Acta Cryst. (1986). A**42**, 405-406

First-order asymmetry in the Renninger interaction of a strong primary reflection with weak beams.

By HELLMUT J. JURETSCHKE,* *School of Physics, University of Melbourne, Parkville, Victoria* 3052, *Australia*

(*Received* 13 *November* 1985; *accepted* 10 *March* 1986)

Abstract

Application of perturbation theory to the modification of a strong two-beam reflection near a three-beam point involving a weak secondary reflection shows that in perfect crystals the first-order asymmetry with azimuthal angle of the integrated intensity in a Renninger scan is caused primarily by changes in absorption. The intensity is always enhanced when the third reciprocal-lattice point is outside the Ewald sphere, and thus this asymmetry does not contain any phase information.

Recent perturbation theories of n-beam X-ray interactions (Juretschke, 1982, 1984; Høier & Marthinsen, 1983) have shown that first-order asymmetries in the wings of multiple-beam-interaction regions of Renninger scans can generally be described quantitatively by introducing an effective structure factor in an otherwise unchanged two-beam formulation. For a primary reflection **H** coupling with **L**, this effective structure factor has the form (σ polarization)

$$F_{HL}=F_H-(k\Gamma\Pi_1/2\xi_L)F_LF_{\bar{L}-\bar{H}}, \qquad (1)$$

where ξ_L is the distance of **L** from the Ewald sphere, $\Gamma=e^2/(\varepsilon_0 m\omega^2 v_{\rm cell})$, $k=\omega/c$, and Π_1 is a geometrical factor less than unity defined in the above references. Equation (1) has been used successfully by Juretschke (1984, 1986) to reproduce all the important structural details of the Renninger scan around **H** = 222 in Ge reported by Nicolosi (1982) and by Post, Nicolosi & Ladell (1984). In this case considerable changes occur over large angular ranges about the n-beam points because F_H is very small compared to F_L and F_{L-H}. Since the sign of the correction term in (1) depends on the sign of $F_LF_{\bar{L}-\bar{H}}/F_H$, the asymmetry is sensitive to the invariant phase of this combination of structure factors.

For a strong primary reflection **H** interacting with a weak contributing term, such as **H** = 311 and **L** = 222 in the diamond structure, (1) predicts negligible changes in the Renninger scan except at very small angular deviations from the three-beam point. In such a case the leading term linear in $1/\xi_L$, and therefore showing asymmetry, is contained in the shift of the Lorentz point, also predicted by the above theory (Juretschke, 1984). This is expressible in a shift of F_o, such that its imaginary part becomes

$$|F''_o|_{HL}=|F''_o-(k\Gamma\Pi_1/4\xi_L)(F_LF_{\bar{L}}+F_{L-H}F_{\bar{L}-\bar{H}})''|. \qquad (2)$$

Equation (2) affects integrated intensities through their absorption corrections. Thus, for a symmetric Bragg reflection in a centrosymmetric crystal, such a first-order correction gives (Afanas'ev & Perstnev, 1969)

$$I_H=(8/3)(\Gamma|F_H|/\sin 2\theta_B)[1-(3\pi/4)|F''_o|/|F'_H|]. \qquad (3)$$

With the assumption that $F_L\sim 0$, the insertion of (2) in (3) gives the leading terms in a modified integrated intensity near the three-beam point:

$$I_{HL}=I_H\{1+(3\pi/4)(k\Gamma\Pi_1/2\xi_L)\times[(F'_{L-H})^2/|F'_H|]|F''_{L-H}/F'_{L-H}|\}. \qquad (4)$$

As predicted, I_{HL} is linear in $1/\xi_L$ and therefore shows asymmetries in the intensity around the three-beam point. However, because of the squares and absolute values in (4), I_{HL} always increases when $\xi_L>0$, *i.e.* when **L** is outside the Ewald sphere. In particular, the asymmetry of (4) is *independent of the phase* of the triplet $F_LF_{\bar{L}-\bar{H}}/F_H$. The extension of (4) to the other polarization mode is straightforward, using the results of Juretschke (1984, 1986).

Compared to the modification of (3) due to (1), (4) predominates in the modified integrated intensity as long as

$$(3\pi/4)|F'_{L-H}/F'_L|\,|F''_{L-H}/F'_{L-H}|\gg 1. \qquad (5)$$

To give a quantitative example, the modification of I_{HL}/I_H is worked out below for the interactions of **H** = 311 with **L** = 222 and **L** = $\bar{2}$22, in Ge (λ = 1·541 Å). The pertinent numerical factors for these interactions are listed in Table 1. They indicate that the left side of (5) is of the order of 10 or more, so that (4) should offer a reliable description of first-order effects.

The resulting curves for $(I_{HL}-I_H)/I_H$ are shown in Fig. 1 for both *L*'s. Both have the same asymmetry, even though the phase of $F_LF_{\bar{L}-\bar{H}}/F_H$ has changed sign. The $\bar{2}$22 curve is smaller, because of, as follows from the entries in Table 1, the difference in Π_1 and the faster relative change of ξ_L with respect to the azimuthal rotation φ_T of the Renninger scan.

Table 1. *Parameters for the interactions* **H**/**L** = 311/222 *and* 311/$\bar{2}$22 *in* Ge(Cu *K*α)

[Structure factors interpolated from the tables in *International Tables for X-ray Crystallography* (1968) and from Hildebrandt, Stephenson & Wagenfeld (1973).]

