

GRAPHICAL METHODS FOR THE DETERMINATION OF RETICULAR DENSITIES AND LATTICE PARAMETERS*

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ABSTRACT

Graphical methods are known for the determination of reticular densities from a gnomonic or stereographic projection made on a plane normal to $[001]$. They are explained in terms of the simple shear and the polar lattice.

Our aim is to generalize these rules for the case of a projection plane normal to an arbitrarily chosen zone $[uvw]$. A general theorem is stated, covering the previous methods as particular cases. Rules for trigonal crystals referred to the Miller axes also follow directly from it. The same method yields both reticular densities and lattice parameters. A working knowledge of the method can be acquired by working out three examples, given to illustrate the rules.

I. PROJECTION PLANE NORMAL TO $[001]$

According to Mallard's gnomonic theorem¹ the length of the projection-line for any face of the type $(hk1)$ is proportional to the reticular area of the crystal face projected. The plane of the gnomonic projection is taken perpendicular to the zone axis $[001]$. In Fig. 1, for instance, the length of the projection-line $P-(\bar{1}\bar{1}1)$ is a measure of the area of the two-dimensional unit-cell of the lattice-

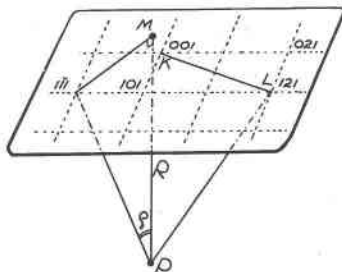


FIG. 1.

plane $(\bar{1}\bar{1}1)$. If the length of the "gnomon" (distance from the projection-point P to the plane of gnomonic projection) is equal to R , then the reticular area of the face $(\bar{1}\bar{1}1)$ is represented by $R/\cos \rho$, in which ρ is the angle between the gnomon and the projection-line $P-(\bar{1}\bar{1}1)$, that is to say the *polar distance* of $(\bar{1}\bar{1}1)$. The reticular

* Translated from the Dutch by J. D. H. Donnay, Johns Hopkins University.

¹ Mallard, E.: *Traité de Cristallographie*, tome. 1, pp. 26 and 63.

density of the face $(\bar{1}\bar{1}1)$, being inversely proportional to its reticular area, is then proportional to $\cos \rho$.

For a general face (hkl) , the method is to be slightly modified. It is well known that, in a gnomonic projection, a face (hkl) is represented by $(h/l \cdot k/l \cdot 1)$. The value of $\cos \rho$ obtained for such a pole, therefore, cannot be a measure of the reticular density of the face (hkl) . The true measure of that reticular density is given by the quotient $(\cos \rho)/l$.

Inspection of this expression immediately shows that another method of reticular density determination will have to be devised in the case of a face $(hk0)$, since the quotient $(\cos \rho)/l$ then leads to the indeterminate form $0/0$. A consequence of Mallard's theorem is that the reticular area of the face (120) , for instance, is represented by the line KL (see Fig. 1) connecting the gnomonic poles of (001) and (121) , in the same way as the reticular area of the face $(\bar{1}\bar{1}1)$ is represented by the line $P-(\bar{1}\bar{1}1)$. In general the reticular area of any face $(hk0)$ is represented by the line obtained by joining the pole (001) with the *substituted pole* $(hk1)$.

When a crystal is given in stereographic projection, the gnomonic projection of the pole $(hk1)$ and of the pole (001) are first determined in the usual manner, then the distance between the two gnomonic poles is measured; for instance, KL in the case of the face (120) , as shown in Fig. 2.

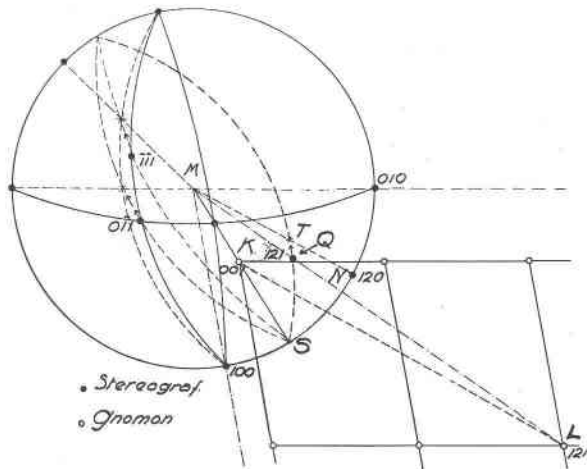


FIG. 2.

