The shapes of the grains in a polycrystalline mass are the result of several kinds of forces, all of which are strong enough to counteract the natural tendency of each grain to grow with well-developed flat faces. The result is a grain roughly polygonal in shape with no obvious aspect of crystallinity. Nevertheless, that grain is a crystal and just as "crystalline" as, for example, a well-developed prism of natural quartz, since the essence of crystallinity is a periodicity of inner atomic arrangement and not any regularity of outward form.

2-12 CRYSTAL DEFECTS

There are a number of types of imperfections in the periodic structure of the individual grains of crystalline solids. These crystallographic defects are broadly classified as point, line and planar defects and can have important consequences in the mechanical, electrical, optical, etc. properties of a material. A large part of materials science and engineering concerns itself with the control and/or characterization of the different defects. Point defects such as substitutional or interstitial impurities were briefly discussed in Sec. 2-9. Edge and screw dislocations and dislocations with character intermediate between the two are linear defects in the periodic array of atoms within a crystal. In metals, multiplication and motion of dislocations occur at relatively low stress, and the relatively easy plastic deformation and high ductility of metals is the product of this. Large strains and very high dislocation densities can be introduced by operations such as forging, rolling, machining, shot peening or ball milling; how these stress and strains can be measured is the subject of portions of Chap. 14 and Chap. 15. There are a variety of planar defects including stacking faults and twins; these are described below.

In Sec. 2-9 the stacking sequence of close packed planes of the fcc and hcp structures was discussed. Stacking faults occur when the normal stacking sequence is interrupted. In the fcc structure, the normal stacking sequence …ABCABCABC…can become …ABCAB*ABC… or …ABCA*CABCA…, for example, by the removal of a C-layer or a B-layer, respectively. The asterisk in the previous sentence is used to indicate the position of the stacking fault. In the hcp system, the stacking sequence…ABABABAB…can become …ABABA*CBCBCB… Faults producing AA, BB or CC neighboring layers have a very high energy of formation, would require extraordinary circumstances to appear and would probably rapidly split into a set of closely-spaced, lower energy faults. In writing sequences such as those shown above, each letter represents a layer of atoms. Each layer extends to the end of the fault, and such planar faults must extend to the edge of the crystal or grain or must terminate at one or more dislocations [2.8, 2.9].

Some crystals have two parts symmetrically related to one another. These, called twinned crystals, are fairly common both in minerals and in metals and alloys. For a detailed discussion of twinning, see Barrett and Massalski [G.10].

The relationship between the two parts of a twinned crystal is described by the symmetry operation which will bring one part into coincidence with the other or with an extension of the other. Two main kinds of twinning are distinguished, depending on whether the symmetry operation is 180° rotation about an axis, called the twin axis, or reflection across a plane, called the twin plane. The plane on which the two parts of a twinned crystal are united is called the composition plane. In the case of a reflection twin, the composition plane may or may not coincide with the twin plane.

Of most interest to those who deal mainly with FCC, BCC, and HCP structures, are the following kinds of twins:

1. Annealing twins, such as occur in FCC metals and alloys (Cu, Ni, α–brass, Al, etc.), which have been cold-worked and then annealed to cause recrystallization.
2. Deformation twins, such as occur in deformed HCP metals (Zn, Mg, Be, etc.) and BCC metals (α–Fe, W, etc.).

Annealing Twins

Annealing twins in FCC metals are rotation twins, in which the two parts are related by a 180° rotation about a twin axis of the form <111>. Because of the high symmetry of the cubic lattice, this orientation relationship is also given by a 60° rotation about the twin axis or by reflection across the {111} plane normal to the twin axis. In other words, FCC annealing twins may also be classified as reflection twins. The twin plane is also the composition plane.

Occasionally, annealing twins appear under the microscope as in Fig. 2-26(a), with one part of a grain (*B*) twinned with respect to the other part (*A*). The two parts are in contact on the composition plane (111) which makes a straight-line trace on the plane of polish. More common, however, is the kind shown in Fig. 2-26(b). The grain shown consists of three parts: two parts (A_1 and A_2) of identical orientation separated by a third part (*B*) which is twinned with respect to A_1 and A_2. *B* is known as a twin band.

Figure 2-27 illustrates the structure of an FCC twin band. The plane of the main drawing is $(1\bar{1}0)$, the (111) twin plane is perpendicular to this plane, and the [111]

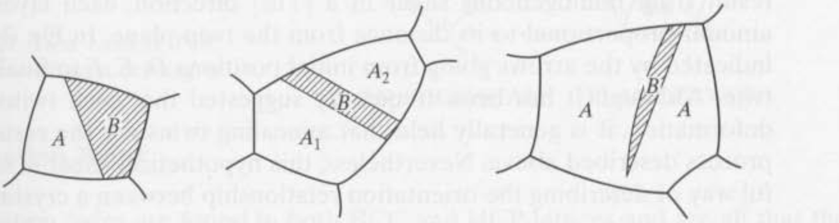

Figure 2-26 Twinned grains: (a) and (b) FCC annealing twins; (c) HCP deformation twin.

twin axis lies in it. Open circles represent atoms in the plane of the drawing and filled circles those in the layers immediately above or below. The reflection symmetry across the twin plane is suggested by the dashed lines connecting several pairs of atoms.

