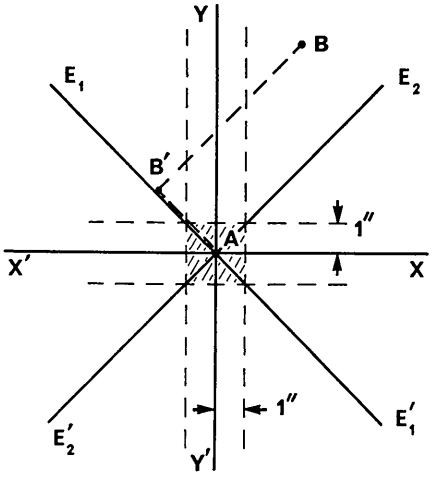

Fig. 1. Region of reciprocal space including the tips *A* and *B* of the active reciprocal lattice vectors of the first and second crystals.

independence of the steps is obtained with rotation ranges as little as half the ±45° shown in Fig. 1.

Fig. 2 shows an example of the beautifully regular fringes formed by superposing one plate of perfect silicon upon another. The plates were about one millimetre thick, so that for each $\mu t \sim 1$. Equally clear and straight fringes were observed over an area of 45 mm². The fringes represent a pure rotation moiré, the rotation, as determined from the fringe period of 17 microns, is 2½″ of arc.

References

BONSE, U. & HART, M. (1965*a*). *Appl. Phys. Lett.* **6**, 155.
BONSE, U. & HART, M. (1965*b*). *Appl. Phys. Lett.* **7**, 99.
BONSE, U. & HART, M. (1965*c*). *Z. Physik*, **188**, 154.
BONSE, U. & HART, M. (1966*a*). *Z. Physik*, **190**, 455.
BONSE, U. & HART, M. (1966*b*). *Z. Physik* **194**, 1.
BONSE, U. & HART, M. (1968) *Acta Cryst.* A**24**, 240.
CHIKAWA, J.-I. (1965). *Appl. Phys. Lett.* **7**, 193.
LANG, A. R. & MIUSCOV, V. F. (1965). *Appl. Phys. Lett.* **7**, 214.

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Vector algebra and the relations between direct and reciprocal lattice quantities.

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Vector methods are used to derive relationships between angles that occur in the direct and the reciprocal lattices, to give pedagogically useful demonstrations of the power of vector algebra and the reciprocal lattice concept. Several relationships involve the unit-cell volumes of the direct or the reciprocal lattices.

The mathematical apparatus used in defining the reciprocal lattice was first outlined by Gibbs (1881, 1906) and Wilson (1909, p. 81) in connection with the geometric problem of expressing a vector in terms of three arbitrary non-coplanar vectors. The application of this formalism to the problems of X-ray diffraction is chiefly due to Ewald (1913*a*, *b*, 1921, 1936) and Bernal (1926). While vector methods are uniformly used to describe and manipulate the reciprocal-lattice relations, equations between direct-lattice and reciprocal-lattice quantities are usually derived by spherical trigonometry. Vector methods may, however, be substituted advantageously, with the important pedagogical purpose of demonstrating further the great power of vector algebra. The following examples are offered as illustrations.

Consider three unit vectors $\mathbf{a}_1^*$, $\mathbf{b}_1^*$, $\mathbf{c}_1^*$, directed along the reciprocal-lattice axes. The vector $\mathbf{a}_1^* \times \mathbf{b}_1^*$ is of length $\sin\gamma^*$ and oriented parallel to the c direct-lattice axis, and the vector $\mathbf{b}_1^* \times \mathbf{c}_1^*$ is of length $\sin\alpha^*$ and oriented parallel to the a direct-lattice axis, while the scalar quantity $(\mathbf{a}_1^* \times \mathbf{b}_1^*) \cdot (\mathbf{b}_1^* \times \mathbf{c}_1^*)$ has the magnitude $\sin\gamma^* \sin\alpha^* \cos\beta$. The following vector identity given by Wilson (1909, p. 76) may readily be established by expansion in terms of the vector components:

$$(\mathbf{a}\times\mathbf{b})\,.\,(\mathbf{c}\times\mathbf{d}) = \begin{vmatrix} \mathbf{a}\,.\,\mathbf{c} & \mathbf{a}\,.\,\mathbf{d} \\ \mathbf{b}\,.\,\mathbf{c} & \mathbf{b}\,.\,\mathbf{d} \end{vmatrix}. \qquad (1)$$