The reticular density of a face ($h\bar{k}0$) can also be determined directly from the stereographic projection. The reticular area of (120) is represented by KL (Fig. 2). Let ϕ_1 be the angle NML and ϕ_2 , the angle NMK . The lines KL and MN are parallel by construction. We have in the triangle MKL (Law of Sines):

$$KL = ML \frac{\sin(\phi_2 - \phi_1)}{\sin \phi_2}$$

Let R be the length of the gnomon, then:

$$ML = R \cdot \tan \rho_{121}$$

Substituting

$$KL = R \cdot \tan \rho_{121} \frac{\sin(\phi_2 - \phi_1)}{\sin \phi_2}$$

In the spherical triangle MSQ , the cotangent formula gives:

$$\sin(\phi_2 - \phi_1) = \frac{\tan MSQ}{\tan MQ}$$

Likewise in the spherical triangle MST :

$$\sin \phi_2 = \frac{\tan MST}{\tan MT} = \frac{\tan MSQ}{\tan MT}$$

Substituting again:

$$KL = R \cdot \tan \rho_{121} \frac{\tan MT}{\tan MQ} = R \cdot \tan MT$$

as $\text{arc } MQ = \rho_{121}$.

The reticular density of the face (120) is thus proportional to $\cot MT$, where the $\text{arc } MT$ is obtained as follows:

(1) Join the center M of the stereographic projection to K the stereographic pole of (001), and produce to S , intersection with the primitive circle.

(2) Draw the zone circle through S and Q , the stereographic pole of (121).

(3) "Slide" Q , the stereographic pole of (121), along that zone circle until it reaches, at point T , the radius MN joining the center M to the stereographic pole N of (120).

II. SIMPLE SHEAR AND POLAR LATTICE

The significance of such a "sliding" in the stereographic projection can best be explained in terms of the properties of the *polar*

*lattice*² (or *reciprocal lattice*). Let the dimensions of the latter be chosen in such a way that the parameter of a reticular row $[hkl]$ of the polar lattice be equal to the reticular area of the plane (hkl) of the crystal lattice. For convenience the reticular planes and rows of the *polar lattice* will be distinguished from those of the crystal lattice by means of the subscript p . Lattice point symbols will be enclosed in double brackets; $[[hkl]]_p$, for instance, represents the point of the polar lattice with "trimetric coordinates" h, k, l .

Consider now the face $(hk0)$. The corresponding row $[hk0]_p$ lies in the axial plane $(001)_p$. On this lattice-row, we find the following succession of points: $[[000]]_p, [[hk0]]_p, [[2h \cdot 2k \cdot 0]]_p$, etc. The parameter of the row $[hk0]_p$ is equal to the distance between the points $[[000]]_p$ and $[[hk0]]_p$, or (parallel lattice-planes being identical) to the distance between the points $[[001]]_p$ and $[[hk1]]_p$, which lie in ${}_1(001)_p$, the first $(001)_p$ plane³ away from the origin (Fig. 3).

If parallel lattice-planes are numbered from the origin: ${}_1(001)_p, {}_2(001)_p, {}_3(001)_p$, etc., the above can be summarized as follows: the reticular area of a face $(hk0)$ is equal to the distance between the two points $[[001]]_p$ and $[[hk1]]_p$ of the plane ${}_1(001)_p$.

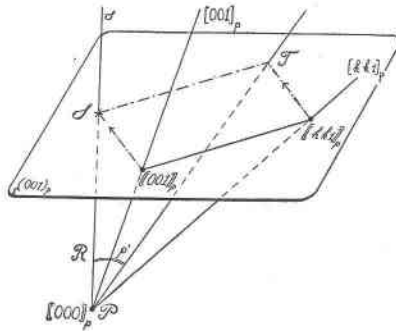


FIG. 3.

