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Computational techniques for stereographic projection

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The geometrical analysis leading to equations which permit the interactive construction of general stereographic projections by means of a computer program compatible with modern microcomputers is given. The stereographic operations covered include the plotting of any pole or direction on a projection of any orientation, and the drawing of the great circle of the plane which is normal to this plane or direction. Other operations considered here are the indexing of any pole at location x, y, the rotation of any one general pole about another, and the direct transfer of diffraction spots on a back-reflection Laüe pattern to the stereographic projection using only the x, y coordinates of the Laüe spots. All of the above operations may be performed in any crystal system since simple equations are included for the calculation of the indices of a Cartesian vector normal to any $(h\,k\,l)$ plane or parallel to any $[u\,v\,w]$ direction in a general crystal. A description of a microcomputer program utilizing the expressions derived is given together with a few examples of graphical output from the program.

1. Introduction

The stereographic projection technique is useful for the graphical solution of many problems involving crystallographic orientation. The technique suffers, however, from the inherent inaccuracy of graphical techniques and from the length of time required to produce solutions of more difficult problems. In addition to overcoming these problems, an interactive computer program for the manipulation of stereographic projections using a microcomputer offers the possibility of using the program as a teaching and research tool. Such a program can be valuable, for instance, in the teaching of stereographic projection techniques, solution of Laüe patterns, solution of pole figures, or finding the orientation of the tensile axis and slip traces on the surface of a single crystal after straining.

The use of the stereographic projection technique is covered in standard texts [1, 2], and techniques for calculating the x, y coordinates of poles and other useful quantities have been discussed by Mackenzie and Bowles [3] and Johari and Thomas [4]. Mackenzie and Bowles [3] gave simple analytical expressions for the x, y coordinates of a general pole on the projection, and for the centre and radius of a general circle. Johari and Thomas [4] reviewed many applications of stereographic projection and presented a computer program which produced standard stereographic projections of any orientation for any crystal system. However, many applications of stereographic projection require for their solution the construction of great or small circles, the rotation of one pole about another, or the determination of the indices of a pole at a general location on a known projection.

The present paper presents the geometrical analysis leading to the equations which are the basis for a computer program which is capable of solving the most general stereographic projection problem using the immediate graphics interaction afforded by the current generation of advanced microcomputers. As an example of one application of the program, the necessary equations are developed for the transfer of the positions of reflections on a back-reflection

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Laüe pattern to the stereographic projection. With the addition of a suitable routine for the solution of the Laüe pattern, this would allow, for instance, the rapid creation of stereographic projections of the orientation of the tensile axis and faces of a single crystal tensile specimen.

The geometrical analysis is presented first, followed by a brief comparison of the present approach with previous work, and a description of the organization of the computer program is included at the end.

2. Derivation of equations

The following discussion is written in terms of vectors in a Cartesian coordinate system. Later, the necessary equations for the description of vectors and plane normals in noncubic crystal systems will be introduced. It is noted here that in deriving computer-compatible solutions to the problems posed herein, it is necessary to ensure that division by zero under any possible set of conditions be avoided. The solutions described below have been carefully examined and determined to be free of such difficulties except as noted.

2.1. Distance of pole from centre

A two-dimensional drawing of the geometrical arrangement by which points on the sphere are projected onto the projection plane is included in Fig. 1. The distance r of the projection P′ of pole P of vector $[hkl]$ from the centre C of the projection is frequently required. The angle CZP is α, the angle between the projection axis and the $[hkl]$ vector. Therefore, by application of Euler's Theorem to arc CP, angle COP is $\alpha/2$.

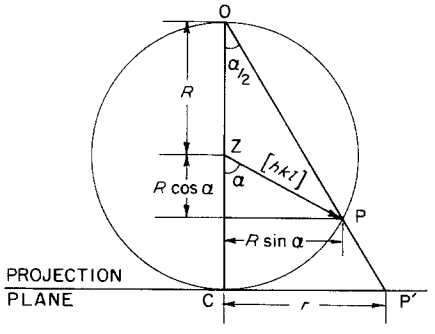

Figure 1 Geometry used to project points onto the projection plane. *ZC* is the projection axis and *ZP* is the vector whose pole P is projected to P′ using projection point O.

If the radius of the sphere is R, then

$$\tan\left(\frac{\alpha}{2}\right) = \frac{R \sin \alpha}{R + R \cos \alpha} = \frac{\sin \alpha}{1 + \cos \alpha}$$

as may be seen from Fig. 1. We also see from Fig. 1 that

$$\tan\left(\frac{\alpha}{2}\right) = \frac{r}{2R}$$

and since the radius of the basic circle of the projection is easily shown to be $R_c = 2R$, we have

$$r = R_c\left(\frac{\sin \alpha}{1 + \cos \alpha}\right) \qquad (1)$$

2.2. Coordinate system

We shall define the unit vector at the centre of the projection as $[abc]$, and those at the east and south poles as $[uvw]$ and $[def]$, respectively. These vectors are defined in terms of a Cartesian coordinate system which is fixed to the crystal lattice. The x, y coordinate system used in the plane of the stereographic projection is centred at the centre of the projection with the x-axis pointing to the right and the y-axis pointing upwards.

2.3. x, y coordinates of $[hkl]$

We may construct a non-unit vector $[pqr]$ which represents the projection of a unit vector $[hkl]$ on to the projection plane by adding a vector V of the appropriate length to $[hkl]$ (see Fig. 2a). Note that the endpoint of $[pqr]$ is not the projected pole of $[hkl]$. V is given by

$$V = -d[abc]$$

where

$$d = [hkl] \cdot [abc] = \cos \alpha$$

since $[hkl]$ and $[abc]$ are unit vectors. Thus,

$$[pqr] = [hkl] - [abc] \cos \alpha \qquad (2)$$

We now define the angles which $[pqr]$ makes with $[uvw]$ and $[def]$ as θ and ϕ, respectively (Fig. 2b). The cosines of these angles can be found from the dot products of $[pqr]$ with $[uvw]$ and $[def]$. Expansion of these dot products using Equation 2 reveals that since the terms involving $[abc] \cdot [uvw]$ and $[abc] \cdot [def]$ are zero we can write

