On Grassmann's method of axial representation, and its application to the solution of certain crystallographic problems.

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**ASSMANN**, in his Memoir, Zur physischen Krystallographie und (j geometrischen Combinationslehre, published in 1829, referred a crystal to three face-normals-rays-as axes of reference; the parameters being the edges along the axes of a parallelepiped having for diagonal a definite length of a known normal which is not co-planar with any pair of the axial rays. Any other normal is then represented as the diagonal of a similarly formed parallelepiped having for its edges along the axes lengths which are rational multiples of the parameters. Grassmann gave no formulæ for finding in general the indices of face-normals from measurements of the angles on the crystal; nor for determining the angles from the crystal-elements and indices. Frankenheim (Crelle's Journal f. Mathematik, VIII, p. 178, 1832) gives an expression for the cosine of the angle between any two rays, but his expression is not in a form such as is now usually adopted. Miller, in his memoir on the method (Proc. Camb. Phil. Soc. II, p. 75, 1868) limited himself to a few general problems relating to zones. The space which could be spared to the subject in my Treatise on Crystallography, 1899, only allowed me to give the relation connecting the ray parameters with those of a crystal referred to zone-axes. But the inclination of any ray to the reference-rays and to any other ray can be easily found by the process adopted in Chapter XIX, Arts. 9, 10, 11, 13 and 14 of my Treatise for the similar relations connecting the direction of a line with axes which are edges of the crystal. The relations obtained when the crystal is referred to axial rays are more immediately applicable to the angles found by goniometric measurement. and are in many respects simpler than the relations given in the above mentioned articles. As, further, Grassmann's axial representation gives many elegant expressions applicable to the solution of problems which occur in the determination of the face symbols and angles of crystals, I have thought that it may prove useful to establish some of the principal relations.

We shall throughout assume that the same three faces are selected to give the axial system, the axial rays being parallel to their normals, and the ordinary axes to their edges of intersection. We shall take Ox, Oyand Oz to be the rays which are, respectively, perpendicular to the faces (100), (010) and (001). We shall denote by OG the parametral ray (111), and shall suppose it to be perpendicular to the face (111) referred to zone axes. We shall denote the ray-parameters by a, b, c, and the angles between the axial rays by a,  $\beta$ ,  $\gamma$ . The corresponding parameters and angles, when the crystal is referred to zone axes, will be denoted by a, b, c,  $a_1$ ,  $\beta_1$ ,  $\gamma_1$ . Any ray (*hkl*) of the crystal is then given by the equations—

and the ray-parameters are connected with those referring to zone-axes by the equations—

or by their equivalents -

Prop. 1. To express the length of a given ray (hkl) in terms of the indices, ray-parameters, and the angles between the axial rays.

Let OLPN, Fig. 1, be the parallelepiped, having OP for diagonal, and for edges along the axes the lengths : --

$$OL = FM = ha$$
,  $OM = LF = kb$ ,  $ON = PF = lc.....(3)$ .

Let the inclination of OP to the axes Ox, Oy, Oz be denoted by  $\lambda$ ,  $\mu$ ,  $\nu$ , respectively.



Since the sum of the orthogonal projections of the three edges OL, LF and FP on OP must be equal to OP, we have—

$$OP = OL \cos \lambda + LF \cos \mu + FP \cos \nu$$
  
= ha cos  $\lambda + kb \cos \mu + lc \cos \nu \dots \dots (4)$ .

Again, taking the orthogonal projections of OP and of the above three edges of the parallelepiped on each of the axial rays in turn, we obtain the following equations :—

$$OP \cos \lambda = OL + LF \cos \gamma + FP \cos \beta = ha + kb \cos \gamma + lc \cos \beta$$
  

$$OP \cos \mu = ha \cos \gamma + kb + lc \cos a$$
  

$$OP \cos \nu = ha \cos \beta + kb \cos a + lc$$
(5).

Multiply both sides of (4) by OP and introduce the values of  $OP \cos \lambda$ , &c., from (5). We then have—

$$OP^{2} = ha(ha + kb \cos \gamma + lc \cos \beta) + kb(ha \cos \gamma + kb + lc \cos a) + lc(ha \cos \beta + kb \cos a + lc) = \Sigma h^{2}a^{2} + 2\Sigma klbc \cos a \dots \dots \dots \dots (6).$$

Prop. 2. To find the direction-cosines of any ray, and the relation which exists between them and the angles between the axial rays.