In general the foot S of the perpendicular s dropped from the origin $[[000]]_p$ on the face ${}_1(001)_p$ does not coincide with the point $[[001]]_p$. Imagine that all the parallel planes ${}_1(001)_p, {}_2(001)_p$, etc. (carrying with them their two-dimensional lattices), be "shoved" over each other so that the points $[[001]]_p, [[002]]_p$, etc., all come to

² Compare, for instance, George Tunell, *Am. Min.*, vol. 18, p. 183, 1933.

³ Mallard calls this plane "*plan limitrophe de l'origine*" (*Traité de Cristallographie*, tome 1, p. 17).

lie on the perpendicular s . This movement brings the point $[[hk1]]_p$ in T . It is easy to see that the reticular area of the face $(hk0)$ is equal to $ST = R \cdot \tan \rho'$ (Fig. 3), where ρ' designates the polar distance of T .

In order to get a simple prescript, we can perform this "sliding" in such a manner, that it obeys the following two conditions:

(1) During the movement the lattice-row $[001]_p$ must remain in the plane defined by $[001]_p$ and the normal s to $(001)_p$.

(2) The deformation of the polar lattice will be a *homogeneous deformation*, that is to say that points lying on a straight line at equal spacings will retain these properties during the deformation.

Under these conditions, the "sliding" considered constitutes a *simple shear*⁴ of the polar lattice. All the points describe rectilinear paths and their displacements are proportional to their distance from a *zero plane* (in which the displacement is of course zero). A *simple shear* is known when its zero plane, its direction, and its angular magnitude are given. The latter, in the present case, is the angle between the lattice-row $[001]_p$ and the normal s to the plane $(001)_p$.

Consider now (in the stereographic projection of Fig. 2) the normals to the faces (001) , (120) , (121) , etc. Apply to this radiating bundle of face-normals a simple shear with the plane of the primitive circle (equatorial plane) for its zero plane and with such a direction and such a magnitude that the normal to the face (001) be brought into coincidence with the normal to the primitive circle.⁵ What is the new position of the normal to the face (121) ?

Notice that:

(1) During the simple shear this normal to (121) remains in the plane α defined by its original position and MS , since each point of the normal to (121) describes a path parallel to MS .

(2) The plane β defined by MN and the normal to (001) is brought by the shear to be perpendicular to the primitive circle along MN , since the normal to (001) becomes perpendicular to the primitive circle, while MN , lying in the zero plane, is not affected by the shear.

⁴ Dutch: *enkelvoudige verschuiving*. German: *einfache Schiebung*. A good example of simple shear is gliding in calcite (see Liebisch: *Grundriss der physikalischen Krystallographie*, 1896, p. 449).

⁵ In Fig. 2, the face symbol 001 has unfortunately been omitted next to the black circllet representing its stereographic projection (between 011 and 010).

The new position of the normal to (121), therefore, lies at the intersection of the two planes α and β referred to above. Its pole is stereographically projected in T (Fig. 2). The procedure to find the reticular density of the face (120) can then be stated as follows:

To the radiating bundle of face-normals, apply a simple shear that will bring the pole (001) to the center of the primitive circle. Find the polar distance ρ' of the *substituted face* (121) after the shear. The reticular density of (120) is $\cot \rho'$.

III. EXAMPLE

Consider two stereographic projections of phthalylphenyl hydrazide⁶ (Figs. 4 and 5). The observed forms are O , C , a , q . The fact that this substance is monoclinic will be ignored so that the

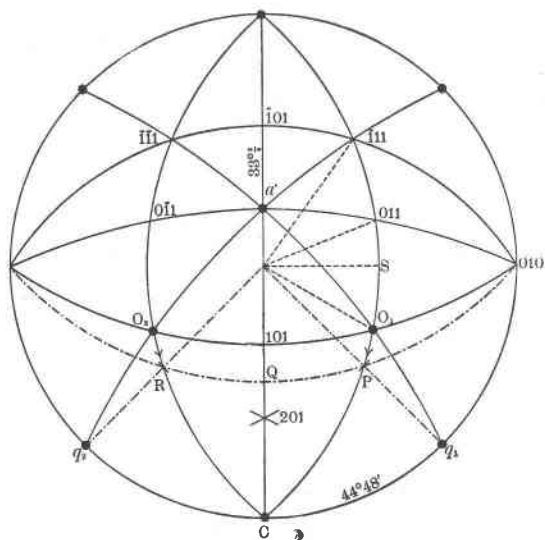


FIG. 4.