$$|[pqr]| \cos \theta = [pqr] \cdot [uvw]$$
$$= [hkl] \cdot [uvw] = \cos \mu$$

and

$$|[pqr]| \cos\phi = [pqr] \cdot [def]$$
$$= [hkl] \cdot [def] = \cos\delta$$

where μ and δ are the angles which $[hkl]$ makes with $[uvw]$ and $[def]$, respectively (Fig. 2c). The quantities cos α, cos δ and cos μ are readily calculated from the dot products of the normalized vectors of the coordinate system with $[hkl]$. The magnitude of $[pqr]$ may be evaluated by squaring the individual terms of Equation 2 and collecting terms to obtain

$$|[pqr]| = (1 - \cos^2\alpha)^{1/2} = \sin\alpha.$$

Finally, we can find the x, y coordinates of pole $[hkl]$ from

$$x = r\cos\theta$$

and

$$y = -r\cos\phi$$

The negative sign in the equation for y is due to the choice of $[def]$ as lying on the $-y$-axis. With the aid of Equations 1 and 2 these can be simplified to give

$$x = R_c \cos\mu/(1 + \cos\alpha) \quad (3a)$$

and

$$y = -R_c \cos\delta/(1 + \cos\alpha) \quad (3b)$$

as previously given by Mackenzie and Bowles [3].

2.4. Great circles

Standard stereographic projections of cubic crystals are generally shown with the {1 0 0} and {1 1 0} great circles drawn, since the intersections of these circles mark the locations of all the {1 0 0}, {1 1 0} and {1 1 1} poles. Simple expressions for the radius and centre of the great circle of the (hkl) plane may be easily derived using Fig. 3. As before, α is the angle of $[hkl]$ from the central pole $[abc]$. The simplest derivation of the radius of the great circle uses the property of stereographic projection that circles on the sphere project as circles on the projection, with the angles between these circles being preserved on the projection. Thus the basic circle and the great circle meet at an angle of α degrees since this is the angle between their normals. Since the angle between the tangents is α, the angle CNO is also α, and so we have $R_c/R_{gc} = \cos\alpha$, or

$$R_{gc} = R_c/\cos\alpha \quad (4)$$

Similarly, since $OC/R_c = \tan\alpha$,

$$OC = R_c \tan\alpha \quad (5)$$

It is readily apparent from Fig. 3 that the angle subtended by the great circle is $180 - 2\alpha$; this allows the computer program to draw only the desired arc of the circle. For $\alpha = 90°$ both R_{gc} and OC are indeterminate, but when this condition occurs the great circle becomes a straight line whose endpoints are readily determined.

2.5. Small circles

Expressions for the radius and centre of a small circle whose normal lies in the projection plane

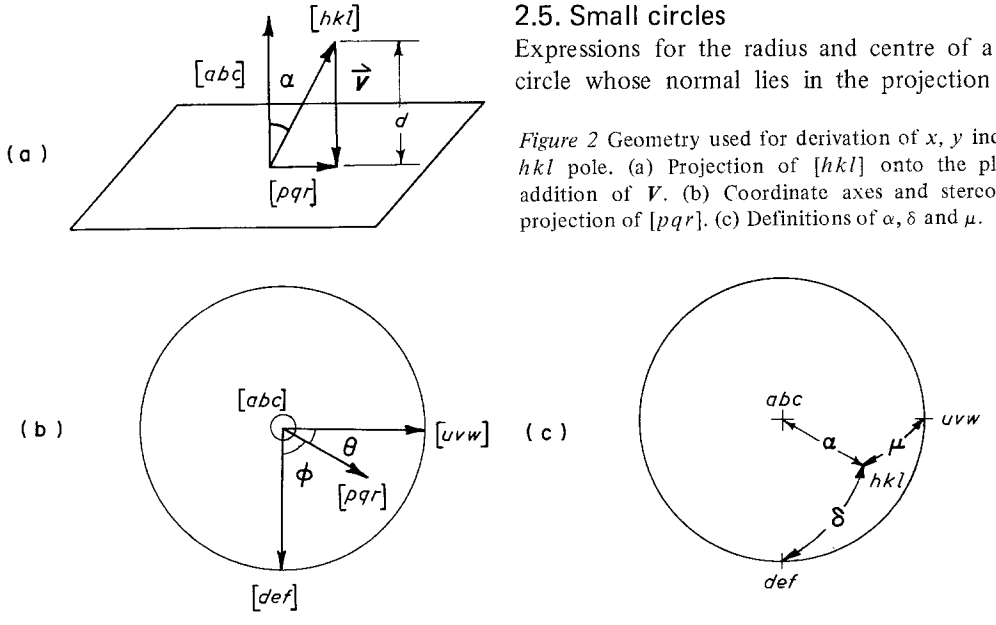

Figure 2 Geometry used for derivation of x, y indices of hkl pole. (a) Projection of $[hkl]$ onto the plane by addition of V. (b) Coordinate axes and stereographic projection of $[pqr]$. (c) Definitions of α, δ and μ.

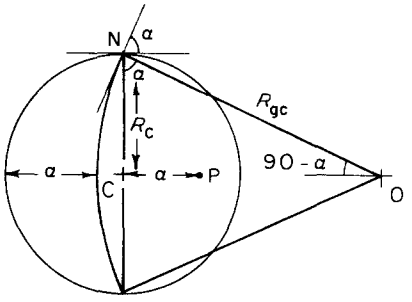

Figure 3 Geometry for construction of great circles. R_c = radius of basic circle; R_{gc} = radius of great circle; P = pole of great circle; O = centre of great circle.

are developed here for the construction of Wulff nets (for demonstration purposes) and because this simplifies the determination of the angle of a pole from another pole on the basic circle. Because the angles between circles are preserved on the projection, triangle OBC in Fig. 4 is a right triangle. Since the small circle is everywhere β degrees from the horizontal great circle (AC), angle BCA = β, whence angle COB = β. Therefore,

$$R_{sc} = R_c/\tan\beta \tag{6}$$

and

$$OC = R_c/\sin\beta \tag{7}$$

The angle subtended by the arc is 2β. R_{sc} and OC become infinite for $\beta = 0^\circ$, but as in the case of great circles this problem can be solved by construction of an appropriate straight line.

