosaic:8"; wavelength band: $\Delta\lambda/\lambda \sim 10^{-3}$; sample: α-quartz; mosaic: 9"; h_1=001 . Due to Umweganregung the sample acts as a secondary monochromator narrowing the wavelength band. 3- and 4-beam cases were calculated in dependence on λ_0, the setting angle ω and the azimuthal orientation φ . Scanning through the 4-beam case is either performed by variation of ω which in turn affects λ_0, or φ , the detectors is fixed at the $2\theta(001)$-position. Intensity curves were recorded in both ways. The intensity profiles are fully reproducible. Asymmetric peaks may be understood as a consequence of phase differences $\Phi(h_2),\Phi(h_3)$. The interference pattern are remarkably extended both in dependence on ω and φ , and subsidiary maxima occur possibly due to other multiple beam cases These observations seem to be in agreement with results from calculations based on dynamical theory of diffraction of α-quartz (Kon,phys. stat.sol(a)54(1979)375 and priv.comm.) and -in favourable cases- might offer a possibility for the ab initio determination of phases. It should be emphasized,however,that crystal perfection is no necessary condition for these observations since asymmetric line profiles may also be explained with the aid of kinematical theory of diffraction.

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11.7-9 TEMPERATURE EFFECT OF X-RAY DIFFRACTION INTENSITIES FROM A PERFECT CRYSTAL FOR THE LAUE CASE

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Considering the variance of susceptibility, χ, produced by the change of temperature, from the revised Taupir-Takagi equation we derived the expression of X-ray diffraction intensities from a perfect crystal as a function of temperature.

We have reported the dynamical diffraction equations for a perfect crystal (Sun Zhangde, Acta cryst., to be published).

$$\begin{aligned}&\nabla^2 D_o - i4\pi(\vec{K}_o\cdot\nabla)D_o + 4\pi^2K^2\chi_o D_o + 4\pi^2K^2C\chi_{\bar{h}}D_h = 0\\ &\nabla^2 D_h - i4\pi(\vec{K}_h\cdot\nabla)D_h + 4\pi^2K^2\chi_o D_h + 4\pi^2K^2C\chi_h D_o = 0\end{aligned} \quad (1)$$

Assuming that the crystal is non-absorbing, the susceptibility of medium could be given by:

$$\chi = -\frac{12\pi n n_i e^2}{3mw^2 + 16\pi^2 n n_i e^2} \quad (2)$$

there n is the number of atoms in unit volume; n_i the number of electrons in an atom; w the frequency of incident X-ray. Under an action of temprature field, the average local deformation of lattice, $\bar{u}$, is obtained by:

$$\bar{u} = \frac{\int u e^{-\frac{U}{kT}} du}{\int e^{-\frac{U}{kT}} du} \approx \frac{\sqrt{2kT}}{\omega_o\sqrt{\pi m}} \quad (3)$$

For a cubic crystal and the symmetric Laue case, the X-ray diffraction intensities at exit surface is derived:

$$\begin{aligned}I = D_{o,h}^2 = &\frac{2}{\pi^3K^2\gamma^2(2+\chi)^2}\left[1 + \frac{6\chi\sqrt{\frac{2kT}{\pi m}}}{(2+\chi)a_o\omega_o}\right]\\ &\cdot \sin^2\left\{\pi K\gamma\left[(2+\chi) - 3\chi\frac{1}{a_o\omega_o}\sqrt{\frac{2kT}{\pi m}}\right] - \frac{\pi}{2}V\right\}\\ &\cdot A_{o,h}^2(\xi)\end{aligned} \quad (4)$$

there

$$A_{o,h}(\xi) = \begin{cases}\frac{1}{V\sqrt{\xi}}J_1(2V\sqrt{\xi}) & \text{for } K_o\\ J_o(2V\sqrt{\xi}) & \text{for } K_h\end{cases}$$

$$\xi = \frac{1}{2}[1 - t/\gamma - B]$$

$$B = \frac{\lambda^2\cdot\frac{1}{\omega_o}\sqrt{\frac{2kT}{\pi m}}}{2d_o a_o\sqrt{4d_o^2\left(1+\frac{2}{a_o\omega_o}\sqrt{\frac{2kT}{\pi m}}\right) - \lambda^2}}$$

The results of computor calculation show:(1) The criterion of geometrical optics is r>t/(1-B), t is the thickness of sample. r will increace with the temperature going up. (2) The distribution of X-ray diffraction intensities would be the pendellosung fringes when the temperature is very low. (3) The intensities decrease and the positions of fringes move outward when the temperature increase.