choice of the axial planes will not depend on symmetry considerations. In the first projection (Fig. 4), C and a are chosen as axial planes; O_1 as unit-face. In the second projection (Fig. 5), the axial planes are q_1 , q_2 , and a ; the unit-face is determined by assigning the symbols (101) and (011) to O_2 and O_1 respectively. The second projection can be obtained from the first by a rotation in the plane of the drawing. In both projections, the reticular densities

⁶ Groth: *Chemische Krystallographie*, vol. 5, p. 168.

TABLE 1
RETICULAR DENSITIES FOR PHTHALYLPHENYL HYDRAZIDE

Face	Fig. 4			Fig. 5		
	Symbol	rho	Reticular density	Symbol	rho	Reticular density
<i>C</i>	100	$49\frac{1}{2}^\circ$	$\cot 49\frac{1}{2}^\circ = .854$	110	67°	$\cot 67^\circ = .424$
<i>q</i>	110	59°	$\cot 59^\circ = .601$	010	59°	$\cot 59^\circ = .601$
<i>q</i>	110	59°	$\cot 59^\circ = .601$	100	59°	$\cot 59^\circ = .601$
<i>O</i>	111	$53\frac{1}{2}^\circ$	$\cos 53\frac{1}{2}^\circ = .595$	011	$53\frac{1}{2}^\circ$	$\cos 53\frac{1}{2}^\circ = .595$
<i>O</i>	111	$53\frac{1}{2}^\circ$	$\cos 53\frac{1}{2}^\circ = .595$	101	$53\frac{1}{2}^\circ$	$\cos 53\frac{1}{2}^\circ = .595$
<i>a</i>	001	$25\frac{1}{2}^\circ$	$\cos 25\frac{1}{2}^\circ = .903$	001	$25\frac{1}{2}^\circ$	$\cos 25\frac{1}{2}^\circ = .903$
	010	49°	$\cot 49^\circ = .869$	110	$66\frac{1}{2}^\circ$	$\cot 66\frac{1}{2}^\circ = .435$
	101	$36\frac{1}{2}^\circ$	$\cos 36\frac{1}{2}^\circ = .804$	112	$36\frac{1}{2}^\circ$	$\frac{1}{2} \cos 36\frac{1}{2}^\circ = .402$
	011	52°	$\cos 52^\circ = .616$	112	52°	$\frac{1}{2} \cos 52^\circ = .308$

It should be kept in mind that the significance of the "reticular density" determined by the method described here is quite different from that of the "reticular density" determined by röntgenographic investigation. It is beyond the reach of geometrical crystallography to deduce the *actual reticular densities* from mere goniometric data. The only results which can be obtained are the *relative densities, after indices have been assigned to the faces*.

This means that, for each crystal, a great many space-lattices can be imagined for which the angles between reticular planes will correspond to the interfacial angles measured on the crystal.¹⁰ All

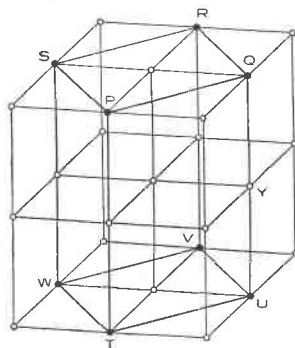


FIG. 6.