The statement that a rotation twin of this kind is related to the parent crystal by a 180° rotation about the twin axis is merely an expression of the orientation relationship between the two and is not meant to suggest that a twin is formed by a physical rotation of one part of the crystal with respect to another. Actually, FCC annealing twins are formed by a change in the normal growth mechanism. Suppose that, during normal grain growth following recrystallization, a grain boundary is roughly parallel to (111) and is advancing in a direction approximately normal to this boundary, namely [111]. To say that the boundary is advancing is to say that atoms are leaving the lattice of the consumed grain and joining that of the growing grain. The grain is therefore growing by the addition of layers of atoms parallel to (111), and these layers are piled up in the sequence *ABCABC* ... in an FCC crystal. If, however, a mistake should occur and this sequence become altered to *CBACBA* ... , the crystal so formed would still be FCC but it would be a twin of the former. If a similar mistake occurred later, a crystal of the original orientation would start growing and a twin band would be formed. With this symbolism, a twin band appears as follows:

$$A\,B\,C\,A\,B\,C\,B\,A\,C\,B\,A\,C\,A\,B\,C\,A\,B\,C$$

parent crystal	twin band	parent crystal
$\longrightarrow$	$\longleftrightarrow$	$\longleftarrow$

In this terminology, the symbols themselves are imaged in the mirror *C*, the twin plane. At the left of Fig. 2-27 the positional symbols *A*, *B*, *C* are attached to various (111) planes to show the change in stacking which occurs at the boundaries of the twin band. Parenthetically, it should be remarked that twin bands visible under the light microscope are thousands of times thicker than the one shown in this drawing.

There is still another way of *describing* the orientation relationship between an FCC crystal and its twin: the (111) layers of the twin are in positions which would result from homogeneous shear in a $[11\bar{2}]$ direction, each layer moving by an amount proportional to its distance from the twin plane. In Fig. 2-27, this shear is indicated by the arrows going from initial positions *D*, *E*, *F* to final positions in the twin. Although it has been frequently suggested that such twins are *formed* by deformation, it is generally held that annealing twins are the result of the growth process described above. Nevertheless, this hypothetical shear is sometimes a useful way of describing the orientation relationship between a crystal and its twin.

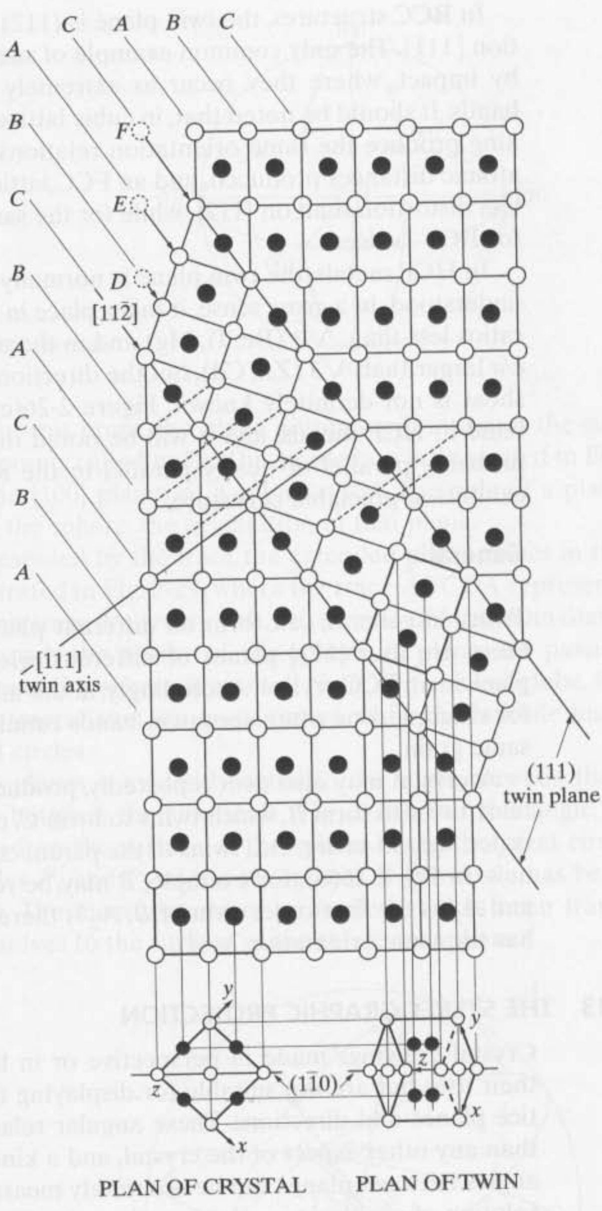

Figure 2-27. Twin band in FCC lattice. Plane of main drawing is $(1\bar{1}0)$.

Deformation Twins

Deformation twins are found in both BCC and HCP lattices and are all that their name implies, since, in both cases, the cause of twinning is deformation. In each case, the orientation relationship between parent crystal and twin is that of reflection across a plane.

In BCC structures, the twin plane is (112) and the twinning shear is in the direction $[11\bar{1}]$. The only common example of such twins is in α–iron (ferrite) deformed by impact, where they occur as extremely narrow twin bands called Neumann bands. It should be noted that, in cubic lattices, both {112} and {111} reflection twinning produce the same orientation relationship; however, they differ in the interatomic distances produced, and an FCC lattice can twin by reflection on {111} with less distortion than on {112}, while for the same reason {112} is the preferred plane for BCC lattices.