For the special case above one writes

$$(\mathbf{a}_1^* \times \mathbf{b}_1^*)\,.\,(\mathbf{b}_1^* \times \mathbf{c}_1^*) = \begin{vmatrix} \mathbf{a}_1^*\,.\,\mathbf{b}_1^* & \mathbf{a}_1^*\,.\,\mathbf{c}_1^* \\ \mathbf{b}_1^*\,.\,\mathbf{b}_1^* & \mathbf{b}_1^*\,.\,\mathbf{c}_1^* \end{vmatrix}. \qquad (2)$$

or

$$\sin\alpha^* \sin\gamma^* \cos\beta = \begin{vmatrix} \cos\gamma^* & \cos\beta^* \\ 1 & \cos\alpha^* \end{vmatrix}. \qquad (3)$$

This gives the usual transformation

$$\cos\beta = \frac{\cos\alpha^* \cos\gamma^* - \cos\beta^*}{\sin\alpha^* \sin\gamma^*}. \qquad (4)$$

This equation is closely related to the cosine formula of spherical trigonometry,

$$\cos R = \frac{\cos r - \cos s \cos t}{\sin s \sin t} \qquad (6)$$

where r, s, and t are the sides of a spherical triangle and R is the angle opposite r.

The volume V of the direct cell extended by the vectors **a**, **b**, and **c** may be found from the following vector identity (Wilson, 1909, p. 87):

$$(\mathbf{P}\,.\,\mathbf{Q}\times\mathbf{R})\,(\mathbf{A}\,.\,\mathbf{B}\times\mathbf{C}) = \begin{vmatrix} \mathbf{P}\,.\,\mathbf{A} & \mathbf{P}\,.\,\mathbf{B} & \mathbf{P}\,.\,\mathbf{C} \\ \mathbf{Q}\,.\,\mathbf{A} & \mathbf{Q}\,.\,\mathbf{B} & \mathbf{Q}\,.\,\mathbf{C} \\ \mathbf{R}\,.\,\mathbf{A} & \mathbf{R}\,.\,\mathbf{B} & \mathbf{R}\,.\,\mathbf{C} \end{vmatrix}. \qquad (7)$$

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This furnishes

$$(\mathbf{a}\,.\,\mathbf{b}\times\mathbf{c})^2 = V^2 = \begin{vmatrix} a^2 & ab\cos\gamma & ac\cos\beta \\ ab\cos\gamma & b^2 & bc\cos\alpha \\ ac\cos\beta & bc\cos\alpha & c^2 \end{vmatrix}$$
$$= a^2b^2c^2[1+2\cos\alpha\cos\beta\cos\gamma-\cos^2\alpha - \cos^2\beta-\cos^2\gamma].$$

More details are contained in a text by Buerger (1942, pp. 349–351). The corresponding expression for V^{*2} may be obtained in the same way. Application of (7) to the evaluation of $(\mathbf{a}\,.\,\mathbf{b}\times\mathbf{c})\,(\mathbf{a}^*\,.\,\mathbf{b}^*\times\mathbf{c}^*)$ yields

$$\begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

and leads at once to the identity $V\,V^*=1$.

An expression for V that contains both direct and reciprocal lattice quantities may be obtained by starting with

$$a=|\mathbf{b}^*\times\mathbf{c}^*|/V^*=b^*c^*\sin\alpha^*/V^*\,. \qquad (9)$$

When b^* and c^* are expressed by direct lattice quantities this becomes

$$a=(c\,a\sin\beta/V)\,(a\,b\sin\gamma/V)\,(\sin\alpha^*/V^*)\,. \qquad (10)$$

Solving for V, and using $V\,V^*=1$ leads to the final result,

$$V=a\,b\,c\sin\alpha^*\sin\beta\sin\gamma\,. \qquad (11)$$

which remains valid when the star is switched to other angles, as in

$$V=a\,b\,c\sin\alpha\sin\beta^*\sin\gamma\,. \qquad (12)$$

Therefore also,

$$(\sin\alpha/\sin\alpha^*)=(\sin\beta/\sin\beta^*)=(\sin\gamma/\sin\gamma^*)\,, \qquad (13)$$