¹⁰ For indications as to how to make a choice between such "isogonal" lattices, see, for instance, Donnay and Mélon: Haüy-Bravais lattice . . . , *Am. Min.*, vol. 18, p. 225, 1933.

these lattices can be derived from each other in the sense that their unit-cells are multiples of each other. Consider (Fig. 6) the space-lattice corresponding to the projection of Fig. 4. By taking the parallelepiped $PQRSTUW$ as a new unit-cell, ignoring all other points, a new lattice can be constructed, which will be in agreement with the second projection of the crystal (Fig. 5). The second lattice is a *multiple lattice* of the first, its unit-cell being a *multiple cell* in the first lattice. Observe that all the points indicated in Fig. 6 belong to the first lattice, but that the second lattice is formed by the black dots only. So the face C (Figs. 4 and 5) or $SQUW$ in Fig. 6 has in the first lattice a reticular area $SQUW/4$, while in the second lattice the reticular area is $SQUW$. In the same manner we find for the face q_1 or $PQUT$ in Fig. 6 the reticular areas in the first and second lattices respectively $PQUT/2$ and $PQUT$; so O_1 or SRY . Therefore the reticular densities of the faces C , q , O , etc., referred to the second lattice, can be obtained by dividing their densities in the first lattice by 4, 2, 2, etc. Again, the numbers thus found can only be taken to indicate the *ratios* between the reticular densities of the faces in question. The unit chosen to express these reticular densities may be changed at will. If, for instance, we wish the reticular density of the face q to be the same in both lattices,¹¹ we divide the edges of the unit parallelepiped $PQRSTUW$ by $\sqrt{2}$. This was done to arrive at the numbers listed in Table 1.

IV. PROJECTION PLANE NORMAL TO $[uvw]$. GENERAL THEOREM

The preceding sections are limited to the case where the plane of projection is normal to the zone $[001]$. Rules for the determination of reticular densities in the case of a projection plane perpendicular to any zone $[uvw]$ will now be derived. The trend of the reasoning will be similar to that of Section II.

A general theorem can be stated as follows:

WHEN A CRYSTAL IS PROJECTED ON A PLANE NORMAL TO AN ARBITRARILY CHOSEN ZONE $[uvw]$,

(1) THE RETICULAR DENSITY OF A FACE (hkl) WHICH DOES NOT LIE IN THE ZONE $[uvw]$ IS GIVEN BY THE FORMULA:

¹¹ The absolute values of the parameters of the "lattices" considered in this paper are not known since they are derived from angular magnitudes only; this is why it has been suggested to call such lattices "relative" or "elastic" in contradistinction with the "absolute" lattice as determined by x -ray investigation.

$$\frac{\cos \rho}{hu + kv + lw},$$

IN WHICH ρ IS THE POLAR DISTANCE OF THE FACE (hkl) ;

(2) THE RETICULAR DENSITY OF A FACE (pqr) WHICH DOES LIE IN THE ZONE $[uvw]$ IS GIVEN BY THE FORMULA:

$$\frac{\cot \rho'}{u^2 + v^2 + w^2},$$

WHERE ρ' IS THE POLAR DISTANCE OF AN AUXILIARY FACE $(p+u \cdot q+v \cdot r+w)$, AFTER APPLICATION OF A SIMPLE SHEAR IF THE POLE OF THE ZONE AXIS $[uvw]$ DOES NOT COINCIDE WITH THE POLE OF THE FACE (uvw) .

The demonstration of the first half of this theorem is based on the following property of the polar lattice. The reticular area of the face (hkl) is equal to the distance between the points $[[000]]_p$ and $[[hkl]]_p$. Let d be that spacing. Consider the series of parallel planes $_1(uvw)_p$, $_2(uvw)_p$, etc., of the polar lattice. One of these planes, $_n(uvw)_p$, passes through the point $[[hkl]]_p$. It is well known that its *serial number*¹² is equal to:

$$n = hu + kv + lw.$$

Now if the plane $_1(uvw)_p$ is chosen as plane of projection,¹³ the length of the projection line of the face (hkl) is equal to $d/(hu + kv + lw)$. This length, however, is also equal to $R/\cos \rho$, where R is the length of the gnomon and ρ is the polar distance of (hkl) . We may therefore write

$$d = \frac{R(hu + kv + lw)}{\cos \rho}.$$

In other words, the reticular density of (hkl) is proportional to $(\cos \rho)/(hu + kv + lw)$.

For a face (pqr) which lies in the zone $[uvw]$, this formula cannot be applied, since it leads to the indeterminate form 0/0. The reason for this is that the line connecting the points $[[000]]_p$ and $[[pqr]]_p$ lies in the $(uvw)_p$ plane passed through the origin. Instead of using these two points, it is more convenient to consider the points

¹² Dutch: *volg nummer*.