In HCP metals, the twin plane is normally $(10\bar{1}2)$. The twinning shear is not well understood; in a gross sense, it takes place in the direction $[\bar{2}\bar{1}1]$ for metals with *c/a* ratios less than $\sqrt{3}$ (Be, Ti, Mg) and in the reverse direction $[21\bar{1}]$ for metals with *c/a* larger than $\sqrt{3}$ (Zn, Cd), but the direction of motion of individual atoms during shear is not definitely known. Figure 2-26(c) illustrates the usual form of a twin band in HCP metals, and it will be noted that the composition "plane," although probably parallel or nearly parallel to the twin plane, is not quite flat but often exhibits appreciable curvature.

General

Twins, in general, can form on different planes in the same crystal. For example, there are four {111} planes of different orientation on which twinning can take place in an FCC crystal. Accordingly, in the microstructure of recrystallized copper, for example, one often sees twin bands running in more than one direction in the same grain.

A crystal may also twin repeatedly, producing several new orientations. If crystal *A* twins to form *B*, which twins to form *C*, etc., then *B*, *C*, etc., are said to be first-order, second-order, etc., twins of the parent crystal *A*. Not all these orientations are new. In Fig. 2-26(b), for example, *B* may be regarded as the first-order twin of A_1, and A_2 as the first-order twin of *B*. A_2 is therefore the second-order twin of A_1 but has the same orientation as A_1.

2-13 THE STEREOGRAPHIC PROJECTION

Crystal drawings made in perspective or in the form of plan and elevation have their uses but are not suitable for displaying the angular relationship between lattice planes and directions. These angular relationships are often more interesting than any other aspect of the crystal, and a kind of drawing is needed on which the angles between planes can be accurately measured and which will permit graphical solution of problems involving such angles. The stereographic projection [2.10] fills this need. For details not given below, see Barrett and Massalski [G.10] and McKie and McKie [G.3].

The orientation of any plane in a crystal can be represented just as well by the inclination of the normal to that plane relative to some reference plane as by the inclination of the plane itself. All the planes in a crystal can thus be represented by a set of plane normals radiating from one point within the crystal. If a reference

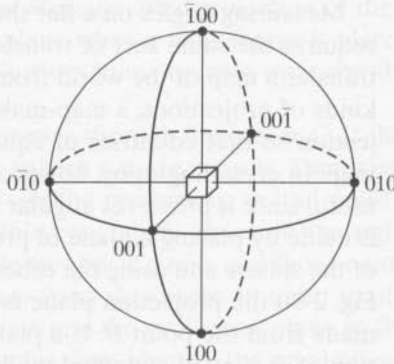

Figure 2-28 {100} poles of a cubic crystal.

sphere is now described about this point, the plane normals will intersect the surface of the sphere in a set of points called *poles*. This procedure is illustrated in Fig. 2-28, which is restricted to the {100} planes of a cubic crystal. The pole of a plane represents, by its position on the sphere, the orientation of that plane.

A plane may also be represented by the trace the extended plane makes in the surface of the sphere, as illustrated in Fig. 2-29, where the trace $ABCDA$ represents the plane whose pole is P_1. This trace is a *great circle*, i.e., a circle of maximum diameter, if the plane passes through the center of the sphere. A plane not passing through the center will intersect the sphere in a *small circle*. On a ruled globe, for example, the longitude lines (meridians) are great circles, while the latitude lines, except the equator, are small circles.

The angle α between two planes is evidently equal to the angle between their great circles or to the angle between their normals (Fig. 2-29). But this angle, in degrees, can also be measured on the surface of the sphere along the great circle $KLMNK$ connecting the poles P_1 and P_2 of the two planes, if this circle has been divided into 360 equal parts. The measurement of an angle has thus been transferred from the planes themselves to the surface of the reference sphere.

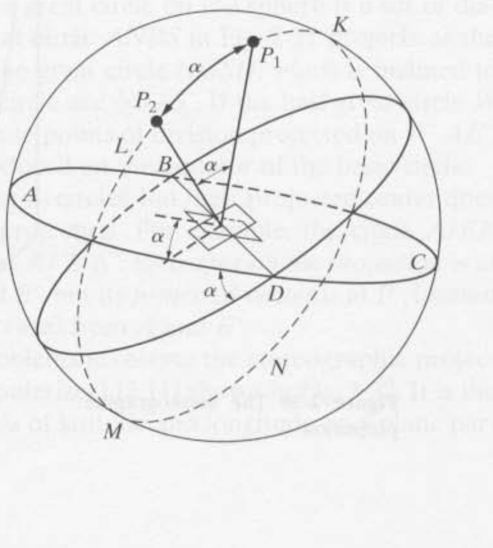

Figure 2-29 Angle between two planes.

Measuring angles on a flat sheet of paper rather than on the surface of a sphere, requires the same sort of transformation as used by the geographer who wants to transfer a map of the world from a globe to a page of an atlas. Of the many known kinds of projections, a map-maker usually chooses a more or less equal-area projection so that countries of equal area will be represented by equal areas on the map. In crystallography, however, an equiangular stereographic projection is most useful since it preserves angular relationships faithfully although distorting areas. It is made by placing a plane of projection normal to the end of any chosen diameter of the sphere and using the other end of that diameter as the point of projection. In Fig. 2-30 the projection plane is normal to the diameter AB, and the projection is made from the point B. If a plane has its pole at P, then the stereographic projection of P is at P', obtained by drawing the line BP and extending it until it meets

