Short Communications

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Use of the Ewald sphere in aligning crystal pairs to produce X-ray moiré fringes. By J. BRÁDLER* AND A. R. LANG,
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One crystal plate can be superposed upon another of the same material to produce observable X-ray moiré fringes in the simultaneously diffracted beam transmitted through the plates. During alignment it is necessary to determine, and then minimize, the small difference vector between the acting reciprocal lattice vectors. By rigid rotation of the crystal pair about the mean reciprocal lattice vector the Ewald sphere is caused to make various angles with the difference vector. This vector can then be fully determined by measuring its component normal to the Ewald sphere at two or more settings of the sphere.

We have recently developed methods for superposing one crystal plate upon another so as to produce X-ray moiré fringes with repeat periods in the range 10–500 microns, such fringes being easily photographed by standard X-ray topographic techniques. Previous X-ray moiré fringe work has been done with (*a*) X-ray interferometers (Bonse & Hart 1965*a, b, c*; 1966*a, b*; 1968) in which parts of a single crystal of silicon are milled away to leave just the interferometer elements upstanding; (*b*) superposed nearly parallel growths of platelet cadmium sulphide crystals (Chikawa, 1965); and (*c*) cracks in quartz at which moiré fringes occur owing to the relative displacement of the two sides of the crack (Lang & Miuscov, 1965). In all the above-cited works the fringes have been formed between elements of crystal grown in a perfect or nearly perfect alignment which has been little disturbed since growth. To produce moiré fringes between crystal elements which have been physically separated from each other involves the stringent requirement of bringing their respective Bragg-plane normals together within a solid-angle range as small as 10^{-10} steradian. This process of alignment, apparently arduous, has been turned into a routine operation by a simple exploitation of the well-known Ewald sphere geometry.

The experimental problem is illustrated by Fig. 1 which shows the region of reciprocal space containing A, the tip of the operating reciprocal lattice vector, g_A, of one crystal slice, and B, the tip of g_B, the operating reciprocal lattice vector of the second slice. The vector g_A points directly towards the observer, and g_B nearly so. The crystals are of the same species, with closely similar lattice parameters, and use the same Bragg reflexion, so that $|g_A| = |g_B|$ very nearly. The crystal plates themselves are each used in symmetrical transmission and one is placed closely behind the other so that both incident and diffracted beams leaving the first crystal subsequently pass through the second crystal. In Fig. 1 $X'AX$ is the trace of the plane containing the rays incident upon and diffracted by a given element of the first crystal. Since the slit-collimated incident beam has a divergence in this plane at least ten times the angular range of reflexion of the crystal, both the first and second crystals are readily set by coarse angular adjustments to realize their

full integrated reflexions. The trace of the Ewald sphere for the ray in the plane $X'A$ which satisfies the Bragg condition exactly in the element of the first crystal considered is shown by YAY', and is sufficiently closely represented by a straight line in the small region of reciprocal space involved. In order to produce observable moiré fringes two conditions must be satisfied. Firstly, B must be brought to lie within a thin band centred on YY' so that the angular range of rays which undergo Bragg reflexion at the second crystal falls within that of rays Bragg reflected by the first crystal. For practical purposes, with the crystals and radiations used, this range can be taken as $\pm 1''$ of arc. It is indicated by the vertical dashed lines on Fig. 1. The distance of B from the Ewald sphere is called y. The second condition is that the distance of B from $X'X$ be not too large for moiré fringes to be resolved. The moiré fringe period (when $|g_A| = |g_B|$) is inversely proportional to this distance which we call τ. For easy recognition on fast coarse-grained X-ray film a fringe spacing not finer than 40 microns is desirable and this corresponds to a range of $\pm 1''$ of arc with the silicon 220 reflexion, and is indicated by the horizontal dashed lines. B is 'home' when it lands in the obliquely shaded area of small y and small τ surrounding A. Now y can be determined, and hence minimized, with progressive fineness, by observations in succession on the half width of the overlapping reflexions from the two crystals, the peak reflected intensity, and the intensity profile across the diffracted beam. On the other hand there is no simple method for finding τ when it is fairly small (say less than $100''$) but still outside the shaded region. The problem is solved by rigid rotation of the crystal pair about the mean reciprocal lattice vector, so that, in a coordinate system fixed to the crystals, as used in Fig. 1, the trace of the Ewald sphere is tilted away from the vertical. A rotation of the crystals clockwise by 45° (looking towards the reciprocal lattice origin) brings the Ewald sphere trace to E_1E_1', and an anticlockwise rotation by 45° from the initial position brings it to E_2E_2'. If in each position y (defined as the distance from the Ewald sphere in its current position) is made very small by appropriate movement of B normal to the Ewald sphere, then B is 'home' in just two, independent, steps: *viz.* the step from B to B' and from B' to A. In practice a few, but not many, more steps may be needed. On the other hand it is found that sufficient