L	222	$\bar{2}$22
$L-H$	$\bar{1}$11	$\bar{5}$11
F'_H	−121	−121
F'_L	1	1
F'_{L-H}	151	−90
$\lvert F''_{L-H}/F'_{L-H}\rvert$	0·04	0·05
Π_1	0·791	0·476
$k\Gamma/2\xi_L$	$0{\cdot}030/\varphi_T$	$0{\cdot}019/\varphi_T$
	(with φ_T in s)	
Sign $(F_LF_{\bar{L}-\bar{H}}/F_H)$	−	+

* Visiting Fellow at the Royal Melbourne Institute of Technology and the University of Melbourne during 1985. Permanent address: Department of Physics, Polytechnic Institute of New York, Brooklyn, New York 11201, USA.

0108-7673/86/050405-02$01.50

It is clear that the changes produced by (4) are not negligible for angular deviations of the order of a min of arc, and should be seen in experiments having the requisite angular resolution and stability. Inclusion of the 10% contributions due to (1) would enhance the 222 curves, and reduce the $\bar{2}22$ curves, by the same factor, but without reversing the sign of the latter. Obviously, the curves in Fig. 1, which only include σ polarization, do not account for a finite incident beam width or for possible broadening by imperfections.

Actual experiments are, of course, also influenced by contributions of order $(1/\xi_L)^2$ to (1), and therefore also to (3), but, since these are intrinsically symmetric in φ_T, they superimpose a symmetric shift on the curves of Fig. 1, without eliminating the asymmetry due to (4). First-order theory giving rise to (4) predominates in the far wings. Second-order terms will begin to contribute to Fig. 1 below about $\frac{1}{2}'$, and much closer to the three-beam point the interaction becomes much more complex.

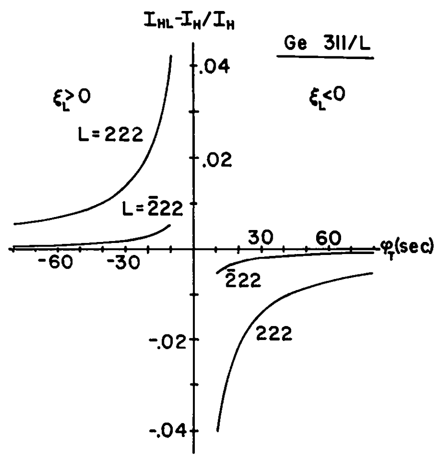

Fig.1. Relative change of integrated intensity of the Ge 311/L interaction in a Renninger scan with azimuthal angle φ_T, for L = 222, $\bar{2}22$, $\lambda = 1{\cdot}541$ Å. ξ_L measures the distance of L from the Ewald sphere. σ polarization only.

In conclusion, under the conditions where this analysis applies, the extraction of invariant phases in three-beam interactions when F_H is large and F_L is very small is not straightforward as long as the asymmetry of the modified absorption terms is not negligible. More generally, the extent to which phase-sensitive contributions control the observable asymmetry in any particular interaction may play a role in the discussion of experimental results under these conditions (*e.g.* Post & Ladell, 1985).

I gratefully acknowledge the hospitality and support of RMIT and Melbourne University during my stay in Melbourne. I also appreciate having been given preliminary results of his recent experiments by Ben Post.

References

Afanas'ev, A. M. & Perstnev, I. P. (1969). *Acta Cryst.* **A25**, 520–523.

Hildebrandt, G., Stephenson, J. D. & Wagenfeld, H. (1973). *Z. Naturforsch. Teil A*, **28**, 588–600.

Høier, R. & Marthinsen, K. (1983). *Acta Cryst.* **A39**, 854–860.

International Tables for X-ray Crystallography (1968). Vol. III. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)

Juretschke, H. J. (1982). *Phys. Rev. Lett.* **48**, 1487–1489.

Juretschke, H. J. (1984). *Acta Cryst.* **A40**, 379–389.

Juretschke, H. J. (1986). *Phys. Status Solidi.* In the press.

Nicolosi, J. (1982). PhD thesis, Polytechnic Institute of New York.

Post, B. & Ladell, J. (1985). Am. Crystallogr. Assoc. Meet., Stanford, CA, August 1985. Abstract M1.

Post, B., Nicolosi, J. & Ladell, J. (1984). *Acta Cryst.* **A40**, 684–688.

Acta Cryst. (1986). A**42**, 406

Lattice complexes and limiting complexes *versus* orbit types and non-characteristic orbits: a comparative discussion. Erratum.

By Elke Koch and Werner Fischer, *Institut für Mineralogie der Universität Marburg, Hans-Meerwein-Strasse, D-3550 Marburg, Federal Republic of Germany.*

(*Received* 28 *November* 1985; *accepted* 24 *June* 1986)

Abstract

In the paper by Koch & Fischer [*Acta Cryst.* (1985), **A41**, 421-426] the words 'or more' are missing on p. 423 (left column, sixth line from bottom). The sentence should read: Then the point configurations of the intersection form another lattice complex or, in very exceptional cases, two or more other lattice complexes (for a proof see Koch, 1974).

All information is given in the *Abstract*.

0108-7673/86/050406-01$01.50