DETERMINATION OF THE SPACE-LATTICE OF A TRICLINIC MINERAL BY MEANS OF THE WEISSENBERG X-RAY GONIOMETER

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In the Weissenberg x-ray goniometer a simultaneous translation of the cylindrical film coupled with the rotation of the crystal permits a unique and rigorous determination of the space-lattice,[1] as Weissenberg[2] has stated. Weissenberg has pointed out that whereas the Debye-Scherrer powder photograph supplies one experimental parameter (the radius of the Debye-Scherrer circle), and the rotation layer-line photograph supplies two experimental parameters, μ, α, by the measurement of the two coordinates of the diffraction spot on the film, the Weissenberg x-ray goniometer supplies three experimental parameters, μ, α, σ. Now a series of parallel net-planes has only three degrees of freedom in a Bravais lattice, namely, the separation of the planes and the two degrees of freedom of the normal used up when its direction is fixed. Thus each net-plane is uniquely determined by the three parameters obtained by means of the Weissenberg goniometer. It should be stated that the modification of the rotation method usually called the oscilla-

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[1] In this paper the term space-lattice is used in the sense of the system of points and is held not to imply the crystallographic axes by means of which the system of points is described since the same system of points can be described by an infinite number of sets of axes in the triclinic system. The present usage is in accord with the following:

Schoenflies, A., Krystallsysteme und Krystallstructur, S. 250, 1891.

Niggli, P., Lehrbuch der Mineralogie, I. Allgemeine Mineralogie, 2. Aufl., S. 19, 1924.

Wyckoff, R. W. G., The Analytical Expression of the Results of the Theory of Space Groups, Second edition, p. 25, 1930.

Hilton, H., Mathematical Crystallography, p. 115, 1903.

Mauguin, Ch., La Structure des Cristaux, p. 8, 1924.

Friedel, G., Leçons de Cristallographie, p. 16, 1926.

[2] *Zeit. f. Physik,* **23,** 229, 1924.

tion method also permits a determination of the lattice of a tri-
clinic crystal by measurements on x-ray photographs alone if the
crystal can be rotated about three crystallographic zone-axes.[3]
However, the Weissenberg goniometer yields a solution of this
problem with one adjustment of the crystal (with any crystal-
lographic zone parallel with the rotation axis) and in a direct and
convenient manner, whereas the solution afforded by the rotation-
oscillation method is roundabout and laborious and in some cases
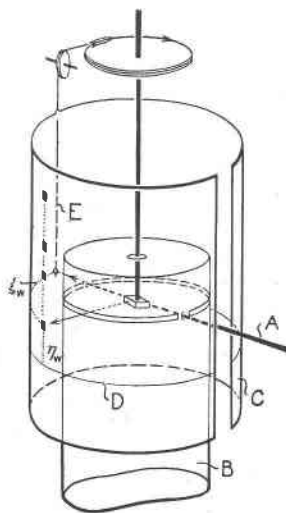physically impracticable owing to the character of the crystals.

FIG. 1. Schematic representation of the Weissenberg x-ray goniometer. (After
Böhm.) *Legend*: A, X-ray beam; B, Layer-line screen; C, Film-cylinder; D, Axis
of ξ_w; E, Axis of η_w.

The first step in an analysis with the Weissenberg goniometer is
to take an ordinary rotation photograph (film-cylinder stationary).
On the rotation picture it is, however, only necessary to measure
the separations of the layer-lines, these measurements determining
the values of the parameter, μ, for the layer-lines. The angular dis-
tance from the equator to the layer-line being μ, one has the rela-
tion, $\tan \mu = s/r$, where s is the distance from the equator to the
layer-line measured on the film and r is the crystal-to-film distance.
The value of μ for each layer-line is then used to set the so-called

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[3] Cf. Bernal, J. D., Equations (25) and (27) on page 144, and equation (3) on
page 125, *Proc. Roy. Soc.* (London), **113A**, 1926.