2.6. Determination of $[hkl]$ from x, y coordinates

The $[hkl]$ indices of a pole located at x, y on the projection can be found by first determining the

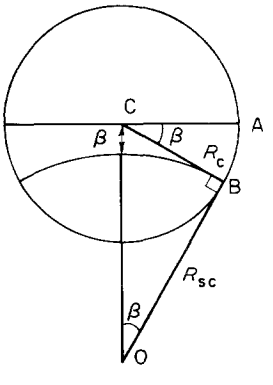

Figure 4 Geometry for construction of small circles centred on an axis lying in the projection plane. R_c = radius of basic circle; R_{sc} = radius of small circle; O = centre of small circle.

cosines of the angles between the pole and the three (Cartesian) coordinate axes, and then solving three simultaneous equations. The cosine of α (the angle between $[hkl]$ and $[abc]$) can be determined from the distance $r = (x^2 + y^2)^{1/2}$. Using Equation 1, we arrive at a quadratic equation in cos α;

$$\cos^2\alpha(Q+1) + \cos\alpha\,(2Q) + (Q-1) = 0$$

where $Q = (r/R_c)^2$. This can be solved to give

$$\cos\alpha = \frac{R_c^2 - (x^2+y^2)}{R_c^2 + x^2 + y^2} \tag{8}$$

To find cos δ we can use Equations 6 and 7 to solve for sin β, where β is the angle of the "horizontal" small circle in Fig. 4 from the centre and is equal to $90 - \delta$. We have the equation of the small circle

$$(x - x_c)^2 + (y - y_c)^2 = R_{sc}^2$$

where $x_c = 0$, y_c is given by the negative of Equation 7, and R_{sc} is given by Equation 6. Substituting and simplifying, we obtain

$$\cos\delta = \sin\beta = \frac{-2yR_c}{R_c^2 + x^2 + y^2} \tag{9}$$

Similarly, we find

$$\cos\mu = \frac{2xR_c}{R_c^2 + x^2 + y^2} \tag{10}$$

The sign difference between Equations 9 and 10 arises from the choice of $[def]$ as lying on the $-y$-axis, whereas $[u\,v\,w]$ is on the $+x$-axis.

Three simultaneous equations are obtained from the dot products of $[hkl]$ with the Cartesian vectors $[abc]$, $[def]$ and $[uvw]$;

$$ha_1 + ka_2 + la_3 = C_\alpha$$
$$hd_1 + kd_2 + ld_3 = C_\delta$$
$$hu_1 + ku_2 + lu_3 = C_\mu$$

where it is understood that all vectors are unit vectors defined in terms of the Cartesian system which is fixed to the crystal lattice. We have used the notation $a_1 = a$, $a_2 = b$, $a_3 = c$, $d_1 = d$, $d_2 = e$, $d_3 = f$, $u_1 = u$, $u_2 = v$, $u_3 = w$, $C_\alpha = \cos\alpha$, $C_\delta = \cos\delta$ and $C_\mu = \cos\mu$ to simplify the equations which follow. Subtracting equations and obtaining solutions for h and k in terms of l we

substitute to get

$$l[u_1(a_3d_2 - a_2d_3) + u_2(a_1d_3 - a_3d_1) + u_3(a_2d_1 - a_1d_2)] + u_1(a_2C_\delta - d_2C_\alpha) + u_2(d_1C_\alpha - a_1C_\delta) = C_\mu(a_2d_1 - a_1d_2)$$

Now, the term multiplying l is $U \cdot \{-(A \times D)\}$ where $U = [uvw]$, $D = [def]$ and $A = [abc]$. Since A and D are perpendicular unit vectors, we see that $A \times D = U$, and taking the dot product we see that the term multiplying l is simply -1. Collecting terms and transposing, we obtain

$$l = (u_2d_1 - u_1d_2)C_\alpha + (u_1a_2 - u_2a_1)C_\delta + (a_1d_2 - a_2d_1)C_\mu \quad (11)$$

Similarly we obtain for h and k

$$k = (u_1d_3 - u_3d_1)C_\alpha + (u_3a_1 - u_1a_3)C_\delta + (a_3d_1 - a_1d_3)C_\mu \quad (12)$$

and

$$h = (u_3d_2 - u_2d_3)C_\alpha + (u_2a_3 - u_3a_2)C_\delta + (a_2d_3 - a_3d_2)C_\mu \quad (13)$$

2.7. Rotation of one pole about another

A closed-form solution for the indices of the vector F lying at the endpoint of the rotation of vector S about vector Z by λ degrees can be obtained by consideration of the geometry illustrated in Fig. 5. Vectors S, Z and F are assumed to be unit vectors. The angle γ between S and Z is easily obtained from $S \cdot Z$. The vector N is a non-unit vector whose length is easily shown to be $\cos\gamma$, and T and G both are normal to N and of length $\sin\gamma$. The components of N are therefore $N_i = Z_i \cos\gamma$, and the components of T are given by $T_i = S_i - Z_i \cos\gamma$, since $N + T = S$.

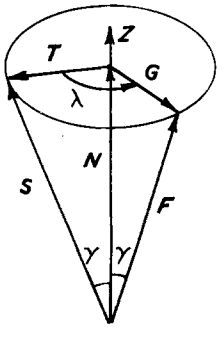

Figure 5 Geometry for determination of indices of vector F, related to S by a rotation of λ degrees about Z. F, Z and S are unit vectors.

The components of F can be found by determining the components of G since $F = N + G$. This can be done through the use of equations for $T \times G$ and $T \cdot G$. We have $T \times G = Z\,TG \sin\lambda = Z \sin^2\gamma \sin\lambda$, and by writing out $T \times G$ we find

$$T_2G_3 - T_3G_2 = Z_1 \sin^2\gamma \sin\lambda \quad (14)$$

$$T_3G_1 - T_1G_3 = Z_2 \sin^2\gamma \sin\lambda \quad (15)$$

and

$$T_1G_2 - T_2G_1 = Z3 \sin^2\gamma \sin\lambda \quad (16)$$

Using Equations 15 and 15 we obtain G_2 and G_3 in terms of G_1 plus known quantities;

$$G_2 = \frac{T_2G_1 + Z_3 \sin^2\gamma \sin\lambda}{T_1}$$

and

$$G_3 = \frac{T_3G_1 - Z_2 \sin^2\gamma \sin\lambda}{T_1}$$

Expanding $T \cdot G$ we get

$$T_1G_1 + T_2G_2 + T_3G_3 = \sin^2\gamma \cos\lambda$$

into which we insert the G_2 and G_3 expressions.