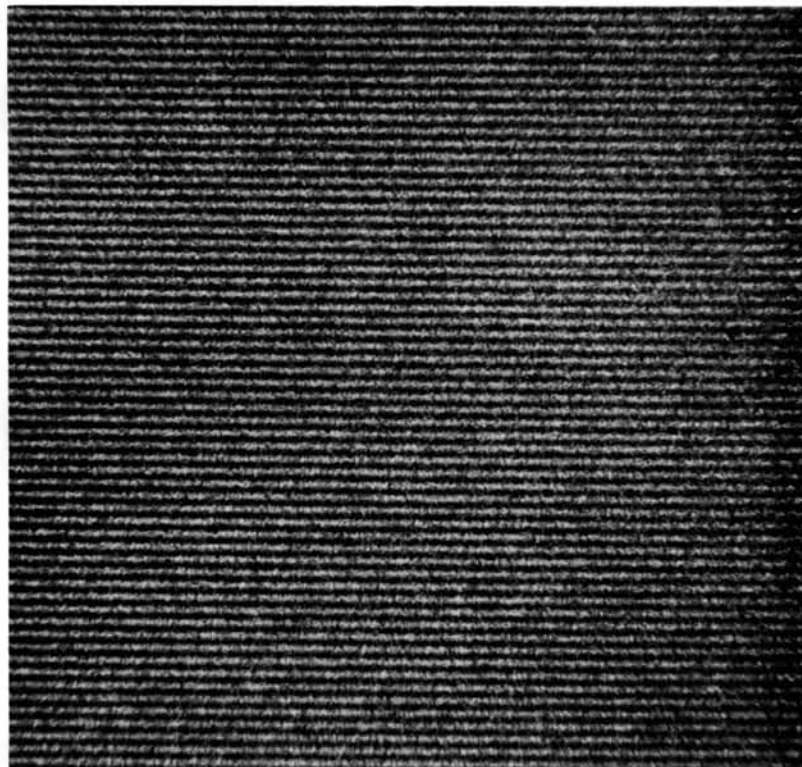* On leave from Institute of Physics, Czechoslovak Academy of Sciences, Prague.

Fig. 2. Pure rotation moiré formed by superposition of one silicon plate upon the other. Reflexion 220, reciprocal lattice vector horizontal, radiation Mo $K\alpha$. Field 1 mm square. Recorded on Ilford L4 nuclear emulsion.
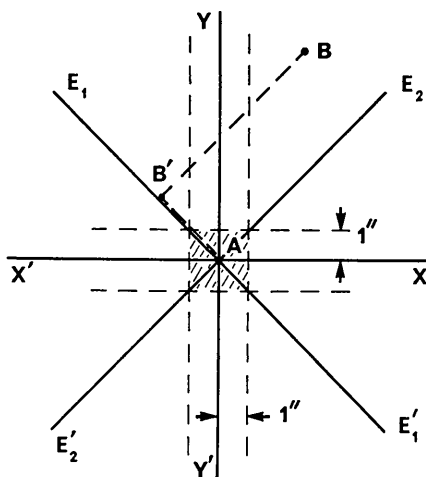
Fig. 1. Region of reciprocal space including the tips A and B of the active reciprocal lattice vectors of the first and second crystals.

independence of the steps is obtained with rotation ranges as little as half the $\pm 45°$ 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 $2\frac{1}{2}''$ of arc.

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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 (1913a, 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 a_1^*, b_1^*, c_1^*, directed along the reciprocal-lattice axes. The vector $a_1^* \times b_1^*$ is of length $\sin \gamma^*$ and oriented parallel to the c direct-lattice axis, and the vector $b_1^* \times c_1^*$ is of length $\sin \alpha^*$ and oriented parallel to the a direct-lattice axis, while the scalar quantity $(a_1^* \times b_1^*) \cdot (b_1^* \times c_1^*)$ 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:

$$(a \times b) \cdot (c \times d) = \begin{vmatrix} a \cdot c & a \cdot d \\ b \cdot c & b \cdot d \end{vmatrix}. \quad (1)$$

For the special case above one writes

$$(a_1^* \times b_1^*) \cdot (b_1^* \times c_1^*) = \begin{vmatrix} a_1^* \cdot b_1^* & a_1^* \cdot c_1^* \\ b_1^* \cdot b_1^* & b_1^* \cdot c_1^* \end{vmatrix}. \quad (2)$$

or

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

This gives the usual transformation

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

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

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

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):

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