The direction cosines are found by introducing in (5) the value of OP given in (6). They are, therefore,—

$$\left. \cos \lambda = \frac{ha + kb \cos \gamma + lc \cos \beta}{\sqrt{\Sigma h^2 a^2 + 2 \Sigma k/bc \cos a}} \\
\cos \mu = \frac{ha \cos \gamma + kb + lc \cos a}{\sqrt{\Sigma h^2 a^2 + 2 \Sigma k/bc \cos a}} \\
\cos \nu = \frac{ha \cos \beta + kb \cos a + lc}{\sqrt{\Sigma h^2 a^2 + 2 \Sigma k/bc \cos a}} \right\} \dots\dots(7)$$

Equations (4) and (5) hold for any ray. Eliminating, therefore, OP, ha, kb, lc from the four equations, we obtain the relation which holds between the direction-cosines: it is—

$$\Delta_{1} = \begin{vmatrix} 1 & \cos \lambda & \cos \mu & \cos \nu \\ \cos \lambda & 1 & \cos \gamma & \cos \beta \\ \cos \mu & \cos \gamma & 1 & \cos \alpha \\ \cos \nu & \cos \beta & \cos \alpha & 1 \end{vmatrix} = 0 \dots (8).$$

Prop. 3. To find expressions for the indices of any ray in terms of the angles which it makes with the axial rays.

Solving equations (5) for ha, kb, lc, we have-

$$\begin{aligned} ha \div & \begin{vmatrix} \cos \lambda & \cos \gamma & \cos \beta \\ \cos \mu & 1 & \cos \alpha \\ \cos \nu & \cos \alpha & 1 \end{vmatrix} = kb \div \begin{vmatrix} 1 & \cos \lambda & \cos \beta \\ \cos \gamma & \cos \mu & \cos \alpha \\ \cos \beta & \cos \nu & 1 \end{vmatrix} \\ = lc \div & \begin{vmatrix} 1 & \cos \beta & \cos \lambda \\ \cos \gamma & 1 & \cos \mu \\ \cos \beta & \cos \alpha & \cos \nu \end{vmatrix} = OP \div \begin{vmatrix} 1 & \cos \gamma & \cos \beta \\ \cos \gamma & 1 & \cos \alpha \\ \cos \beta & \cos \alpha & 1 \end{vmatrix} ...(9). \end{aligned}$$

Again, if the value of OP given in (4) be introduced into the equations (5), we obtain the following equations, which may be sometimes useful:

 $\begin{aligned} &ha \sin^2 \lambda + kb(\cos \gamma - \cos \lambda \cos \mu) + lc(\cos \beta - \cos \lambda \cos \mu) = 0 \\ &ha(\cos \gamma - \cos \lambda \cos \mu) + kb \sin^2 \mu + lc(\cos \alpha - \cos \mu \cos \nu) = 0 \\ &ha(\cos \beta - \cos \lambda \cos \nu) + kb(\cos \alpha - \cos \mu \cos \nu) + lc \sin^2 \nu = 0 \end{aligned}$ (10).

Prop. 4. To find the equation of the plane perpendicular to a ray (hkl), *i.e.* of the face (hkl).

Suppose the plane to pass through the point P, which is the extremity of the diagonal of the parallelepiped having for edges ha, kb, lc; and let the ray make the angles  $\lambda$ ,  $\mu$ ,  $\nu$  with the axial rays.

The sum of the orthogonal projection on OP of the coordinates x, y, z of any point which lies in the plane is equal to OP.