¹³ According to the usual practice. See E. Mallard: *Traité de Cristallographie*, vol. 1, pp. 26 and 63.

The determination of reticular densities is somewhat more intricate for *trigonal crystals* referred to the Miller system of coördinate axes. It follows from the general theorem for $u=v=w=1$. For any face (hkl) which does not lie in the vertical zone, the reticular density is then $(\cos \rho)/(h+k+l)$, in which ρ is the polar distance of (hkl) . For a vertical face (pqr) , the reticular density is equal to $\frac{1}{3} \cot \rho'$, where ρ' is the polar distance of the substituted face $(p+1 \cdot q+1 \cdot r+1)$.

For pseudo trigonal crystals described with reference to Miller axes, the above formulae are also applicable provided the necessary simple shear be applied before reading ρ' for the faces of the vertical zone.

Tarbuttite provides a good example of the last case. Guided by the *complex symbol* found by Fedorov for that mineral, we have departed from Spencer¹⁴ in adopting the pseudotrigonal orientation projected in Fig. 7. The letters used to designate the crystal forms are those of Spencer's original description. The Fedorov orientation can be obtained from that of Spencer by the transformation $010/\bar{1}00/101$. The reticular densities are listed in Table 2.

TABLE 2
RETICULAR DENSITIES OF TARBUITITE

Face	Symbol	Substituted face	Reticular density
<i>c</i>	001	—	$\cos 44^\circ = .719$
<i>b</i>	100	—	$\cos 49^\circ = .656$
<i>f</i>	010	—	$\cos 50^\circ = .643$
<i>a</i>	0 $\bar{1}$ 1	102	$\frac{1}{3} \cot 30\frac{1}{2}^\circ = .566$
<i>u</i>	$\bar{1}$ 01	012	$\frac{1}{3} \cot 31^\circ = .554$
<i>k</i>	$\bar{1}$ 10	021	$\frac{1}{3} \cot 34^\circ = .494$
<i>s</i>	011	—	$\frac{1}{2} \cos 30^\circ = .433$
<i>m</i>	$\bar{1}\bar{1}$ 1	—	$\cos 66\frac{1}{2}^\circ = .399$
<i>g</i>	12 $\bar{1}$	—	$\frac{1}{2} \cos 46^\circ = .348$
—	111	—	$\frac{1}{3} \cos 4^\circ = .333$
<i>i</i>	$\bar{2}$ 11	$\bar{1}$ 22	$\frac{1}{3} \cot 48^\circ = .300$
<i>t</i>	012	—	$\frac{1}{3} \cos 30^\circ = .289$
<i>l</i>	201	—	$\frac{1}{3} \cos 33\frac{1}{2}^\circ = .278$
<i>o</i>	21 $\bar{2}$	—	$\cos 75^\circ = .259$
<i>d</i>	$\bar{2}$ 21	—	$\cos 76\frac{1}{2}^\circ = .233$
<i>e</i>	221	—	$\cos 77^\circ = .225$

¹⁴ Spencer, L. J., *Min. Mag.*, vol. 15, p. 22, 1908.

Remember that, for instance, the angle $\rho' = 30\frac{1}{2}^\circ$ for the substituted face (102) is read on the stereographic projection after the pole (111) has been brought to the center of the primitive circle by the proper *simple shear* (here $3\frac{1}{2}^\circ$).

VI. CENTERED LATTICES

The preceding sections all have reference to crystals which can be described by means of *simple lattices*. If one is dealing with a *centered lattice*, the reticular densities are first determined as if the lattice were simple, then corrected as follows:

(1) For a *body-centered lattice*, the reticular densities of the faces for which $(h+k+l)$ is even are multiplied by two.

(2) For an *all-face-centered lattice*, the reticular densities of the faces with all indices odd are multiplied by two.

(3) For a lattice *centered in one face xy only*, the reticular densities of the faces for which $(h+k)$ is even are multiplied by two.