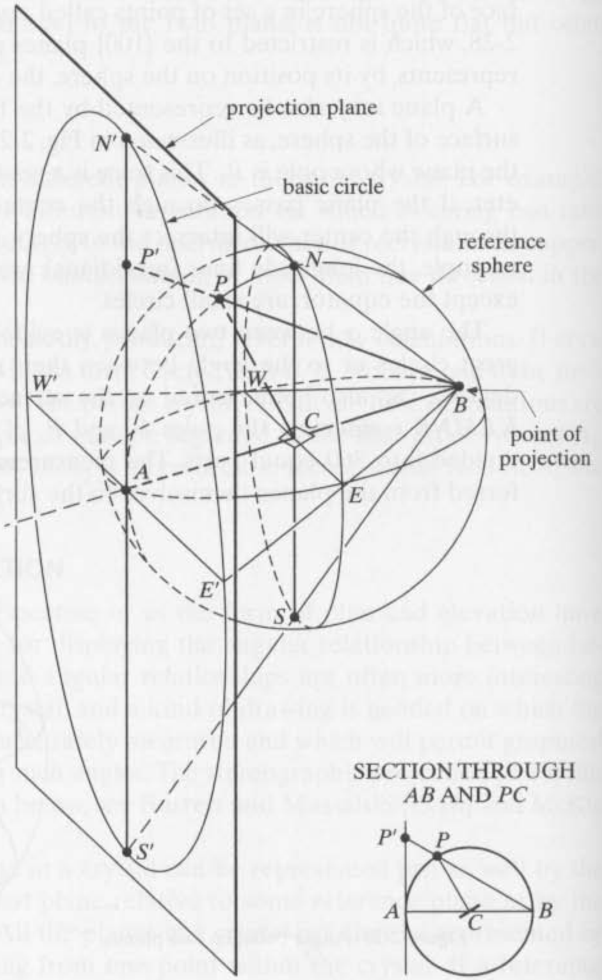

Figure 2-30 The stereographic projection

the projection plane. Alternately stated, the stereographic projection of the pole *P* is the shadow cast by *P* on the projection plane when a light source is placed at *B*. The observer, incidentally, views the projection from the side opposite the light source.

The plane *NESW* is normal to *AB* and passes through the center *C*. It therefore cuts the sphere in half and its trace in the sphere is a great circle. This great circle projects to form the *basic circle N′E′S′W′* on the projection, and all poles on the left-hand hemisphere will project within this basic circle. Poles on the right-hand hemisphere in Fig. 2-30 will project outside this basic circle, and those near *B* will have projections lying at very large distances from the center. In order to plot such poles, the point of projection must move to *A* and the projection plane to *B*; minus signs designate the new set of points while plus signs identify, the previous set (projected from *B*). Note that movement of the projection plane along *AB* or its extension merely alters the magnification; this plane is usually tangent to the sphere, as illustrated, but it can pass through the center of the sphere, for example, in which case the basic circle becomes identical with the great circle *NESW*.

A lattice plane in a crystal is several steps removed from its stereographic projection, and it may be worth-while at this stage to summarize these steps:

1. The plane *C* is represented by its normal *CP*.
2. The normal *CP* is represented by its pole *P*, which is its intersection with the reference sphere.
3. The pole *P* is represented by its stereographic projection *P′*.

After gaining some familiarity with the stereographic projection, the student will be able mentally to omit these intermediate steps and will then refer to the projected point *P′* as the pole of the plane *C* or, even more directly, as the plane *C* itself.

Great circles on the reference sphere project as circular arcs on the projection or, if they pass through the points *A* and *B* (Fig. 2-31), as straight lines through the center of the projection. Projected great circles always cut the basic circle in diametrically opposite points, since the locus of a great circle on the sphere is a set of diametrically opposite points. Thus the great circle *ANBS* in Fig. 2-31 projects as the straight line *N′S′* and *AWBE* as *W′E′*; the great circle *NGSH*, which is inclined to the plane of projection, projects as the circle arc *N′G′S′*. If the half great circle *W AE* is divided into 18 equal parts and these points of division projected on *W′ AE′*, a graduated scale, at 10° intervals, is produced on the equator of the basic circle.

Small circles on the sphere also project as circles, but their projected center does not coincide with their center on the projection. For example, the circle *AJEK* whose center *P* lies on *AEBW* projects as *AJ′E′K′*. Its center *on the projection* is at *C*, located at equal distances from *A* and *E′*, but its *projected center* is at *P′*, located an equal number of degrees (45° in this case) from *A* and *E′*.

The device most useful in solving problems involving the stereographic projection is the *Wulff net* (named after its popularizer) [2.11] shown in Fig. 2-32. It is the projection of a sphere ruled with parallels of latitude and longitude on a plane par-