 $\therefore OP = x \cos \lambda + y \cos \mu + z \cos \nu.$ 

Introducing the values of  $\cos \lambda$ ,  $\cos \mu$ ,  $\cos \nu$  from (5) and the value of  $OP^2$  from (6), we have—

$$(x-ha) (ha+kb\cos\lambda+lc\cos\beta)+(y-kb) (ha\cos\gamma+kb+lc\cos\alpha) +(z-lc) (ha\cos\beta+kb\cos\alpha+lc)=0 \dots (11).$$

The parallel plane through the origin is—

 $x(ha+kb\cos\gamma+lc\cos\beta)+y(ha\cos\gamma+kb+lc\cos\alpha) + z(ha\cos\beta+kb\cos\alpha+lc)=0.....(12).$ 

Prop. 5. To find the angle  $\phi$  between any two rays (hkl) and  $(h_1k_1l_1)$ .

Let OP in Fig. 1 be the ray (hkl), and let its inclination to the axial rays be  $\lambda$ ,  $\mu$ ,  $\nu$ . Then the relations established in the preceding propositions hold for it. Suppose the ray  $(h_1k_1l_1)$  to be given by the diagonal  $OP_1$  of a similar parallelepiped, and its direction-angles to be  $\lambda_1$ ,  $\mu_1$ ,  $\nu_1$ . Then the orthogonal projection of OP on  $OP_1$  must be equal to the sum of the projections of the edges OL, LF, FP on  $OP_1$ .

Hence,  $OP \cos \phi = OL \cos \lambda_1 + LF \cos \mu_1 + FP \cos \nu_1$ =  $ha \cos \lambda_1 + kb \cos \mu_1 + lc \cos \nu_1$ .....(13).

But  $\cos \lambda_1$ ,  $\cos \mu_1$ ,  $\cos \nu_1$ ,  $OP_1$  are connected together by equations similar to those given in (5). Multiplying both sides of (13) by  $OP_1$ , and replacing  $OP_1 \cos \lambda_1$ , &c., by their equivalents, we have—

$$OP.OP_1 \cos\phi = ha(h_1a + k_1b\cos\gamma + l_1c\cos\beta) + kb(h_1a\cos\gamma + k_1b + l_1c\cos\alpha) + lc(h_1a\cos\beta + k_1b\cos\alpha + l_1c).$$

Hence-

$$\cos\phi = \frac{\Sigma h h_1 a^2 + \Sigma b c (k l_1 + l k_1) \cos a}{\sqrt{\Sigma h^2 a^2 + 2\Sigma k l b c \cos a} \sqrt{\Sigma h_1^2 a^2 + 2\Sigma k_1 l_1 b c \cos a}} \dots \dots (14).$$

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This expression is simpler and more easily computed than either of the expressions (44) and (47) of pages 569 and 570 of my *Treatise on* Crystallography. It can also be easily transformed into either of them by the relations (2). Thus to get (47) we need only substitute for a, b, c from (2), when we have—

$$\cos \phi =$$

$$\frac{\Sigma \frac{hh_1}{a^2} \sin^2 a + \Sigma \frac{kl_1 + lk_1}{bc} \sin \beta \sin \gamma \cos a}{\sqrt{\Sigma \frac{h^2}{a^2} \sin^2 a + 2\Sigma \frac{kl}{bc} \sin \beta \sin \gamma \cos a} \sqrt{\frac{\Sigma \frac{h_1^2}{a^2} \sin^2 a + 2\Sigma \frac{k_1 l_1}{bc} \sin \beta \sin \gamma \cos a}}$$

Equation (44) is found by a similar substitution from  $(2^*)$ , and the relations of a spherical triangle—

$$\cos \alpha = \cos \beta \, \cos \gamma + \sin \beta \, \sin \gamma \, \cos \, (A = \pi - a_1), \&c.$$

We shall now show how this method can be applied to the solution of crystallographic problems. Thus let us take an anorthic crystal, and let it be required to find the linear elements from a knowledge of some of the angles. Adopting the letters and notation of page 161 of my *Treatise*, let us suppose the zone [BLC] = [010, 001] to be known. Introducing the indices 0,1,1 of L into the first and second equations of (7), we have—

$$\cos (AL = 100 \land 011) = \frac{b \cos \gamma + c \cos \beta}{\sqrt{b^2 + c^2 + 2 bc \cos a}} \dots (15)$$
  
and 
$$\sec^2(D = 0.10 \land 011) = \frac{b^2 + c^2 + 2 bc \cos a}{(b + c \cos a)^2};$$
  
$$\therefore \tan^2 D = \sec^2 D - 1 = \frac{c^2(1 - \cos^2 a)}{(b + c \cos a)^2};$$
  
$$\therefore \tan D = \frac{c \sin a}{b + c \cos a} \dots (16)$$
  
Also 
$$\frac{\sin D}{c \sin a} = \frac{\cos D}{b + c \cos a} = \frac{\sin (a - D)}{b \sin a};$$
  
$$\therefore \frac{b}{c} = \frac{\sin (a - D)}{\sin D} = \frac{\sin D}{\sin D}, \dots (17)$$

