Crystallography. — *Calculation of the stereographic pole figure of the cubic lattice for any given direction [HKL]*. I. By W. MAY. (Communicated by Prof. J. M. BURGERS.)

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1. *Introduction.*

The method of SCHIEBOLD and SACHS [1]) is often used when the orientation of a single crystal must be determined. A transmission LAUE photograph of the single crystal is taken and from this (generally asymmetric) photograph a stereographic pole figure is prepared. By means of a stereographic net the pole figure is rotated till an important zone lies on the reference circle; this operation brings the projection of the corresponding zone axis in the centre of this circle. By preparing beforehand stereographic pole figures for the more important crystallographic directions of the crystal lattice (standard projections), it is possible to find a correspondence between the rotated projection and one of the standard projections. Indices can then be assigned to every LAUE spot and the axes can be plotted.

On a LAUE photograph nearly always more than one zone can be observed, but it complicates the process too much if for every zone axis a standard projection is prepared. SCHIEBOLD and SACHS, who worked out the method for the cubic face-centered lattice, have limited themselves to 5 standard projections, viz. for the directions [1 1 0], [0 0 1], [1 1 2], [1 3 0], [1 1 1]; one of the corresponding zones is practically always present in the LAUE pattern. The above sequence of crystallographic directions is that of decreasing packing density. Our experience with a large number of LAUE photographs of aluminium single crystals confirms this limitation; the various projections were used according to the following percentage scale: [1 1 0] 60 %, [0 0 1] 21 %, [1 1 2] 11 %, [1 3 0] 7 %, [1 1 1] 1 %.

In order to obtain precise results, it is necessary to construct these standard projections, as reproduction of those given by SCHIEBOLD and SACHS is rather inaccurate (for a radius of 7 cm the error is about 2°), especially when an enlargement is required. The construction can be made in several ways:

a. construction with the aid of a stereographic net, by laying off the calculated angles between the direction of the standard projection and the poles of the planes. It is quite probable that SCHIEBOLD and SACHS have

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1) E. SCHIEBOLD und G. SACHS, Z. Krist. **63** (1926) 34.

constructed their projections in this way [2]). It is clear that this method is not very accurate either, as the accuracy of a stereographic net with a radius of 10 cm is about $\frac{1}{2}°$. As the net is also used for the orientation determination, the possible error is doubled and comes to 1°.

b. construction with the aid of descriptive geometry. This method has clearly the drawback that this construction becomes very complicated and that errors will occur frequently. The accuracy will be slightly better than method *a*.

c. calculation of the coordinates of the projection. With this method any desired degree of accuracy can be obtained so that the precision of the standard projection is only limited by the plotting of the calculated distances and does not exceed a few tenths of a degree. In the following sections this calculation is given in detail.

2. *General course of the calculation.*

In fig. 1 the axes X and Y are mutually perpendicular and lie in the plane of projection. In their point of intersection O a perpendicular Z is

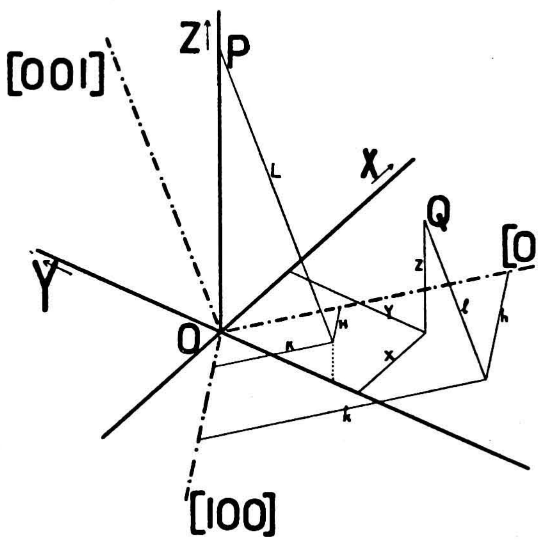

Fig. 1.

erected so that $OXYZ$ is a three-dimensional set of rectangular axes. The cubic lattice is represented by the three axes [1 0 0], [0 1 0] and [0 0 1] and forms a second set. Let the direction $[HKL]$ of the cubic lattice

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2) We have not been able to find another method published; see for example:
Internationale Tabellen zur Bestimmung von Kristallstrukturen, Berlin 1935, II, 687.
R. GLOCKER, Materialprüfung mit Röntgenstrahlen, 2. Aufl., Berlin 1936, 364.
F. HALLA und H. MARK, Röntgenographische Untersuchung von Kristallen, Leipzig 1937, 199.
C. S. BARRETT, Structure of Metals, New-York, 1943, 33.
A. TAYLOR, An Introduction to X-Ray Metallography, London 1945, 251.

coincide with the Z axis, $[HKL]$ being the direction for which the standard projection must be calculated. This involves that the pole (HKL) lies in the centre of the projection and therefore the poles of the corresponding zone planes lie on the reference circle. It is further supposed that [0 0 1] lies in the OYZ-plane; then the X axis lies in the plane O — [1 0 0]— [0 1 0] [3]. In this way the pole (0 0 1) is always situated on the positive side of the Y axis of the projection, as is also the case in the standard projections of SCHIEBOLD and SACHS.