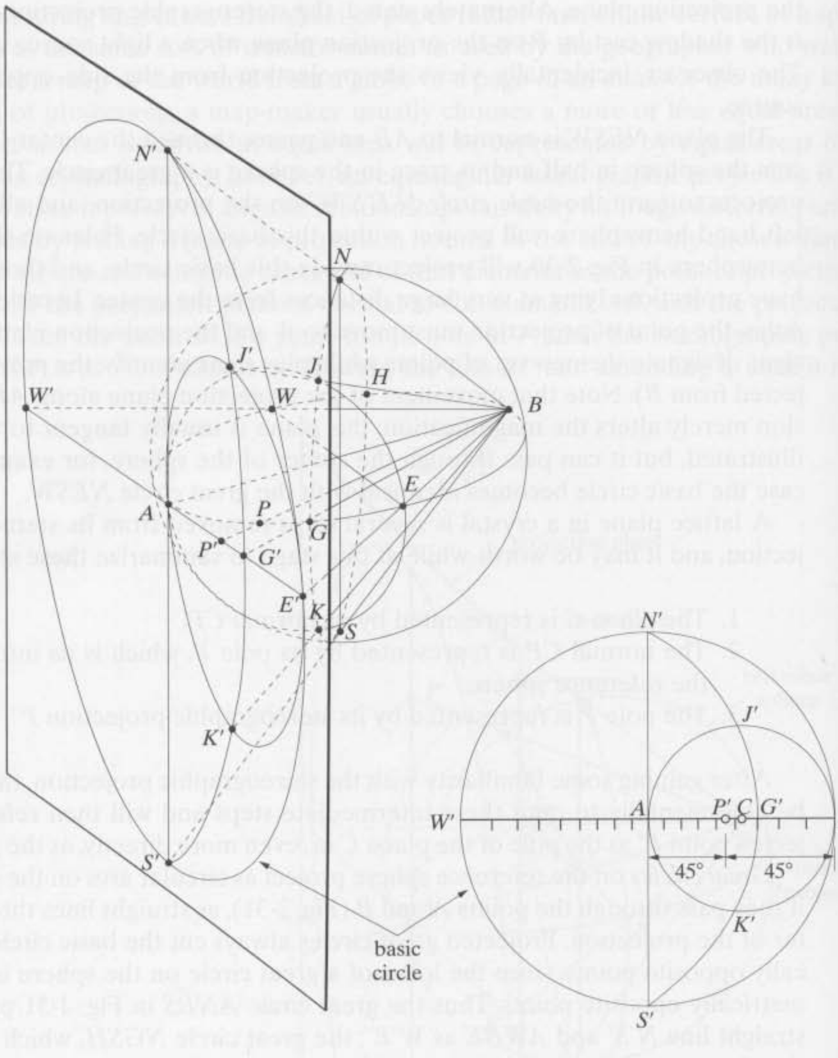

Figure 2-31 Stereographic projection of great and small circles.

allel to the north-south axis of the sphere. The latitude lines on a Wulff net are small circles extending from side to side and the longitude lines (meridians) are great circles connecting the north and south poles of the net. These nets are available in various sizes and can be plotted readily from equations available elsewhere [G.16], one of 18-cm diameter giving an accuracy of about one degree, which is satisfactory for most problems; to obtain greater precision, either a larger net or mathematical calculation must be used. Wulff nets are used by making the stereographic projection on tracing paper and with the basic circle of the same diameter as that of the Wulff

Table 2–4
Interplanar Angles (in degrees) in Cubic Crystals between Planes of the Form $\{h_1k_1l_1\}$ and $\{h_2k_2l_2\}$

	$\{h_1k_1l_1\}$						
$\{h_2k_2l_2\}$	100	110	111	210	211	221	310
100	0 90						
110	45 90	0 60 90					
111	54.7	35.3 90	0 70.5 109.5				
210	26.6 63.4 90	18.4 50.8 71.6	39.2 75.0	0 36.9 53.1			
211	35.3 65.9	30 54.7 73.2 90	19.5 61.9 90	24.1 43.1 56.8	0 33.6 48.2		
221	48.2 70.5	19.5 45 76.4 90	15.8 54.7 78.9	26.6 41.8 53.4	17.7 35.3 47.1	0 27.3 39.0	
310	18.4 71.6 90	26.6 47.9 63.4 77.1	43.1 68.6	8.1 58.1 45	25.4 49.8 58.9	32.5 42.5 58.2	0 25.9 36.9
311	25.2 72.5	31.5 64.8 90	29.5 58.5 80.0	19.3 47.6 66.1	10.0 42.4 60.5	25.2 45.3 59.8	17.6 40.3 55.1
320	33.7 56.3 90	19.1 54.0 66.9	22.2 80.8	17.0 29.8 41.9	10.9 37.6 55.6	11.5 42.3 49.7	21.6 37.9 52.1
321	36.7 57.7 74.5	11.3 40.9 55.5	36.9 51.9 72.0 90	7.1 33.2 53.3	25.2 29.2 40.2	22.4 27.0 36.7	15.3 32.3 40.5
331	46.5	13.1	22.0				
510	11.4						
511	15.6						
711	11.3						

Largely from R. M. Bozorth, *Phys. Rev.* **26**, 390 (1925); rounded off to the nearest 0.1°. A much longer list is given on p. 120-122 of Vol. 2 of [G.11].