Rearrangement yields

$$(T_1^2 + T_2^2 + T_3^2)G_1 + (T_2Z_3 - T_3Z_2)\sin^2\gamma \sin\lambda = T_1 \sin^2\gamma \cos\lambda$$

However, since $(T_1^2 + T_2^2 + T_3^2) = T_2 = \sin^2\gamma$, we can divide through by $\sin^2\gamma$ to get

$$G_1 = T_1 \cos\lambda + (T_3Z_2 - T_2Z_3)\sin\lambda$$

Now we use $F_i = G_i + N_i = G_i + Z_i \cos\gamma$, which with some rearrangement yields

$$F_1 = S_1 \cos\lambda + Z_1 \cos\gamma(1 - \cos\lambda) + (S_3Z_2 - S_2Z_3)\sin\lambda \quad (17)$$

By repeating the same procedure we obtain

$$F_2 = S_2 \cos\lambda + Z_2 \cos\gamma(1 - \cos\lambda) + (S_1Z_3 - S_3Z_1)\sin\lambda \quad (18)$$

and

$$F_3 = S_3 \cos\lambda + Z_3 \cos\gamma(1 - \cos\lambda) + (S_2Z_1 - S_1Z_2)\sin\lambda \quad (19)$$

2.8. Application to noncubic crystals

Extension of the techniques so far described so that they are applicable to noncubic crystals

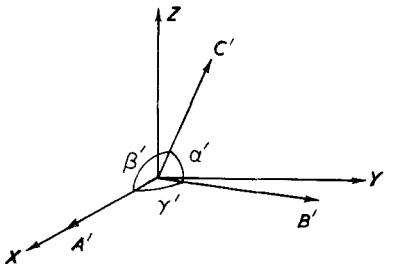

Figure 6 Relation of the Cartesian coordinate system X, Y, Z to the crystal axes A', B' and C'.

allows rapid, accurate application of stereographic projection techniques to any crystal system, thus greatly decreasing the time required for the solution of such problems. The first step is to express the basis vectors A', B' and C' of the crystal lattice as vectors in a Cartesian coordinate system, X, Y and Z. This is sufficient to allow representation of crystal directions as Cartesian vectors. In order to express plane normals as Cartesian vectors, we define the basis vectors of the reciprocal lattice, R', S' and T', using the cross products of the vectors A', B' and C' (see, for instance, Appendix 1 of Cullity [1]). Then, given the indices of the $(h\,k\,l)$ plane, we can write its normal in the Cartesian system as

$$H = hR' + kS' + lT' \tag{20}$$

Fig. 6 shows the most natural choice of the relationship of the crystal and Cartesian coordinate systems. Since A' lies along X, its components are

$$\begin{aligned} A_1' &= A' \\ A_2' &= A_3' = 0 \end{aligned} \tag{21}$$

The components of B', which lies in the same plane as the X- and Y-axes of the Cartesian system, are

$$\begin{aligned} B_1' &= B' \cos\gamma' \\ B_2' &= B' \sin\gamma' \\ B_3' &= 0 \end{aligned} \tag{22}$$

The components of C' can be found by writing expressions for the dot products $A'\cdot C'$ and $B'\cdot C'$, after first temporarily normalizing A' and B' and assuming C' to also be a unit vector. We find

$$\begin{aligned} C_1' &= \cos\beta' \\ C_2' &= \frac{\cos\alpha' - \cos\beta'\cos\gamma'}{\sin\gamma'} \\ C_3' &= (1 - C_1'^2 - C_2'^2)^{1/2} \end{aligned} \tag{23}$$

These components are then multiplied by C' to convert to a vector of the correct length. Note that the computer must execute these functions in the order given here. From $R' = B' \times C'$ we obtain

$$\begin{aligned} R_1' &= B_2'C_3' \\ R_2' &= -B_1'C_3' \\ R_3' &= B_1'C_2' - B_2'C_1' \end{aligned} \tag{24}$$

Note that it is unnecessary to divide through by the volume of the unit cell unless one wishes to calculate interplanar spacings from the lengths of the reciprocal lattice vectors.

From $S' = C' \times A'$ we find

$$\begin{aligned} S_1' &= 0 \\ S_2' &= C_3'A_1' \\ S_3' &= -C_2'A_1' \end{aligned} \tag{25}$$

and from $T' = A' \times B'$ we find

$$\begin{aligned} T_1' &= T_2' = 0 \\ T_3' &= B_2'A_1' \end{aligned} \tag{26}$$

Inserting these into Equation 20 we obtain the components of H;

$$\begin{aligned} H_1 &= hB_2'C_3' \\ H_2 &= C_3'(kA_1' - hB_1') \\ H_3 &= C_2'(hB_1' - kA_1') + B_2'(lA_1' - hC_1') \end{aligned} \tag{27}$$

Plane normals are plotted using H_1, H_2 and H_3 in place of h, k and l in calculating cos α, cos δ and cos μ for insertion into Equation 3a, b. To plot a direction $[h\,k\,l]$, we write

$$D' = hA' + kB' + lC'$$

which gives

$$\begin{aligned} D_1 &= hA_1' + kB_1' + lC_1' \\ D_2 &= kB_2' + lC_2' \\ D_3 &= lC_3' \end{aligned} \tag{28}$$

D_1, D_2 and D_3 are then used in place of h, k and l.