This equation, which gives the parametral ratio  $\frac{b}{c}$ , is given by Grassmann, p. 138; but as he endeavours to connect the ratio with the distances between consecutive particles, his expression differs slightly from

the above. It can, by means of the relations (2), be easily transformed into the equations giving the parameters on the corresponding zone-axes. This latter expression is—

By introducing into (7) the values (101) and (110), we get corresponding expressions for the other parametral ratios. They are—

$$\frac{c}{a} = \frac{\sin E_i}{\sin E}$$
, and  $\frac{a}{b} = \frac{\sin F_i}{\sin F}$ .....(19).

Again, if L is 0kl, we have from the second equation of (7)—

$$\cos BL_{i} = \frac{kb + lc \cos a}{\sqrt{k^{2}b^{2} + l^{2}c^{2} + 2kl bc \cos a}},$$
whence  $\tan BL_{i} = \frac{lc \sin a}{kb + lc \cos a}$ ......(20).  
and  $\frac{\sin BL_{i}}{\sin (a - BL_{i})} = \frac{\sin BL_{i}}{\sin CL_{i}} = \frac{lc}{kb}$ ......(21)

Dividing (21) by (17), we have the anharmonic ratio of the four poles  $\{BL_{L}LC\}$ , which is—

The deduction of special formulæ for the systems of greater symmetry is easy. We shall at present limit ourselves to the consideration of the rhombohedral system.

Rhombohedral system.

In this system the normals to the fundamental trigonal pyramid or rhombohedron are selected as the axial rays, and the triad axis as the parametral ray (111).

Hence  $a = \beta = \gamma$ ; and a = b = c = 1 (say). Equations (5) become  $OP \cos \lambda = h + (k+l)\cos a = h(1 - \cos a) + \theta \cos a$   $OP \cos \mu = h(1 - \cos a) + \theta \cos a$   $OP \cos \nu = l(1 - \cos a) + \theta \cos a$   $\left. \dots \dots (23); \right.$ 

Where  $\theta = h + k + l$ .

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Also,  $OP^2 = \Sigma h^2 + 2 \cos \alpha \Sigma kl = \theta^2 \cos \alpha + (1 - \cos \alpha)\Sigma h^2 \dots (24).$ And,

$$\cos \lambda = \frac{h(1 - \cos a) + \theta \cos a}{\sqrt{\Sigma h^2 + 2 \cos a \Sigma h l}}$$

$$\cos \mu = \frac{h(1 - \cos a) + \theta \cos a}{\sqrt{\Sigma h^2 + 2 \cos a \Sigma h l}}$$

$$\cos \nu = \frac{l(1 - \cos a) + \theta \cos a}{\sqrt{\Sigma h^2 + 2 \cos a \Sigma h l}}$$
(25).

 $\Delta_1$  becomes—

$$\frac{(1-\cos a)^2(1+2\,\cos a)-(1-\cos^2 a)\Sigma\,\cos^2 \lambda}{+2\,\cos a(1-\cos a)\Sigma\,\cos \,\lambda\,\cos \,\mu}.$$

Since this is equal to zero, we obtain as the relation between the direction-cosines-

 $(1+\cos a)\Sigma\cos^2\lambda-2\cos a\Sigma\cos\lambda\cos\mu=(1-\cos a)(1+2\cos a)....(26).$ 

When the ray coincides with the triad axis,  $\lambda = \mu = \nu = D = 111 \wedge 100$ . Equation (26) then reduces to—

$$3(1 - \cos \alpha) \cos^2 D = (1 - \cos \alpha) (1 + 2 \cos \alpha);$$
  

$$\therefore \quad 3 \cos^2 D = 1 + 2 \cos \alpha \dots \dots (27).$$
  
Hence 
$$2 \cos \alpha = \frac{2 - \tan^2 D}{1 + \tan^2 D} \dots \dots (28).$$

Again,  $3 \sin^2 D = 2(1 - \cos a) = 4 \sin^2 \frac{a}{2} \dots \dots (29).$ 

This last equation is equivalent to the well-known formula-

 $\sin r'r/2 = \sin 60^\circ \sin D;$ 

Where r and r' are two poles of the fundamental rhombohedron.