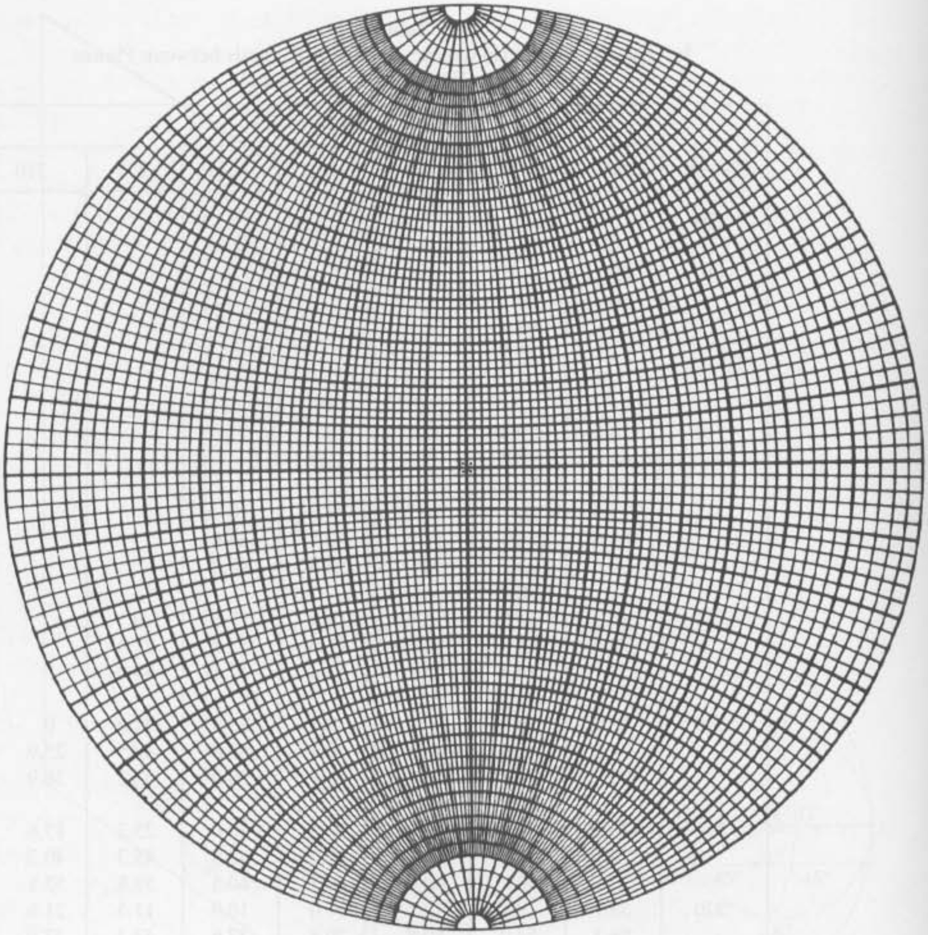

Figure 2-32 Wulff net drawn to 2° intervals.

net; the projection is then superimposed on the Wulff net, with the centers always coinciding.

Drawing the stereographic projection on tracing paper is not only more economical than drawing it directly on a Wulff net, but it also allows differentiation between the frame of reference of the crystal (represented by the stereographic projection on the paper) and the frame of reference of the laboratory, i.e., of the equipment on which the crystal is positioned for various measurements (the Wulff net). The sample and laboratory reference frames are not identical and both are needed. The sample may be mounted in a number of orientations on the equipment, and it may be necessary to realign the sample relative to the apparatus, e.g. with <001> in different orientations relative to vertical and to the incident beam direction $\mathbf{S_0}$.

To return to the problem of the measuring the angle between two crystal planes, Fig. 2-29 showed that this angle could be measured on the surface of the sphere along the great circle connecting the poles of the two planes. This measurement can also be carried out on the stereographic projection *if, and only if, the projected poles lie on a great circle*. In Fig. 2-33, for example, the angle between the planes[8] A and B or C and D can be measured directly, simply by counting the number of degrees separating them along the great circle on which they lie. Note that the angle C-D equals the angle E-F, there being the same difference in latitude between C and D as between E and F.

If the two poles do not lie on a great circle, then the projection is rotated relative to the Wulff net until they do lie on a great circle, where the desired angle measurement can then be made. Figure 2-34(a) is a projection of the two poles P_1 and P_2 shown in perspective in Fig. 2-29, and the angle between them is found by the rotation illustrated in Fig. 2-34(b). This rotation of the projection is equivalent to rotation of the poles on latitude circles of a sphere whose north-south axis is perpendicular to the projection plane.

As shown in Fig. 2-29, a plane may be represented by its trace in the reference sphere. This trace becomes a great circle in the stereographic projection. Since every point on this great circle is 90° from the pole of the plane, the great circle may be found by rotating the projection until the pole falls on the equator of the underlying Wulff net and tracing that meridian which cuts the equator 90° from the pole, as illustrated in Fig. 2-35. If this is done for two poles, as in Fig. 2-36, the angle between the corresponding planes may also be found from the angle of intersection of the two great circles corresponding to these poles; it is in this sense that the stereographic projection is said to be angle-true. This method of angle measurement is not as accurate, however, as that shown in Fig. 2-34(b).

Often poles must be rotated around various axes. Rotation about an axis normal to the projection is accomplished simply by rotation of the projection around the center of the Wulff net. Rotation about an axis lying in the plane of the projection is performed by, first, rotating the *axis* about the center of the Wulff net until it coincides with the north-south axis if it does not already do so, and, second, moving the poles involved along their respective latitude circles the required number of degrees. Suppose it is required to rotate the poles A_1 and B_1 shown in Fig. 2-37 by 60° about the NS axis, the direction of motion being from W to E on the projection. Then A_1 moves to A_2 along its latitude circle as shown. B_1, however, can rotate only 40° before reaching the edge of the projection; then it moves 20° in from the edge to the point B'_1 on the other side of the projection, staying always on its own latitude circle. The final position of this pole on the positive side of the projection is at B_2 diametrically opposite B'_1.

(The student should carefully note that the angle between A_1 and A_2, for example, in Fig. 2-37 is *not* 60°. The pole A_2 is the position of A_1 after a 60° rotation about

[8] Here the planes are represented by their normals, as was discussed above.