In the cubic lattice the direction $[hkl]$ (that is the line connecting the origin with the point hkl) is perpendicular to the plane (hkl), so that one may say that plane (hkl) is represented by point hkl. Let Q in fig. 1 represent the point hkl; then first the coordinates X, Y and Z of Q must be calculated. Then the point of intersection of the direction $[hkl]$ with the reference sphere (centre O) is stereographically projected upon the plane OXY and the coordinates x and y of the projection are calculated from X, Y, Z.

3. *X, Y, Z as a function of H, K, L, h, k, l.*

The problem of the calculation of the coordinates of a point in a second set of rectangular axes when the coordinates in the first set are given, the

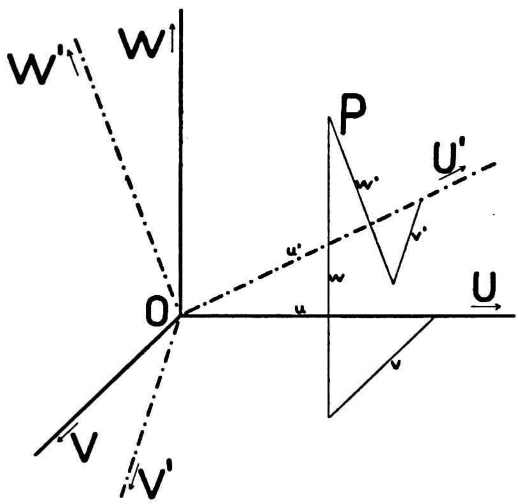

Fig. 2.

TABLE I.

	U	V	W
U'	a_1	b_1	c_1
V'	a_2	b_2	c_2
W'	a_3	b_3	c_3

sets having the same origin and a given mutual position, is solved in elementary analytical geometry. If in table I a_i, b_i and c_i $(i = 1, 2, 3)$ represent the cosines of the angles between the two sets $OUVW$ and

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[3]) This can be easily proved as follows: $OX \perp$ plane OYZ and therefore $OX \perp$ [001]; now [100] and [010] are both $\perp$ [001] and therefore OX, [100] and [010] lie in the same plane, perpendicular to [001].

$OU'V'W'$ (fig. 2), then the transformation equations for the coordinates are:

$$\left.\begin{aligned} u &= a_1 u' + a_2 v' + a_3 w' \\ v &= b_1 u' + b_2 v' + b_3 w' \\ w &= c_1 u' + c_2 v' + c_3 w' \end{aligned}\right\} \quad \ldots\ldots\ldots \quad (1)$$

Let the set $OUVW$ of fig. 2 be set $OXYZ$ of fig. 1 and set $OU'V'W'$ the cubic lattice, then we have:

$$\left.\begin{aligned} u &= -Y;\ v = -X;\ w = +Z \\ u' &= +k;\ v' = +h;\ w' = +l. \end{aligned}\right\} \quad \ldots\ldots \quad (2)$$

The cosines are related to each other by six independent equations:

$$a_i^2 + b_i^2 + c_i^2 = 1 \ (i = 1, 2, 3) \qquad a_i a_j + b_i b_j + c_i c_j = 0 \ (i = 1, 2, 3; \ j = 1, 2, 3; \ i \neq j).$$

From this and the location of the cubic lattice (section 2) they can be calculated (see table II):

TABLE II.

$$\left.\begin{aligned} a_1 &= +\frac{KL}{\sqrt{(H^2+K^2)\cdot\Sigma H^2}};\ b_1 = -\frac{H}{\sqrt{H^2+K^2}};\ c_1 = +\frac{K}{\sqrt{\Sigma H^2}} \\ a_2 &= +\frac{HL}{\sqrt{(H^2+K^2)\cdot\Sigma H^2}};\ b_2 = +\frac{K}{\sqrt{H^2+K^2}};\ c_2 = +\frac{H}{\sqrt{\Sigma H^2}} \\ a_3 &= -\frac{H^2+K^2}{\sqrt{\Sigma H^2}} \quad ;\ b_3 = 0 \quad ;\ c_3 = +\frac{L}{\sqrt{\Sigma H^2}} \end{aligned}\right\}. \quad (3)$$

Putting (2) and (3) in (1) gives:

$$X = \frac{Hk - Kh}{\sqrt{H^2+K^2}};\ Y = \frac{H(Hl - Lh) + K(Kl - Lk)}{\sqrt{(H^2+K^2)\cdot\Sigma H^2}};\ Z = \frac{Hh + Kk + Ll}{\sqrt{\Sigma H^2}} \quad (4)$$

where $\Sigma H^2 = H^2 + K^2 + L^2$.

