

11.7-17 DYNAMICAL DIFFRACTION OF X-RAYS AT GRAZING INCIDENCE. By O. Sakata, H. Hashizume and I. Minato, Research Laboratory of Engineering Materials, Tokyo Institute of Technology, Nagatsuta, Midori, Yokohama, 227 Japan.

The X-ray standing wave technique for the localization of surface atoms has been used so far with crystals in the Bragg-case geometry. Since the standing wave intensity is modulated along the diffracting vector  $h$ , the Laue-case geometry with  $h$  nearly parallel to the surface is more preferable for the studies of lateral structures of the surface. For this purpose total external reflection at grazing incidence angles is used to create a standing wave extending on both sides of the boundary surface (P. L. Cowan, 1985, Phys. Rev., 32, 5437-5439). Dynamical X-ray diffraction in this geometry involves two angles that can be controlled independently: the angle of incidence  $\phi_0$  and the deviation angle  $\Delta\theta$  from the exact Laue incidence. The geometry is best inspected using a three-dimensional dispersion surface. Fig. 1a shows a section of this surface (solid line) and of the reflecting spheres for the external waves (broken line) by a plane parallel to the boundary surface and passing through the reciprocal lattice point  $H$ .  $P_0'$  shows the projection of wave point  $P_0$  for the incident wave. Crystal wave fields are excited when line  $P_0 - P_0'$  cuts through the dispersion surface. It can be shown that the sectioned reciprocal space is divided into four regions, I to IV, where there are zero, one or two standing waves. For  $P_0'$  located in region I simple specular reflection occurs with no standing wave formed even when the Laue condition is exactly met. In region II the external diffracted wave is evanescent and the standing wave is confined in shallow depths of a few tens Angstrom on the both sides of the interface (P. L. Cowan, *ibid.*). Here the real part of the external wave vector remains parallel to the crystal surface. Calculations show that an abrupt change occurs in the specularly reflected beam intensity whenever  $P_0'$  traverses the sectioned dispersion surface. The  $\phi_0$  angles where the change occurs define critical angles of total reflection for the two wave fields associated with the two branches of the dispersion surface. A 100% specular reflectivity is expected from non-absorbing crystals only when  $P_0'$  is located in region I. Otherwise the incident energy is partly spent in exciting the crystal fields.

We have confirmed some of the above predictions in experiments using a germanium or gallium arsenide crystal at a synchrotron radiation source, where secondary fluorescent X-rays were measured from the specimen together with the specular and diffracted beams.

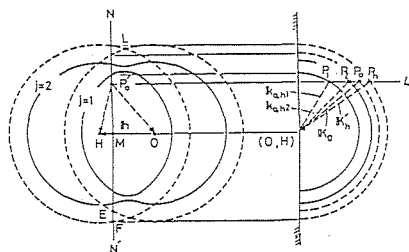
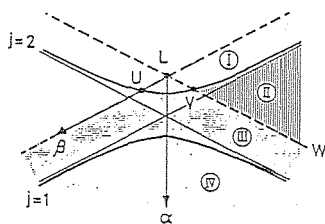


Fig. 1a (left), 1b (right) and 1c (bottom)



11.7-18 EXPERIMENTAL DETERMINATION OF TRIPLET PHASES AND ENANTIOMORPHS OF NON-CENTROSYMMETRIC STRUCTURES. By K. Huemmer, H. Bondza, E. Weckert, Inst. für Angewandte Physik, Lehrstuhl für Kristallographie, University of Erlangen, FRG.

Experimental results of phase determination by the method of three-beam interaction successfully applied to non-centrosymmetric light atom crystal structures with medium cell size are reported. Calculations based on the dynamical diffraction theory predict that the psi-scan profiles near a three-beam position show characteristics which depend on the triplet phase sum of the structure factors involved in a three-beam interference  $F(-h)F(g)F(h-g)$  (K. Huemmer, H. Billy, Acta Cryst. (1986), A42, 127-133).

The measurements were carried out with a special Psi-Circle-Diffractometer and a rotating Cu-anode equipment. The incident-beam divergence is reduced to  $0.02^\circ$  owing to a small effective focus size ( $0.1 \times 0.1 \text{ mm}^2$ ) in conjunction with a large crystal to source distance. The six diffractometer axes are computer controlled, the angular resolution of each circle is  $0.001^\circ$ .

The experimental results confirm our theoretical considerations. In addition, the measurements show that the phase-dependent interference effects may be superposed on phase-independent Umweganregung or Aufhellung effects. Comparing the psi-scan profiles of the two centrosymmetric correlated three-beam cases  $h/g$  and  $-h/-g$ , whose triplet phases have opposite sign but equal values, it is possible to evaluate the phase-independent effects. Thus, the triplet phases can be determined with an accuracy of about  $45^\circ$ . A computer program for this procedure will be prepared. As the triplet phases of  $\pm\phi_0$  can well be distinguished the absolute configuration of the structure can be unambiguously fixed.

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11.7-19 DETERMINATION OF THREE-PHASE INVARIANTS FROM FOUR-BEAM EFFECTS - USE OF EFFECTIVE STRUCTURE FACTORS. By K. Marthinsen and R. Høier, Department of Physics and Mathematics, University of Trondheim-NTH, Norway.

A variety of many beam diffraction effects observed with x-rays or electrons may be understood from a perturbed two-beam point of view, and for these cases an effective structure factor is introduced. This factor may be calculated using the second Bethe approximation recently formulated for the x-ray case (Høier, R. and Marthinsen, K. (1983) Acta Cryst. A39, 854). The effective structure factor,  $F_{ho}^{n,p}$ , is calculated for each polarization direction  $p$ , in the  $n$ -beam case.  $F_{ho}^{n,p}$  may generally replace  $F_{ho}^{n,p}$  in two-beam intensity expressions.

It is well known that three-phase invariants may be determined from three-beam effects, and recently it has also been shown experimentally that a four-beam effect may yield the same information (Post et al. (1986) Acta Cryst. A42, 178). Such effects may be explained from  $F_{ho}^{n,p}$ . The reciprocal lattice points,  $h$ ,  $g$ , and  $f$ , is in this case positioned at the corners of a symmetrical trapezium. Tilting around one of the parallel sides,  $h$ , with two-fold symmetry, one obtains:

$$|F_{ho}^{4,p}| = |F_{ho}^{2,p}| \left[ (1 + a^p(s) \cdot \frac{|F_{hg}| |F_{go}|}{|F_{ho}|} \cos\psi)^2 + (a^p(s) \cdot \frac{|F_{hg}| |F_{go}|}{|F_{ho}|})^2 (1 - \cos^2\psi) \right]^{\frac{1}{2}}$$

where  $a^p(s)$  varies inversely with the deviation parameter  $s = s_g = s_f$  (see Høier, R. & Marthinsen, K., ref. above).  $\psi = \phi_{0h} + \phi_{0g} + \phi_{0f}$  is the three-phase invariant. The intensity in the  $h$ -beam for the non-centrosymmetric four-beam case is hence determined by the three-beam interactions in which  $h$  are involved. Selected four-beam cases may thus be utilized to determine three-phase invariants experimentally.