layer-line screen of the Weissenberg goniometer. This screen is a metal cylinder of diameter slightly less than that of the cylindrical film; the screen is cut by a peripheral slit (the plane of the peripheral circular slit is at right angles to the axis of the cylinder) which permits the diffraction spots of only one layer-line to register on the film at each setting of the screen. The spots of this layer-line are spread out over the cylindrical film by the translation of the film carriage during the rotation of the crystal. After exposure and development, the film is laid upon a flat surface[4] and the rectangular coordinates of each diffraction spot are measured. For these measurements one coordinate axis, the η_w-axis, is a line that was parallel with the rotation axis during the exposure and passed through the center of the direct x-ray beam. In the case of a layer-line of a triclinic crystal the direction of the η_w-axis on the film is fixed by two reference spots made by the direct beam with exposures of two or three seconds; the lateral position of the η_w-axis is fixed by two diffraction spots of the same plane of the space-lattice, the two spots lying at equal distances on opposite sides of the η_w-axis. The ξ_w-axis is an arbitrary line at right angles to the η_w-axis. From the ξ_w- and η_w-coordinates[5] of each diffraction spot the point of the reciprocal lattice[6] corresponding to it is quickly and easily obtained by the graphical construction of Schneider.[7] From ξ_w and η_w are obtained α and σ by the equations of Weissenberg

$$\alpha = \xi_w \frac{360}{2\pi r_F},$$

$$\sigma = \eta_w \frac{360}{\eta_{360}},$$

[4] The measurement of the film can be carried out very well by means of an illuminated sheet of opal flashed glass held in a wooden frame to which the film can be clamped. A glass strip with a hair-line extends across the film and slides along a scale at right angles to the hair-line. A vernier attached to the glass strip allows the position of the hair-line to be read on the scale.

[5] It should be noted that the symbol ξ of Weissenberg has an entirely different signification from the symbol ξ of Bernal. Therefore Schneider has very properly used ξ_w in place of Weissenberg's ξ for the rectangular coordinate of the diffraction spot on the Weissenberg film and has followed Bernal's use of ξ for the cylindrical coordinate of the point of the reciprocal lattice.

[6] For the definition and properties of the reciprocal lattice see Bernal, J. D., *Op. cit.*, pp. 118–125. (Bernal defines the reciprocal lattice somewhat more generally than Ewald did in his original description.)

[7] *Zeit. f. Krist.*, **69**, 41, 1928.

where r_F denotes the radius of the film and η_{360} the translation of the film carriage corresponding to a rotation of the crystal of 360°. Schneider's graphical construction is illustrated in Figs. 2 and 3.
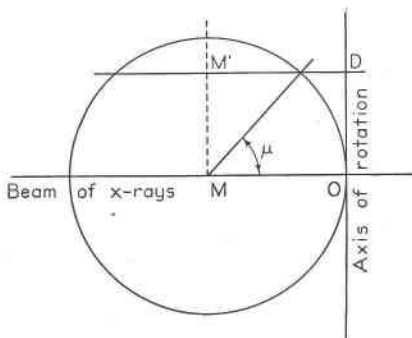

FIG. 2. Cross-section along the rotation-axis and through the center of the sphere of reflection. (Slightly modified after Schneider.)

Fig. 3 shows the piercing point of the rotation axis, D, also the circle, S_k, with radius r, cut out of the sphere of reflection by the plane of the diagram, and the center of the circle of reflection, M'.
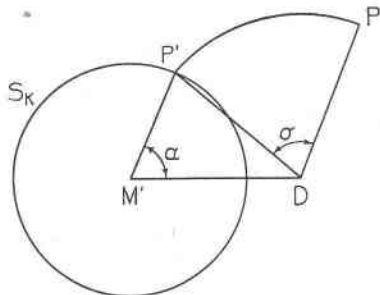

FIG. 3. Construction of the points of the reciprocal lattice. (After Schneider.)