The reverse transformations are useful for finding the crystal indices of a pole or direction whose Cartesian indices are known. For poles, given H_1, H_2 and H_3 we can use

$$\begin{aligned} h &= H_1/B_2'C_3' \\ k &= \frac{H_2 + H_1B_1'/B_2'}{C_3'A_1'} \\ l &= \frac{H_3 + kC_2'A_1' - h(B_1'C_2' - B_2'C_1')}{B_2'A_1'} \end{aligned} \tag{29}$$

Note that the computer must execute the l function after first computing h and k. For directions, given D_1, D_2 and D_3 we use the reverse transformation

$$l = D_3/C_3'$$
$$k = \frac{D_2 - lC_2'}{B_2'} \quad (30)$$
$$h = \frac{D_1 - kB_1' - lC_1'}{A_1'}$$

Note that the computer must execute these functions in the order given. The computer program must plot the poles and directions using the Cartesian indices to calculate x and y, but it must label the points using the crystal indices. If the crystal indices are found from Cartesian indices using Equation 29 or 30, they will generally be irrational and should therefore be converted to integers.

2.9. Back-reflection Laüe patterns

An example of a possible application of the stereographic projection techniques described here is that of the solution of back-reflection Laüe patterns. The x, y coordinates of points on a back-reflection Laüe pattern can be read directly into a microcomputer by means of a graphics tablet. A few simple equations will be presented which allow the direction calculation of the x, y coordinates of points on the stereographic projection from the coordinates x_L, y_L of the corresponding points on the Laüe pattern. This makes it possible to create an accurate stereographic projection from a Laüe pattern with no recourse to graphical methods. The projection can be set up with the standard 0 0 1 orientation and the points assigned "dummy" indices as they are entered. With these indices the cross products of poles on the same zone can be used to find the dummy indices of the zone axes, and angle between poles can be determined. The operator can then solve the orientation in the usual way. Alternatively, a computer program could be written to automatically solve for the orientation.

Fig. 7 shows the necessary aspects of the back-reflection Laüe geometry. The angle between a reflecting plane normal and the incident beam is σ and the diffracted beam is coplanar with the incident beam and plane normal and makes an angle 2σ with the incident beam. Since the crystal-to-film distance, IC, is known and the distance of the diffracted beam spot from the film centre is $r_L = (x_L^2 + y_L^2)^{1/2}$, σ is readily calculated from

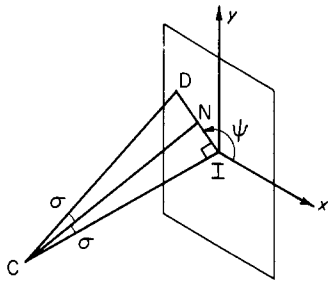

Figure 7 Geometry of back-reflection Laüe pattern. C = point on crystal surface; I = film centre; CN = plane normal; CD = diffracted beam; IC = incident beam. The coordinates of D are x_L, y_L.

$$\sigma = \frac{1}{2}\tan^{-1}\left[\frac{(x_L^2 + y_L^2)^{1/2}}{IC}\right] \quad (31)$$

Using Equation 1 we can calculate the distance r of the (hkl) pole on the projection from the centre of the projection from

$$r = R_c \tan(\sigma/2) \quad (32)$$

Now, the vector from the film centre to the diffracted beam makes an angle ψ with the x-axis, as does the vector IN which is the projection of the plane normal on the film. Therefore this angle must be preserved on the projection, which leads to $x_L/r_L = x/r = \cos\psi$ and $y_L/r_L = y/r = \sin\psi$, or

$$x = \frac{x_L r}{(x_L^2 + y_L^2)^{1/2}}$$
$$y = \frac{y_L r}{(x_L^2 + y_L^2)^{1/2}} \quad (33)$$

3. Comparison with previous work

This discussion will follow the sequence in which the geometrical analysis was presented. Methods for the computation of the x, y coordinates of the projection of the endpoint of a Cartesian vector onto the plane have been previously given by Mackenzie and Bowles [3] and by Johari and Thomas [4]. The method described in the present paper leads to the solution given by Equation 3, which is the same as that given previously by Mackenzie and Bowles. The derivation is included here for completeness, since it was not given by Mackenzie and Bowles. The method used by Johari and Thomas was far more cumbersome.

The treatment given here for the construction of great circles and small circles having centres on an axis in the projection plane has the advantage that it provides very simple expressions for the angular range of the arc of the circle which lies within the basic circle, which is very useful in the computer program. Mackenzie and Bowles [3] gave equations for the centre and radius of a general circle of angular range η from a central pole hkl (that is, the circle is the locus of the endpoints of all vectors at η degrees from $[hkl]$). The radius is given by

$$R_{sc} = \left(\frac{\sin \eta}{\cos \alpha + \cos \eta} \right)$$

and the centre coordinates are

$$x = \left(\frac{\cos \mu}{\cos \alpha + \cos \eta} \right)$$

and

$$y = \left(\frac{\cos \delta}{\cos \alpha + \cos \eta} \right)$$

where α, δ and μ are the angles between $[hkl]$ and the vectors $[abc]$, $[def]$ and $[uvw]$ as before. These relations reduce to the ones given earlier for the radii and centre distanes of circles. However, they do not give the angular range of the arcs. The equation of the general circle has not been found necessary here, and has not been used.

The derivation of expressions for the computation of hkl from x, y involves the solution of three simultaneous equations involving $\cos\alpha$, $\cos\delta$ and $\cos\mu$. Mackenzie and Bowles [3] gave expressions which reduce to those given here in Equations 8 to 10 for these cosines, but did not provide the solution to the resulting equations, which is necessary for the determination of the indices of a point on a general projection. The solution can also be obtained by means of a subroutine involving Cramer's Rule. However, the closed form solution is given here because it is somewhat more compact in computer code. In fact, due to the similar forms of Equations 11 and 13, the equations are solved in a short FOR loop in the program by permuting the subscripts.

The solution of the problem of the rotation of one general pole about another was not previously discussed by either Mackenzie and Bowles or Johari and Thomas. The expressions of Mackenzie and Bowles for the centre and radius of a general circle give the locus of possible locations of the final pole, but no simpler method of finding the final location has been found than that given in Equations 17 to 19.

