Acta Cryst. (1976). A**32**, 918

Angle settings for rotation around the diffraction vector for four-circle diffractometers.* By B. C. Wang, C. S. Yoo, J. Pletcher and M. Sax, *Biocrystallography Laboratory, Veterans Administration Hospital, Pittsburgh, Pennsylvania* 15240, *and the Department of Crystallography, University of Pittsburgh, Pittsburgh, Pennsylvania* 15260, *U.S.A.*

(*Received* 30 *October* 1975; *accepted* 23 *April* 1976)

Simple graphical representations have been found which have led to the discovery of new geometrical relations between the angle settings, χ_0, ω, χ and $\varphi-\varphi_0$, of a four-circle single-crystal diffractometer, and the azimuthal angle, ψ, of the diffraction vector. The new geometric relations greatly simplify the derivation of the trigonometric equations which relate the angle settings with the rotation around the diffraction vector. One of these equations, $\tan\chi=\tan\chi_0/\cos(\varphi-\varphi_0)$, is given here for the first time. The others are similar in form to those derived previously with matrix methods.

Introduction

What are the relations between the angle settings, ω, χ, and φ and the azimuthal angle ψ (psi) on a conventional four-circle single-crystal diffractometer? This question is often asked in other more practical ways, such as: how to calculate the angle settings for a given value of ψ or how (what angles to use) to locate a particular reflection at the angle settings other than the bisecting position often used for data collection. Equations for relating the new angle settings χ, ω and φ to the original angle settings,† χ_0, ω_0 and φ_0, have been reported by several authors. For example, Santoro & Zocchi (1964) related the setting angles in terms of the Cartesian coordinates of the reciprocal lattice points and the length of the reciprocal vector. Arndt & Willis (1966) expressed these relations in terms of an offset angle ε_0 and the reciprocal lattice coordinates ξ, ζ and τ. Busing & Levy (1967) pointed out that the angle settings can be extracted from an orthogonal matrix **R** which is the product of four orientation matrices $\mathbf{\Psi}$, $\mathbf{\Omega}_0$, $\mathbf{X}_0$ and $\mathbf{\Phi}_0$. The angle settings were then expressed in terms of the elements of the matrix **R**. Hamilton (1974), on the other hand, used a treatment similar to that of Busing & Levy (1967) and led to the simpler relations expressing χ, ω, φ, and ψ in terms of the diffractometer angles. However, all these relations either were expressed in terms of variables other than the diffractometer angle settings or they were derived from a solution of elegant but complicated equations of crystal orientation. There was no simple graphical representation which allowed one to visualize instantly the geometrical relations between the angle settings and the azimuthal angle. We report here such a representation and the new geometrical relations, as well as the derivation of the equations relating the various angles. A detailed description for deriving the representation is given because it is useful in teaching diffractometry on the one hand, and because it provides a clear picture of the relations between the various angles on the other.

Geometrical relations

We begin by considering Fig. 1. The Cartesian coordinate system shown there has been chosen such that the *XY* and the diffraction planes are parallel and such that the *X* axis points in the direction of the diffraction vector. In other words, the Bragg condition may be satisfied if a particular reciprocal lattice point is moved onto the *X* axis. Now assume that when $\omega=0$, $\chi=0$ and $\varphi=\varphi_0$ we are able to bring this particular reciprocal lattice point to location *A*. Clearly, there are an infinite number of ways to move the lattice point from *A* into the diffraction position *D*, which is on the *X* axis. A special way to achieve this is to move along *AD*, or a more general route is to follow *AB–BC–CD*. The former involves a single rotation of the crystal about the χ axis while the latter consists of rotations about the φ, χ and ω axes. Although the final position of the reciprocal lattice point is the same in both cases, the latter route will produce a rotation of the reciprocal lattice about *OD*, the diffraction vector, as compared to the orientation of the lattice after it has traversed the former path. Since *AD*, *AB*, *BC* and *CD* are the paths of a reciprocal lattice point when rotations about diffractometer axes are made, relations must exist between their lengths and the angles of rotations, χ_0, ω, χ and $\Delta\varphi$, which is $\varphi-\varphi_0$. Indeed, these relations can be represented in Figs. 1 and 2(*a*) by the four angles around the apex, *O*, of a distorted rectangular pyramid, *O–A′BC′D′*. The points *A′*, *B*, *C′* and *D′* are the projections of *A*, *B*, *C* and *D* on the plane that is parallel to the *YZ* plane and that passes through point *B*. The rotation around the diffraction vector, *i.e.* the azimuthal angle, ψ,* can be represented by the angle between *BC″* and *BE″* [Figs. 1 and 2(*b*)] which are the tangents of the arcs *BC* and *BE* respectively at *B*. We now explain these relations.