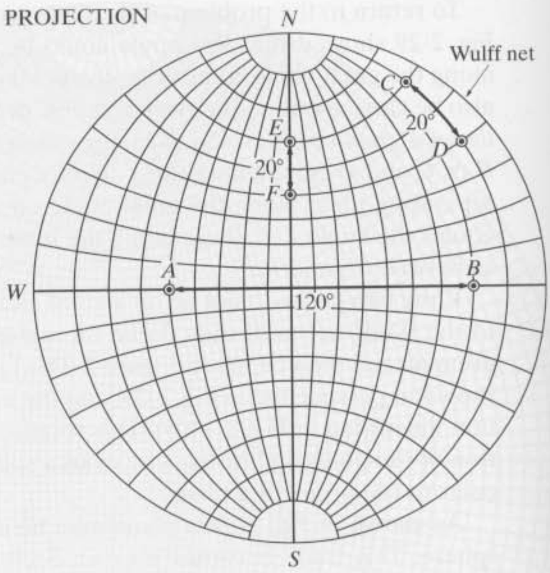

Figure 2-33 Stereographic projection superimposed on Wulff net for measurement of angle between poles. For illustrative purposes this net is graduated at 10° intervals..

NS, which is not the same thing. Consider the two great circles NA_1S and NA_2S; these are the traces of two planes between which there is a true dihedral angle of 60°. Any pole initially on NA_1S will be on NA_2S after a 60° rotation about *NS*, but the angle between the initial and final positions of the poles will be less than 60°, unless they lie on the equator, and will approach zero as the poles approach *N*.)

Rotation about an axis inclined to the plane of projection is accomplished by compounding rotations about axes lying in and perpendicular to the projection plane. In this case, the given axis must first be rotated into coincidence with one or the other of the two latter axes, the given rotation performed, and the axis then rotated back to its original position. Any movement of the given axis must be accompanied by a similar movement of all the poles on the projection.

For example, suppose A must be rotated about B_1 by 40° in a clockwise direction (Fig. 2-38). In (a) the pole to be rotated A_1 and the rotation axis B_1 are shown in their initial position. In (b) the projection has been rotated to bring B_1 to the equator of a Wulff net. A rotation of 48° about the *NS* axis of the net brings B_1 to the point B_2 at the center of the net; at the same time A_1 must go to A_2 along a parallel of latitude. The rotation axis is now perpendicular to the projection plane, and the required rotation of 40° brings A_2 to A_3 along a circular path centered on B_2. The operations which brought B_1 to B_2 must now be reversed in order to return B_2 to its original position. Accordingly, B_2 is brought to B_3 and A_3 to A_4, by a 48° reverse rotation about the *NS* axis of the net. In (c) the projection has been rotated back to its initial position, construction lines have been omitted, and only the initial and final positions of the rotated pole are shown. During its rotation about B_1, A_1 moves along the small circle shown. This circle is centered at *C* on the projection and not at its projected center B_1. To find *C*, use the fact that all points on the cir-

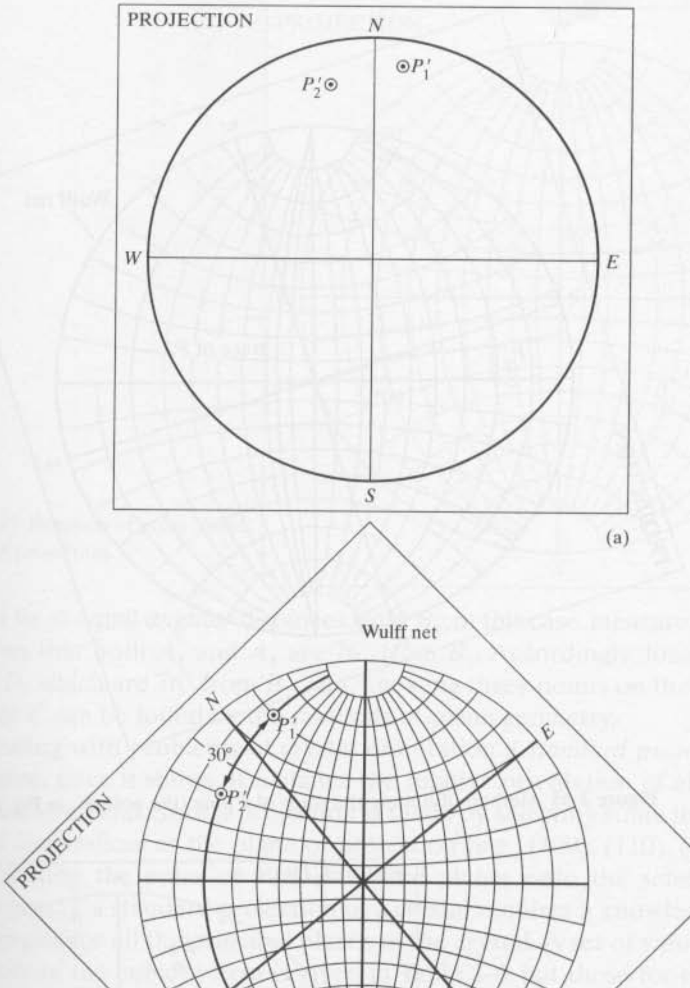

Figure 2-34 (a) Stereographic projection of poles P_1 and P_2 of Fig. 2-29. (b) Rotation of projection to put poles on same great circle of Wulff net. Angle between poles = 30°.