The solution to the problem of conversion of crystal indices of planes to the x, y coordinates of the pole on the projection was not given by Mackenzie and Bowles [3], but a solution was given by Johari and Thomas [4]. Johari and Thomas began with the same choice of the relationship between the coordinate systems as used here (Fig. 6), and they derived expressions for unit vectors which are equivalent to those in Equations 21 to 23. However, at this point their approach diverged strongly from that used here. They derived expressions for the Cartesian vectors [100], [010] and [001], and employed these to arrive at expressions for the endpoint of the (hkl) plane normal in Cartesian space. Their approach necessitated the calculation of the length of the general reciprocal lattice vector in a triclinic crystal (which is very lengthy), and the solutions for the endpoint of the plane normal were also quite long in comparison with that embodied in Equations 24 to 26. The complete code for the calculation of the x, y coordinates of the pole of the (hkl) plane in a general crystal is given below using the present approach;

```
370 INPUT "ENTER A,B,C";A,B,C
380 INPUT "ENTER ALPHA, BETA, GAMMA";AL,BE,GA
390 AL = AL * PI / 180:BE = BE * PI / 180:GA = GA * PI / 180
400 A1 = A:A2 = 0:A3 = 0
410 B1 = B * COS (GA):B2 = B * SIN (GA):B3 = 0
420 C1 = COS (BE)
430 C2 = ( COS (AL) - COS (BE) * COS (GA)) / SIN (GA)
440 C3 = SQR (1 - C1 * C1 - C2 * C2)
450 C1 = C * C1:C2 = C * C2:C3 = C * C3
460 REM FUNCTIONS H1, H2 and H3 CONVERT A XTAL POLE HKL TO
        AN RL POLE H1, H2, H3
470 DEF FN H1(X) = H * B2 * C3
```

```
480 DEF FN H2(X) = C3 * (K * A1 − H * B1)
490 DEF FN H3(X) = C2 * (H * B1 − K * A1) + B2 * (L * A1 −
        H * C1)

1280 IF PD$ = "P" THEN L = FN H3(0): K = FN H2(0):
        H = FN H1(0)
1290 HM = SQR (H * H + K * K + L * L)
1300 CA = (A * H + B * K + C * L) / (AM * HM)
1310 IF CA < 0 GOTO 1250
1320 CD = (D * H + E * K + F * L) / (DM * HM)
1330 CU = (U * H + V * K + W * L) / (UM * HM)
1340 X = RC * CU/(1 + CA)
1350 Y = −RC * CD / (1 + CA)
```

Lines 370 and 380 request the lattice parameters, and lines 390 to 450 define Al etc. according to Equations 21 to 23. Lines 470 through 490 define functions according to Equations 24 to 26, and lines 1280 through 1330 compute the vector for the plane normal and then compute cos α, cos δ and cos μ (CA, CD and CU) from dot products. (DM and UM have been previously defined in the program as the magnitudes of $[def]$ and $[uvw]$, respectively.) Finally, lines 1340 and 1350 compute x and y. This code is considerably more condensed than that employed by Johari and Thomas. It is also noted that Johari and Thomas did not provide for the plotting of directions as well as poles. It should be noted that variables A, B and C are initially defined as the lattice parameters A', B' and C' and are later redefined to denote the projection axis $[abc]$. The lattice parameters are first used to define the necessary functions for conversions between the crystal and Cartesian coordinate systems.

The procedure given here for the direct transfer of Laüe coordinates to the stereographic projection has not been previously presented and should prove quite useful.

An important difference between the present work and that of previous authors is that the techniques presented here represent a complete set of tools which allow the creation of general projections complete with great circles, and the solution of the most general stereographic problem using live interaction graphics on a modern microcomputer. This was the impetus for the solution of the problems involving the drawing of circles, the indexing of unknown poles, and the rotation of one general pole about another.

4. Program description

The complete computer program allows generation on the screen of a stereographic projection of any orientation for any crystal system, complete with all the {100} and {110} great circles, within about one minute on an Apple II or IIe microcomputer. Examples are shown in Figs. 8 and 9 for cubic and orthorhombic crystals. It will be noted that the resolution of these figures is limited by the screen resolution of the microcomputer, since the plots were made on a dot-matrix printer using a screen-dump routine. Modification of the program to utilize an x–y plotter or to more effectively use the resolution of the dot-matrix printer will provide much better results.

For hexagonal crystals, a minor modification

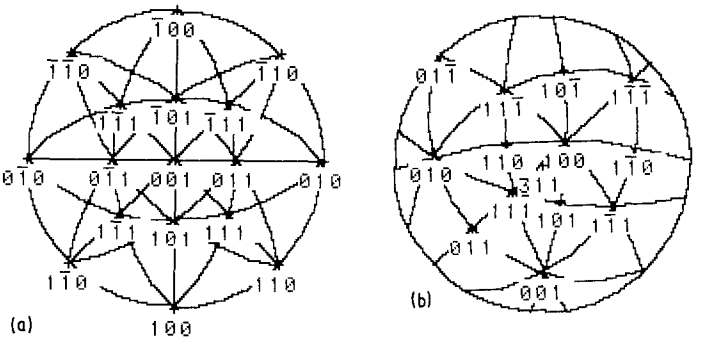

Figure 8 Stereographic projections of a cubic crystal. (a) 001; (b) 311.

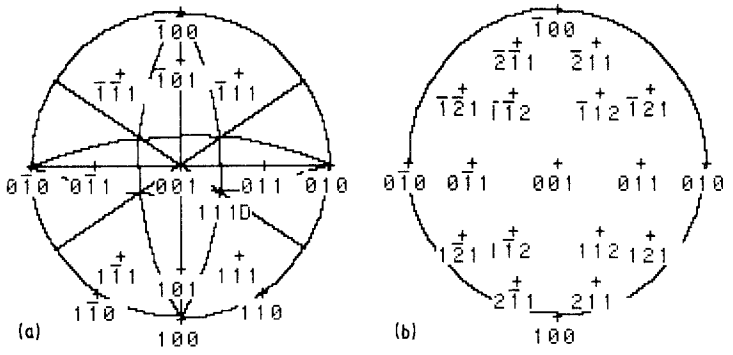

Figure 9 Stereographic projections of an orthorhombic crystal with crystal axes $a = 1$, $b = 1.5$, $c = 2.5$. (a) 001; note that the direction [111] is indicated as 111D; (b) same orientation, but showing all the 112 poles, drawn using menu selection 8.

is made to convert crystal directions and poles into four-axis Miller–Bravais indices, and the appropriate additional great circles are drawn as in Fig. 10. Separate versions of the program have been created for the cubic and hexagonal systems, and a general version is used for the remaining systems. In crystal systems other than cubic, the user is able to specify whether he wishes to plot poles or directions, and direction indices are indicated by a trailing "D" (Fig. 9).