(*A*) *The diffractometer setting angles* φ_0, φ, χ_0, χ, ω_0 and ω

From Fig. 1, if the reciprocal lattice point of interest is moved from *A* to *D* following the former route mentioned earlier, *i.e.* *AD*, then $\chi_0=\angle AOD$, $\varphi=\varphi_0$ and $\omega=\omega_0=0$. If the latter route is used, *i.e.* *AB–BC–CD*, then $\Delta\varphi=\varphi-\varphi_0=\angle DOE=\angle D'OC'$, $\chi_0=\angle AOD=\angle BOC'$, $\chi=\angle BO'C=\angle A'OD'$, $\omega_0=0$ and $\omega=\angle DOC$. But right triangles, *A′OB* and *D″OC* are congruent ($\because CD''=BA'$, $OC=OB$, and $\angle OA'B=\angle OD''C=\pi/2$). Therefore $\omega=\angle DOC=\angle A'OB$.

(*B*) *The azimuthal angle*, ψ

Define a unit vector, **u**, in reciprocal space pointing in the same direction as the tangent of the arc *AD* at *A* (Fig. 1) and consider the two different routes mentioned earlier for moving a particular lattice point from *A* to *D*. We then observe what happens to the orientation of this newly defined vector **u** when it reaches *D*. Obviously after follow-

* Presented at the American Crystallographic Association Winter Meeting, Clemson, South Carolina, January, 1976.

† These settings are defined to be the χ and φ angles at which the crystal diffracts for $\omega=\omega_0=0$ and for $\psi=0$.

* $\psi_0=0$ is defined as the value of ψ at $\omega=\omega_0=0$.

ing the first route (along AD, about χ) **u** will be aligned with the tangent of arc AD at D. Along the second route, **u** becomes aligned with BE''; however, after the particular reciprocal lattice point is first moved from A to B, as well as at the completion of the route (B to C to D), **u** will no longer be in the direction of the tangent of AD at D. Instead, another unit vector in reciprocal space, say **v**, which points in the direction of BC'', when the lattice point of interest is at B, will be tangent to AD at D. Therefore, the angle of rotation due to the difference in route is just that between **u** and **v** or equivalently between BC'' and BE''. Accordingly, ψ can be represented by $\angle C''BE''$.

Calculation of angles

If we assume that $OB=1$, then from Fig. 2(a) it is evident that

$$\sin \omega = A'B/OB = \cos \chi_0 \sin \Delta\varphi\ , \qquad (1)$$

$$\cos \chi = OD'/OA' = \cos \chi_0 \cos \Delta\varphi / \cos \omega\ . \qquad (2)$$

Equation (1) is similar to equation (12) of Hamilton (1974) except that the sign convention for ω is different. The positive directions of the angles are indicated by the curved arrows in Fig. 1. Hamilton's sign convention for ω is opposite in sense to the one assigned for our Picker diffractometer. Equation (2), however, is the same as Hamilton's equation (13). An alternative simpler expression for χ, which may have certain conceptual advantages, but has not been previously mentioned, indicates that χ can be independent of ω,

$$\tan \chi = A'D'/OD' = \tan \chi_0 / \cos \Delta\varphi\ . \qquad (2')$$

Therefore both ω and χ can be expressed in terms of χ_0 and $\Delta\varphi$.