The expression (14) for the cosine of the angle between the rays (hkl) and  $(h_1k_1l_1)$  becomes—

$$\cos\phi = \frac{\Sigma h h_1 + \cos\alpha \Sigma (k l_1 + k_1 l)}{\sqrt{\Sigma h^2 + 2 \cos\alpha \Sigma k l} \sqrt{\Sigma h_1^2 + 2 \cos\alpha \Sigma k_1 l_1}} \dots \dots (30).$$

If  $\cos \alpha$  is replaced by its equivalent given in (28), we obtain the following expressions for the cosine :--- $\cos \phi =$ 

$$\begin{split} \frac{2\{\Sigma hh_1 + \Sigma(kl_1 + k_ll)\} + \tan^3 D\{\Sigma \Sigma hh_1 - \Sigma(kl_1 + k_ll)\}}{\sqrt{2(\Sigma h^2 + 2\Sigma kl) + 2 \tan^2 D(\Sigma h^2 - \Sigma kl)} & \sqrt{2(\Sigma h_1^2 + 2\Sigma k_ll_1) + 2 \tan^2 D(\Sigma h_1^2 - \Sigma k_ll_1)} \\ &= \frac{2\theta \theta_1 + \tan^2 D\Sigma(k - l)(k_1 - l_1)}{\sqrt{2\theta^2 + \tan^2 D\Sigma(k - l)^2} & \sqrt{2\theta_1^2 + \tan^2 D\Sigma(k_1 - l_1)^2}} \dots (31); \\ &\text{where } \theta_1 = h_1 + k_1 + l_1. \end{split}$$

By means of the equations above given, and the relations of the spherical triangles formed by P with the axial poles and with the poles C, N, m, m', m'', a', &c., marked in Fig. 2, we can easily establish the relations in general use for the solution of problems respecting rhombohedral crystals.



Or employing the general equations (30) and (31), and C being (111), we have—

$$\cos CP = \frac{\theta \sqrt{1 + 2 \cos a}}{\sqrt{3\{\Sigma h^2 + 2 \cos a\Sigma kI\}}}$$
$$= \frac{\theta \sqrt{2}}{\sqrt{2\theta^2 + \tan^2 D\Sigma (k - l)^2}} \dots (32).$$

By transforming the first equivalent, we have-

=

$$\tan CP = \frac{\sqrt{(1-\cos a)\Sigma(k-l)^2}}{\theta\sqrt{(1+2\cos a)}}\dots\dots(38).$$

By transforming the second equivalent, we obtain-

$$\tan CP = \frac{\sqrt{\Sigma(k-l)^2}}{\theta\sqrt{2}} \tan D.....(34) ;$$

and this can be shown to be the result of replacing  $\cos a$  in (33) by its equivalent in terms of  $\tan D$ .

Again, taking  $2\xi$ ,  $2\eta$  to be the angles, respectively, over the obtuse and acute polar edges of a scalenohedron  $\{hkl\}$ , and  $2\zeta$  to be that over each of its median edges, we have —

$$\cos 2\xi = \cos hkl_{\Lambda}hlk = \frac{h^2 + 2kl + \cos \left\{\theta^2 - (h^2 + 2kl)\right\}}{\Sigma h^2 + 2\cos \left\{\Sigma hl\right\}}$$
$$= \frac{2\theta^2 + \tan^2 D \left\{3(h^2 + 2kl) - \theta^2\right\}}{2\theta^2 + \tan^2 D \Sigma (k-l)^2} \dots \dots (35).$$