Here $r = \cos \mu$. P is the point of the reciprocal lattice in the "initial position" (the "initial position" corresponds to the line chosen as the ξ_w-axis of coordinates), and P' the location of the same point at the moment of reflection.

The construction of the net-plane corresponding to the layer-line which is being analyzed is then accomplished as follows: The distance $M'D$ is laid off equal to unity (10 centimeters is convenient) and the circle of reflection is drawn with center M' and radius

$r = \cos \mu$ (10 cos μ centimeters if $M'D$ be taken as 10 centimeters). Then the angle α is laid off from $M'D$ (counterclockwise for the side of the film that occupied the upper half of the film carriage, clockwise for the other side) and the point P' is found. Lastly the angle σ is laid off from DP' (clockwise or counterclockwise according to the direction of rotation of the crystal; with a uniform experimental procedure the sense of this angle is always the same for the same instrument). The construction is repeated for each diffraction spot on the Weissenberg photograph.

The analysis of the first layer-line, together with the spacing of the layer-lines obtained from the preliminary rotation photograph, suffices to build up the reciprocal lattice of any crystal, and the space-lattice is of course completely determined by and easily obtained from the reciprocal lattice since each plane of the space-lattice is perpendicular to the line from the origin through the point of the reciprocal lattice, and the spacing, $d_{(hkl)}$, of the plane in the space-lattice is connected with the distance of the point of the reciprocal lattice from the origin, $\rho_{(hkl)}$, by the equation

$$\rho_{(hkl)} \cdot d_{(hkl)} = k^2$$

where k^2 is an arbitrary constant usually set equal to the wavelength, λ, of the x-rays.

The data for a triclinic crystal obtainable with certainty and ease by means of the Weissenberg goniometer are thus: the coordinates of the points of the space-lattice; the indices of the plane of the space-lattice producing each diffraction spot; and the approximate intensity of the diffraction from each plane of the space-lattice estimated by means of the density of the spot on the film.

The choice of the crystallographic axes remains to be made and is not determined by the knowledge of the space-lattice since the same triclinic space-lattice can be described by means of an infinite number of different unit cells. However, the determination of the space-lattice by means of the Weissenberg goniometer makes it easy to choose the axes in such a way as to satisfy the law of Bravais as stated by Friedel,[8] according to which the pinacoids shall have the greatest spacings or reticular densities, and in the three zones between the pinacoids the unit prism and unit domes shall have the greatest spacings except the pinacoids themselves.

The relationship between the linear elements, that is, the axial

[8] *Op. cit.*, p. 20. Cf. also p. 17 and pp. 142–144.

ratios, a/b and c/b, and the axial angles, α, β, γ, and the unit cell dimensions, a_0, b_0, c_0, α, β, γ, is well known; that a similar close relationship exists between the polar elements of Victor Goldschmidt and the elements of the reciprocal lattice seems not to be well known but is very useful to remember. The angles of the reciprocal lattice, α^*, β^*, γ^* (notation of Bernal), are identically the polar angles, λ, μ, ν, of Victor Goldschmidt and the reciprocal lattice elements, a^*, b^*, c^* (notation of Bernal), differ from Goldschmidt's p_0, q_0, $r_0(=1)$ only by a constant, or in other words, $a^*/c^* = p_0/r_0$ and $b^*/c^* = q_0/r_0$. In the crystallographic system of Victor Goldschmidt each crystal face is represented by the point at which its normal intersects a horizontal plane, the plane of the gnomonic projection, and in the reciprocal lattice each plane of the space-lattice is represented by the point on its normal at a distance from the origin equal to $\lambda/d_{(hkl)}$. The reciprocal lattice can be considered to be made up of the points at the corners of Victor Goldschmidt's "Polarform" plus the points at the corners of the "Polarform" after translation successively parallel to each of its edges successive distances equal to the length and multiples of the length of the edge along which the translation took place, if the scales of the reciprocal lattice and "Polarform" be properly chosen. Owing to the common polar character of these two representations their elements are necessarily closely related.