4. *x and y as a function of H, K, L, h, k, l.*

The point of intersection of the line OQ with the reference sphere (centre O, radius R) is now projected stereographically in the plane of projection OXY. *It will be clear that this is wholly equivalent to projecting the plane* (hkl).

In fig. 3*a* is drawn the plane through the Z axis and point Q and the intersection of this plane with the reference sphere. In fig. 3*b* the projection plane is given. It is easy to see that:

$$OS = R \tan \tfrac{1}{2} \angle ROV = R\sqrt{\frac{1-\cos\angle MQO}{1+\cos\angle MQO}} = R\sqrt{\frac{OQ - MQ}{OQ + MQ}}.$$

$$OS = R\sqrt{\frac{\sqrt{X^2+Y^2+Z^2}-Z}{\sqrt{X^2+Y^2+Z^2}+Z}} = R\frac{\sqrt{X^2+Y^2}}{\sqrt{X^2+Y^2+Z^2}+Z} = R\frac{\sqrt{X^2+Y^2}}{\sqrt{\Sigma h^2}+Z},$$

where $\Sigma h^2 = h^2 + k^2 + l^2$.

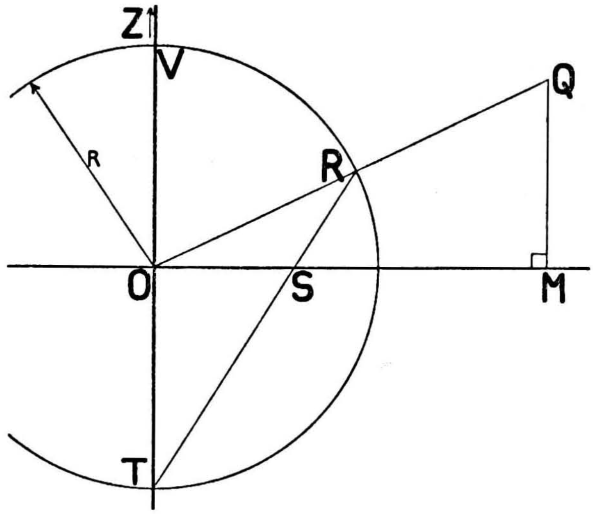

Fig. 3*a*.

Fig. 3*b* shows that:

$$x = \frac{OS}{\sqrt{X^2+Y^2}} X \text{ and } y = \frac{OS}{\sqrt{X^2+Y^2}} Y.$$

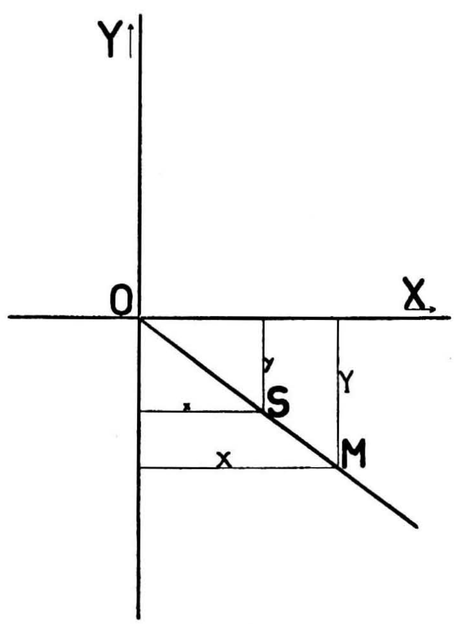

Fig. 3*b*.

With equations (4) this gives:

$$\left.\begin{aligned} x &= \frac{(Hk-Kh)\cdot\sqrt{\Sigma H^2}}{(\sqrt{\Sigma H^2\cdot\Sigma h^2}+Hh+Kk+Ll)\cdot\sqrt{H^2+K^2}}\,R\,; \\ y &= \frac{H(Hl-Lh)+K(Kl-Lk)}{(\sqrt{\Sigma H^2\cdot\Sigma h^2}+Hh+Kk+Ll)\cdot\sqrt{H^2+K^2}}\,R\,. \end{aligned}\right\} \quad . \quad . \quad (5)$$

With these equations it is possible to calculate the coordinates of the stereographic projection of every plane in the cubic lattice for any given direction $[HKL]$.

It is possible to extend this method to other symmetry systems, but the difficulties in handling the more and more complicated equations will grow rapidly.