VII. DETERMINATION OF PARAMETERS

The gist of the method lies in the following remarks:

(1) The reticular density of a plane is the reciprocal of its reticular area; the linear density of a row is the reciprocal of its parameter.

(2) (a) The determination of the reticular areas of a crystal K_1 resolves itself into the determination of the parameters of its polar crystal K_2 .

(b) The determination of the reticular densities of a crystal K_1 resolves itself into the determination of the linear densities of its polar crystal K_2 .

Inversely, since the crystal K_1 is the polar crystal of K_2 (just as K_2 is the polar of K_1), the determination of the reticular densities of K_2 is equivalent to the determination of the reciprocals of the parameters of K_1 . Hence in order to find the parameters of K_1 graphically, the first step is to derive the stereographic projection of K_2 from the given stereographic projection of K_1 . The face poles of K_1 are the points where the edges of K_2 intersect the sphere of projection, or, in other words, *the stereographic projection of K_2 is at the same time the cyclographic projection of K_1* . Hence, the rules of reticular density determination, applied to the cyclographic projection of a crystal, yield the reciprocals of the parameters of that crystal.

The stereographic projection of a crystal K_1 being given, the corresponding cyclographic projection is found by plotting the pole of

each zone circle (this is easily done by means of a Wulff net) and then by rotating the projection until the polar crystal K_2 is projected on a face of the given crystal K_1 .

EXAMPLE.—Starting from the stereographic projection of sodium molybdo-tellurate¹⁵, the corresponding cyclographic projection (Fig. 8) is derived in that manner. The values of some of the parameters, graphically determined on the projection are listed in Table 3.

The order of accuracy of the graphical solution may be judged by

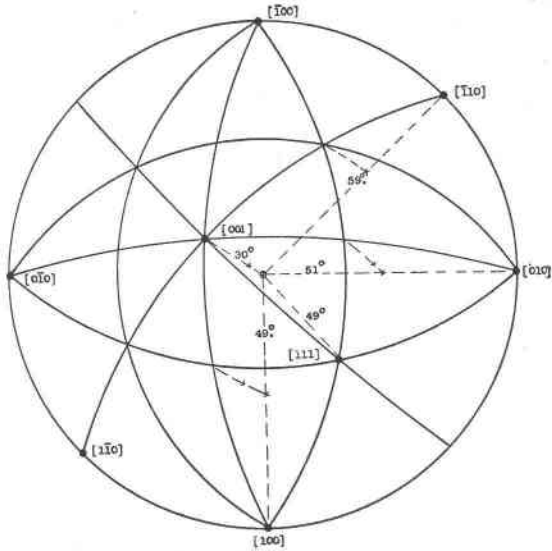


FIG. 8.

TABLE 3
PARAMETERS OF SODIUM₂MOLYBDO-TELLURATE

Lattice row	Parameter	Parameter ($b=1$)
[100]	$\tan 49\frac{1}{2}^\circ = 1.171$	0.948
[010]	$\tan 51^\circ = 1.235$	1.000
[001]	$\sec 30^\circ = 1.156$	0.940
[110]	$\tan 59\frac{1}{2}^\circ = 1.698$	1.234
[111]	$\sec 49^\circ = 1.524$	1.375

¹⁵ Donnay and Mélon: *Am. Min.*, vol. 18, p. 243, Fig. 6, 1933.

comparison of these results with the computed values on record:

$$\bar{a}:\bar{b}:\bar{c}=0.9548:1:0.9344.$$

In this case, the error is less than one *per cent*.

The above method for the determination of parameters only applies to simple lattices. In the case of a *body-centered lattice*, the parameters found for rows with all three indices odd must be divided by two. If the lattice is of the *face-centered* type, the parameters of the rows with two indices odd should be divided by two. For a lattice centered in one face *xy* only, the parameters of the rows for which $(h+k)$ and l are even should be divided by two.

The graphical determination of reticular densities and parameters described in this paper is sufficiently accurate for a number of purposes when made on the usual Wulff net (10 cm. radius). For greater accuracy the Schiebold stereographic net (50 cm. radius), sold by the firm R. Seifert in Hamburg, may be found serviceable.

ACKNOWLEDGMENTS

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