The angle of rotation, ψ, about the diffraction vector has been pointed out in the foregoing paragraph to be the angle between BC'' and BE'' [Figs. 1 and 2(b)]. It can be shown (see Appendix) that $\angle BE''C''=\pi/2$, where E'' and C'' are the intercepts of BC'' and BE'' with the XY plane. From Fig. 2(b), we have

$$BC' = BE'' \cos \chi_0 = BC'' \cos \psi \cos \chi_0\ .$$

Also,

$$BC' = BC'' \cos \chi\ .$$

Therefore,

$$\cos \chi = \cos \psi \cos \chi_0\ . \qquad (3)$$

Equations (1), (2'), and (3) are all that is necessary in relating the various angles. By knowing any two of the five variables, χ_0, χ, ω, $\Delta\varphi$ and ψ, the other three can be calculated. For example, if a rotation of ψ from ψ_0 is needed when χ_0 is known, then χ can be calculated from (3), $\Delta\varphi$ can then be evaluated by substituting χ_0 and χ into (2'), and finally ω can be calculated by entering χ_0 and $\Delta\varphi$ into (1). The new angle settings which will rotate the diffraction vector by an amount of ψ will then be ω, χ and $\varphi_0+\Delta\varphi$.

APPENDIX

One of the ways to show that $\angle BE''C''=\pi/2$ is as follows: from Fig. 2(b),

$$C'O = BC'/\tan \chi_0$$
$$C'O' = BC'/\tan \chi$$
$$C'E'' = BC' \tan \chi_0$$
$$C'C'' = BC' \tan \chi\ .$$

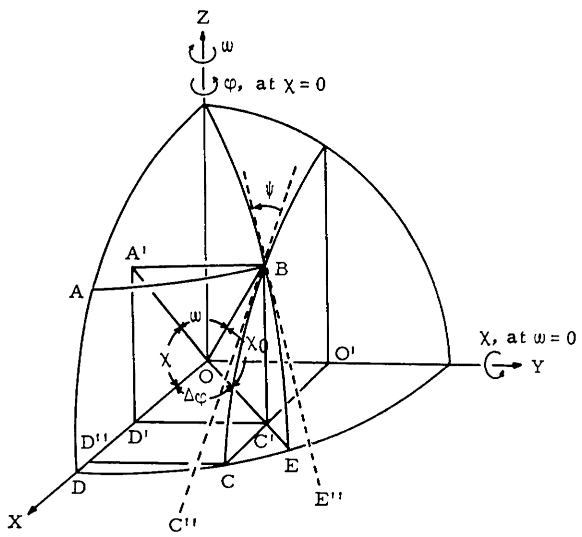

Fig. 1. Coordinate system and diffractometer angles. The φ and χ axes shown here are at $\chi=0$ and $\omega=0$. The positive directions of the angles of rotation are indicated by the curved arrows.

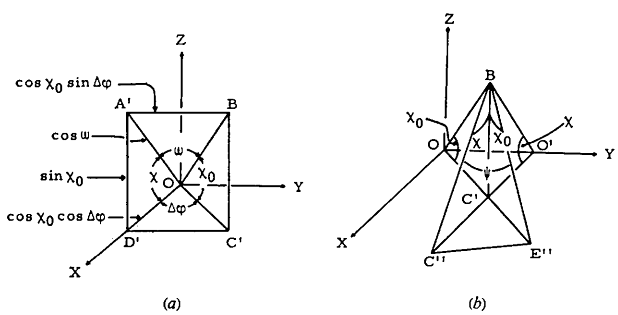

Fig. 2. Parts of Fig. 1 that have been excised and isolated for clarity.

Thus,

$$C'O/C'O' = C'C''/C'E''$$

and

$$\angle C'E''C'' = \angle C'O'O = \pi/2\ ,$$

i.e.

$$C''E'' \perp C'E''\ .$$

Since

$$\Delta C'E''B \perp \Delta E'E''C''$$

therefore

$$BE'' \perp E''C''\ ,$$

that is,

$$\angle BE''C'' = \pi/2\ .$$

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