Any point on the screen may be indexed by moving a cursor to that point, and rotation of one pole about another general pole may be accomplished by specifying the poles either by use of a cursor or by direct entry of the pole indices. Fig. 11 shows the "menu" for the program. The various selections cause the program to branch to the appropriate subroutines, which will be described shortly. Fig. 12 shows a flow chart for the initial portion of the program, which allows the user to specify the crystal lattice parameters and orientation. A new orientation may be chosen at any time by means of menu selection 9, which simply returns to the point at which the orientation of the central pole is chosen. For noncubic crystals, after the lattice parameters a, b and c and α', β' and γ' are entered the program defines functions which allow calculation of Cartesian indices from crystal indices and vice versa, using Equations 21 to 30.

The following paragraphs will outline the operation of the various subroutines which are activated by the menu selections, and are organized in the order indicated by the menu. Fig. 13 shows a flow chart for the plotting of a pole or direction with or without its great circle. Menu selection 2 enters this routine after first asking for crystal indices, whether a pole or direction is to be plotted, and whether the great circle is to be plotted. The responses to the latter two questions are used to define token variables which determine the branches taken within the subroutine. Two special cases deserve comment. First, poles (vectors) making an obtuse angle with the central vector $[abc]$ would plot outside the basic circle.

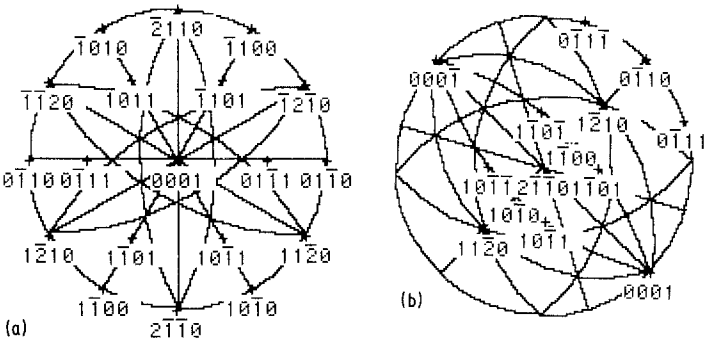

Figure 10 Stereographic projections of an hexagonal crystal with c/a ratio = 1.633. (a) 0 0 0 1; (b) $2\bar{1}\bar{1}0$.

```
1  MENU
2  PLOT HKL POLE
3  DRAW ALL 100 & 110 GREAT CIRCLES
4  INDEX POLE WITH CURSOR
5  ROTATE POLE A ABOUT POLE B
6  DRAW ROTATED WULFF NET
7  CLEAR SCREEN
8  PLOT ALL HKIL POLES
9  NEW ORIENTATION
10 CHANGE INDEX ENTRY MODE
11 CHANGE INDEX OUTPUT MODE
12 SAVE TO DISC
13 END
```

Figure 11 Menu for the hexagonal version of the program. See text for explanation of the various selections.

This is avoided by checking the dot product with $[abc]$ and, if it is negative, reversing the signs of the indices before proceeding. Thus the negative of such a pole is plotted, and this must lie inside the basic circle. Secondly, for plotting the great circle of a pole lying on the outer circle, the radius calculated will be infinite. Thus circumstance may be recognized by the condition $[abc] \cdot [hkl] = 0$, and in this case a straight line is plotted.

The circle drawing routine referred to in Fig. 13 simply draws straight line segments between specified points. These points are calculated for great circles by assuming the centre of the great circle to lie on the x-axis and using Equations 4 and 5 to calculate several points on the circle, after which all points are rotated by the required amount using standard rotation of axes formulae. The same circle drawing routine is used for drawing the small circles on the Wulff net; the Wulff net subroutine uses Equations 6 and 7 to calculate the points.

The subroutine which is called by menu selection 3 automatically draws the great circles of all the {100} and {110} poles by simply defining the

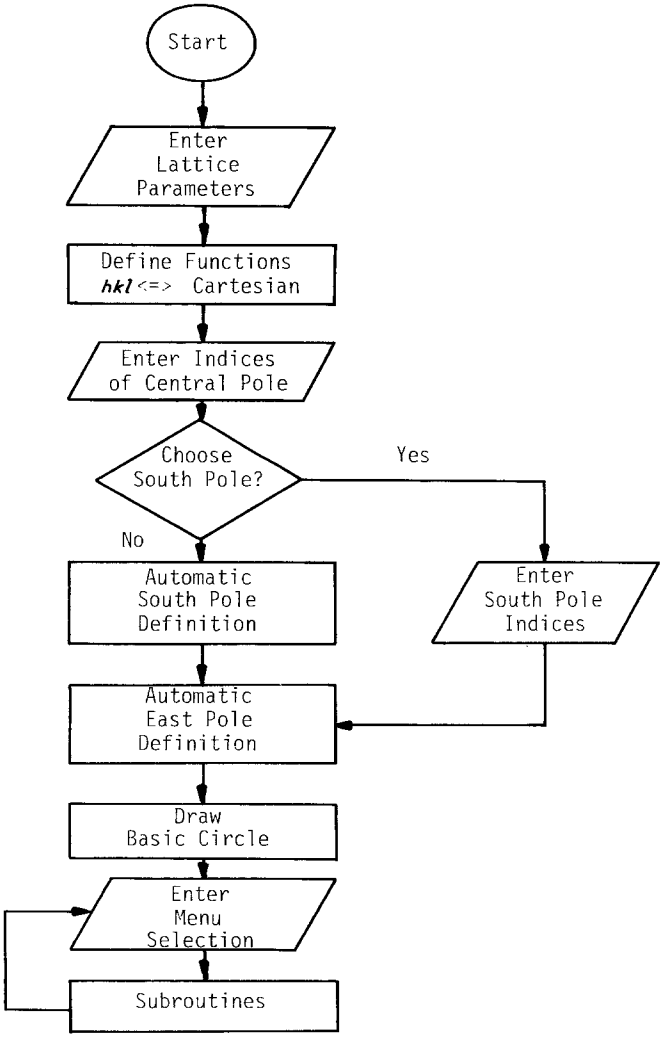

Figure 12 Flow chart of the initial portion of the program.