which is the equivalent of the sine law of spherical trigonometry:

$$\sin r/\sin R=\sin s/\sin S=\sin t/\sin T\,. \qquad (14)$$

Relationships reciprocal to (11) and (12), of the form

$$V^*=a^*\,b^*\,c^*\sin\alpha\sin\beta^*\sin\gamma^* \qquad (15)$$

are, of course, correct also.

Another expression for V follows from solving $a^*=b\,c\sin\alpha/V$ for V:

$$V=b\,c\sin\alpha/a^*\,. \qquad (16)$$

Cyclic variation yields two additional formulas, and analogous expressions exist for V^*.

Combining (12) and (16) yields

$$a\,a^*\sin\beta^*\sin\gamma=1\,, \qquad (17)$$

which invites comparison with $\mathbf{a}\,.\,\mathbf{a}^*=1$, that is,

$$a\,a^*\cos(\mathbf{a},\mathbf{a}^*)=1\,. \qquad (18)$$

It follows that

$$\cos(\mathbf{a},\mathbf{a}^*)=\sin\beta^*\sin\gamma=\sin\beta\sin\gamma^*\,, \qquad (19)$$

where (13) has also been used. The argument of the cosine is the angle between the zone direction [100] and the normal to the (100) plane. An expression for $\cos(\mathbf{a},\mathbf{a}^*)$ containing direct lattice quantities only follows from solving equation (12) for $\sin\beta^*\sin\gamma$ and insertion into (19),

$$\cos(\mathbf{a},\mathbf{a}^*)=V/a\,b\,c\sin\alpha\,. \qquad (20)$$

Likewise, in reciprocal space quantities,

$$\cos(\mathbf{a},\mathbf{a}^*)=V^*/a^*\,b^*\,c^*\sin\alpha^*\,. \qquad (21)$$

Expressions analogous to (19), (20), and (21) follow by cyclic permutation.

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References

BERNAL, J. D. (1926). *Proc. Roy. Soc.* A **113**, 120.

BUERGER, M. J. (1942). *X-ray Crystallography*. New York: John Wiley.

EWALD, P. P. (1913*a*). *Physik. Z.* **14**, 465.

EWALD, P. P. (1913*b*). *Physik. Z.* **14**, 1038.

EWALD, P. P. (1921). *Z. Kristallogr.* **56**, 129.

EWALD, P. P. (1936). *Z. Kristallogr.* **93**, 396.

GIBBS, J. W. (1881). *Elements of Vector Analysis*. New Haven, Connecticut: Privately printed.

GIBBS, J. W. (1906). *The Scientific Papers of J. Willard Gibbs*, Vol. II, p. 25. London: Longmans, Green & Co.

WILSON, E. B. (1909). *Vector Analysis. A text-book for the use of Students of Mathematics and Physics Founded upon the Lectures of J. Willard Gibbs*. 2nd Ed. New York: Charles Scribner's Sons.

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Possibility of 'Bijvoet differences' in the non-centrosymmetric structures of the elements.

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It is proposed that it would be interesting to look for and measure Bijvoet differences in the noncentrosymmetric structures of the elements like α-manganese and the hexagonal, isomorphous tellurium and selenium. This would check directly the validity of some of the usual assumptions regarding temperature factors in X-ray diffraction.

The purpose of this communication is to point out the possibility of directly checking the usual assumptions on the temperature factors in X-ray diffraction in cases where the anomalous scattering is appreciable, through experiments on the non-centrosymmetric structures of some elements.

Considering such a structure with n atoms in the unit cell, the structure factors of the pair of reflexions, hkl and $\bar{h}\bar{k}\bar{l}$, would be

$$F(hkl)_\pm=\sum_1^n (f+\Delta f'+i\Delta f'')\,(A_j\pm iB_j)\,(\text{temperature factor})_j, \qquad (1)$$