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Hence 
$$2 \sin^2 \hat{\xi} = \frac{2 (k-l)^2 \sin^2 \frac{a}{2}}{\Sigma h^2 + 2 \cos a \ \Sigma k l} = \frac{3(k-l)^2 \tan^2 D}{2\theta^2 + \tan^2 D \ \Sigma (k-l)^2}$$
.....(36).  
Similarly,  
 $\cos 2\eta = \cos (hkl \Lambda khl) = \frac{l^2 + 2hk + \cos a \{\theta^2 - (l^2 + 2hk)\}}{\Sigma h^2 + 2 \cos a \ \Sigma k l}$   
 $= \frac{2\theta^2 + \tan^2 D \{3(l^2 + 2hk) - \theta^2\}}{2\theta^2 + \tan^2 D \ \Sigma (k-l)^2}$ .....(37).  
 $\therefore 2 \sin^2 \eta = \frac{2(h-k)^2 \sin^2 \frac{a}{2}}{\Sigma h^2 + 2 \cos a \ \Sigma k l} = \frac{3(h-k)^2 \tan^2 D}{2\theta^2 + \tan^2 D \ \Sigma (k-l)^2}$ .....(38).  
And  
 $\cos 2\zeta = \cos hk^l \Lambda \bar{l} \ \bar{k} \ \bar{h} = \frac{-(k^2 + 2hl) - \cos a \{\theta^2 - (h^2 + 2hl)\}}{\Sigma h^2 + 2 \cos a \ \Sigma \ k l}$ 

$$=\frac{-2\theta^2-\tan^2 D \left\{3(k^2+2hl)-\theta^2\right\}}{2\theta^2+\tan^2 D \left[\Sigma(k-l)^2\right]}.$$
(39).

Hence

$$2 \cos^{2} \zeta = \frac{2 (h-l)^{2} \sin^{2} \frac{a}{2}}{\sum h^{2}+2 \cos a \ \Sigma k l} = \frac{3(h-l)^{2} \tan^{2} D}{2\theta^{2}+\tan^{2} D \ \Sigma (k-l)} \dots \dots (40).$$

Now each of the angles  $\xi$ ,  $\eta$ ,  $\zeta$  is less than 90°, for the angles over the scalenohedral edges are each less than 180°. Therefore taking, as we are at liberty to do, h, k and l to be in descending order of magnitude, and their sum to be greater than unity, the positive values must be taken when the square roots of equations (36), (38) and (40) are extracted. We have, therefore,—

$$\sin \hat{\xi} = \frac{(k-l) \sin \frac{a}{2}}{\sqrt{2h^2 + 2\cos a 2kl}} = \frac{(k-l) \sqrt{3} \tan D}{\sqrt{4\theta^2 + 2 \tan^3 D 2(k-l)^2}};$$
  

$$\sin \eta = \frac{(h-k) \sin \frac{a}{2}}{\sqrt{2h^2 + 2\cos a 2kl}} = \frac{(h-k) \sqrt{3} \tan D}{\sqrt{4\theta^2 + 2 \tan^3 D 2(k-l)^2}};$$
  

$$\cos \zeta = \frac{(h-l) \sin \frac{a}{2}}{\sqrt{2h^2 + 2\cos a 2kl}} = \frac{(h-l) \sqrt{3} \tan D}{\sqrt{4\theta^2 + 2 \tan^2 D 2(k-l)^2}}$$

Hence,

$$\frac{\sin \xi}{k-l} = \frac{\sin \eta}{h-k} = \frac{\cos \zeta}{h-l} = \frac{\sin \frac{a}{2}}{\sqrt{2h^2 + 2\cos a\Sigma kl}}$$
$$= (by \text{ transformation from (32)}) \frac{\sqrt{3}\sin CP}{\sqrt{2\Sigma(k-l)^2}} = \frac{\sqrt{3}\tan D}{\sqrt{4\theta^2 + 2}\tan^2 D\Sigma(k-l)^2}$$
$$= (\text{from (32)}) \frac{\sqrt{3}\tan D\cos CP}{2\theta} \dots \dots (42);$$
and  $\sin \xi + \sin \eta = \cos \zeta \dots \dots (43).$ 

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