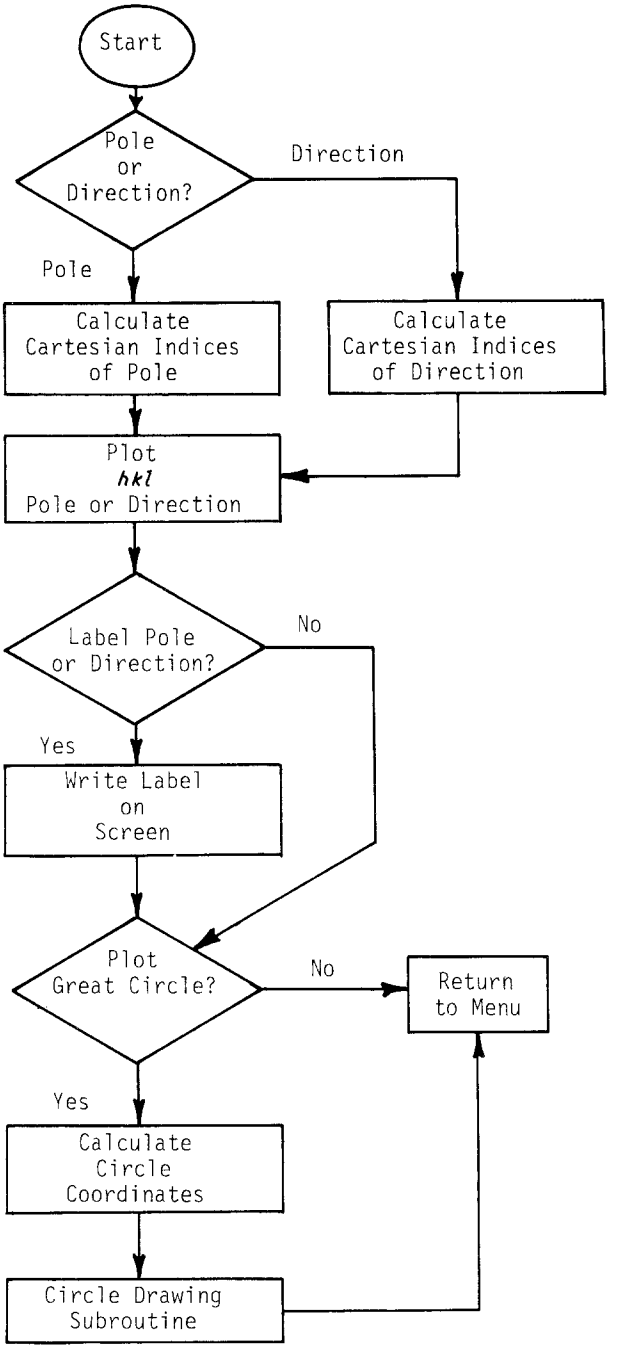

Figure 13 Flow chart of the subroutine for plotting a pole or direction with or without its great circle and label.

indices and calling the subroutine illustrated in Fig. 13. Similarly, menu selection 8 permutes the indices and plots all poles (or directions) of type *hkl* (see Fig. 9b).

Menu selection 4 activates a subroutine which allows indexing of a pole by means of a cursor, utilizing Equations 8 to 13 to calculate the indices of the pole or direction, and then converts the indices to integers. Naturally, the accuracy of positioning the cursor is limited by the screen resolution of the computer. Since the indices are generally irrational, there is necessarily some error in the integer indices, and the user may request the decimal indices if desired. Equations 9 and 10 could be used to allow the user to enter the pole position by means of the angles from the east and south if desired, which would be useful if it were desired to work directly from

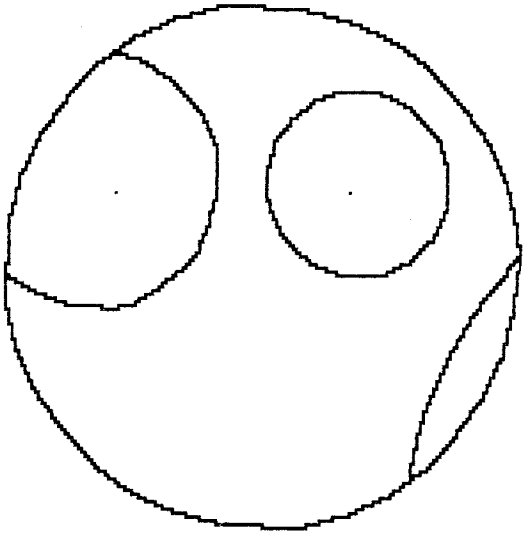

Figure 14 Rotation of a general pole about another general pole by 360°. Two examples are shown.

an actual tracing since these angles could be measured using a Wulff net.

The subroutine called by menu selection 5 to rotate one pole about another first allows definition of the poles by means of the cursor routine or direct input of indices. It then calculates the decimal Cartesian indices of these poles using the subroutine just described, and then applies Equations 14 to 19 to find the final position of the pole after rotation. The rotation procedure is drawn on the screen by calculating the several intermediate locations on the circle swept out by the pole as it rotates, as shown in Fig. 14.

Menu selection 6 calls a subroutine which calculates the coordinates of the points on all the "meridians" and "parallels" (great and small circles) on a Wulff net with 30° increments, rotates these circles by the amount requested, and calls the circle drawing subroutine to draw the rotated Wulff net. This routine is included primarily for instructional purposes.

Menu selection 8 simply calls the pole and great circle routine (Fig. 13) with the appropriate token variables defined so that the {1 1 1} poles are labelled but the circles are not drawn.

Menu selections 10 and 11 allow the user to change the index entry and printout modes to either the standard three-axis or the four-axis Miller–Bravais system in the hexagonal version of the program.

A listing of the program is not included here because of its length and because of the complicated naming of the many variables required. A copy of the listing will be provided by the author upon request.

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