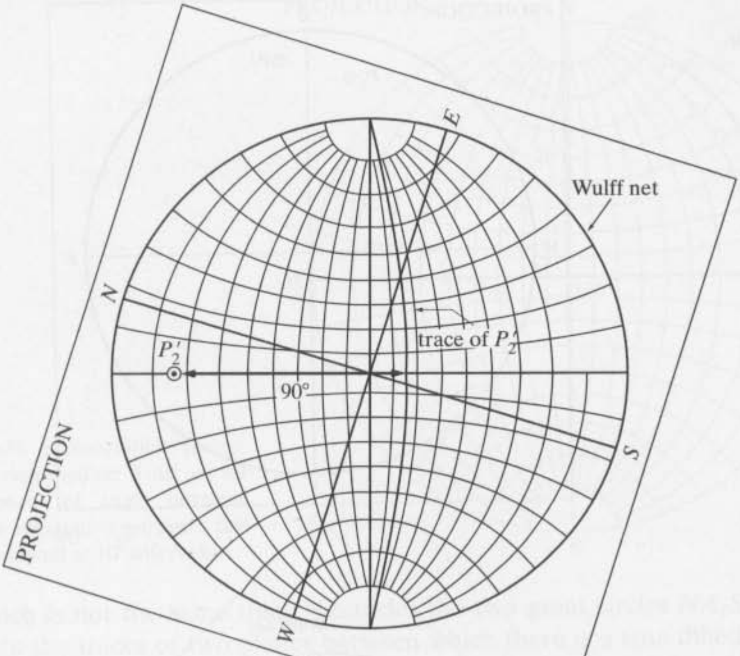

Figure 2-35 Method of finding the trace of a pole (the pole P'_2 in Fig. 2-34).

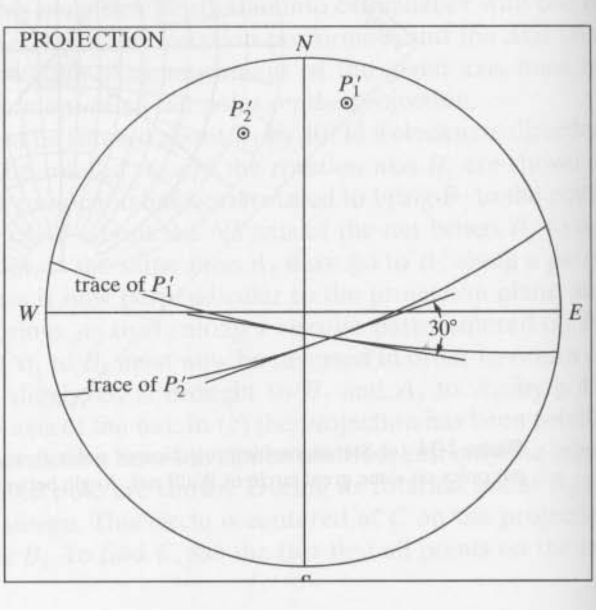

Figure 2-36 Measurement of an angle between two poles (P_1 and P_2 of Fig. 2-29) by measurement of the angle of intersection of the corresponding traces.

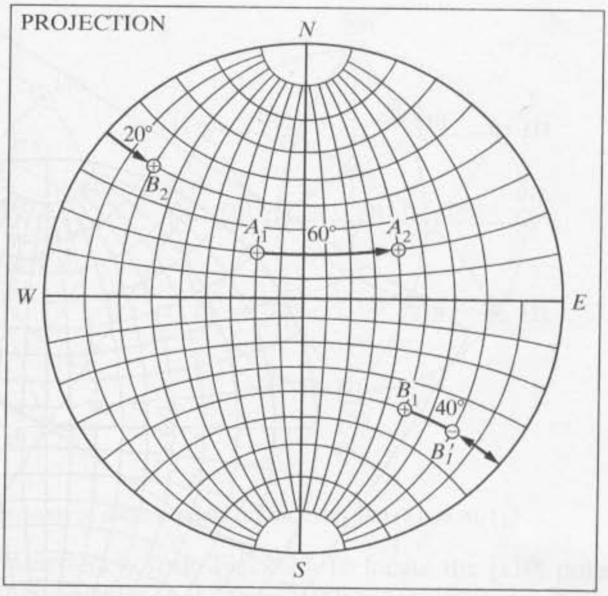

Figure 2-37 Rotation of poles about *NS* axis of projection.

cle must lie at equal *angular* distances from B_1; in this case, measurement on a Wulff net shows that both A_1 and A_4 are 76° from B_1. Accordingly, locate other points, such as D, which are 76° from B_1, and, knowing three points on the required circle, its center C can be found by the methods of plane geometry.

In dealing with problems of crystal orientation a *standard projection* is of very great value, since it shows at a glance the relative orientation of all the important planes in the crystal. Such a projection is made by selecting some important crystal plane of low indices as the plane of projection [e.g., (100), (110), (111), or (0001)] and projecting the poles of various crystal planes onto the selected plane. The construction of a standard projection of a crystal requires a knowledge of the interplanar angles for all the principal planes of the crystal. A set of values applicable to all crystals in the cubic system is given in Table 2-4, but those for crystals of other systems depend on the particular axial ratios involved and must be calculated for each case by the equations given in Appendix 3. A simple spreadsheet program suffices if interplanar angles are needed beyond those listed in Table 2-4 (for cubic crystals). Much time can be saved in making standard projections by making use of the zonal relation: the normals to all planes belonging to one zone are coplanar and at right angles to the zone axis. Consequently, the poles of planes of a zone will all lie on the same great circle on the projection, and the axis of the zone will be at 90° from this great circle. Furthermore, important planes usually belong to more than one zone and their poles are therefore located at the intersection of zone circles. It is also helpful to remember that important directions, which in the cubic system are normal to planes of the same indices, are usually the axes of important zones.

Figure 2-39(a) shows the principal poles of a cubic crystal projected on the (001) plane of the crystal or, in other words, a standard (001) projection. The location of

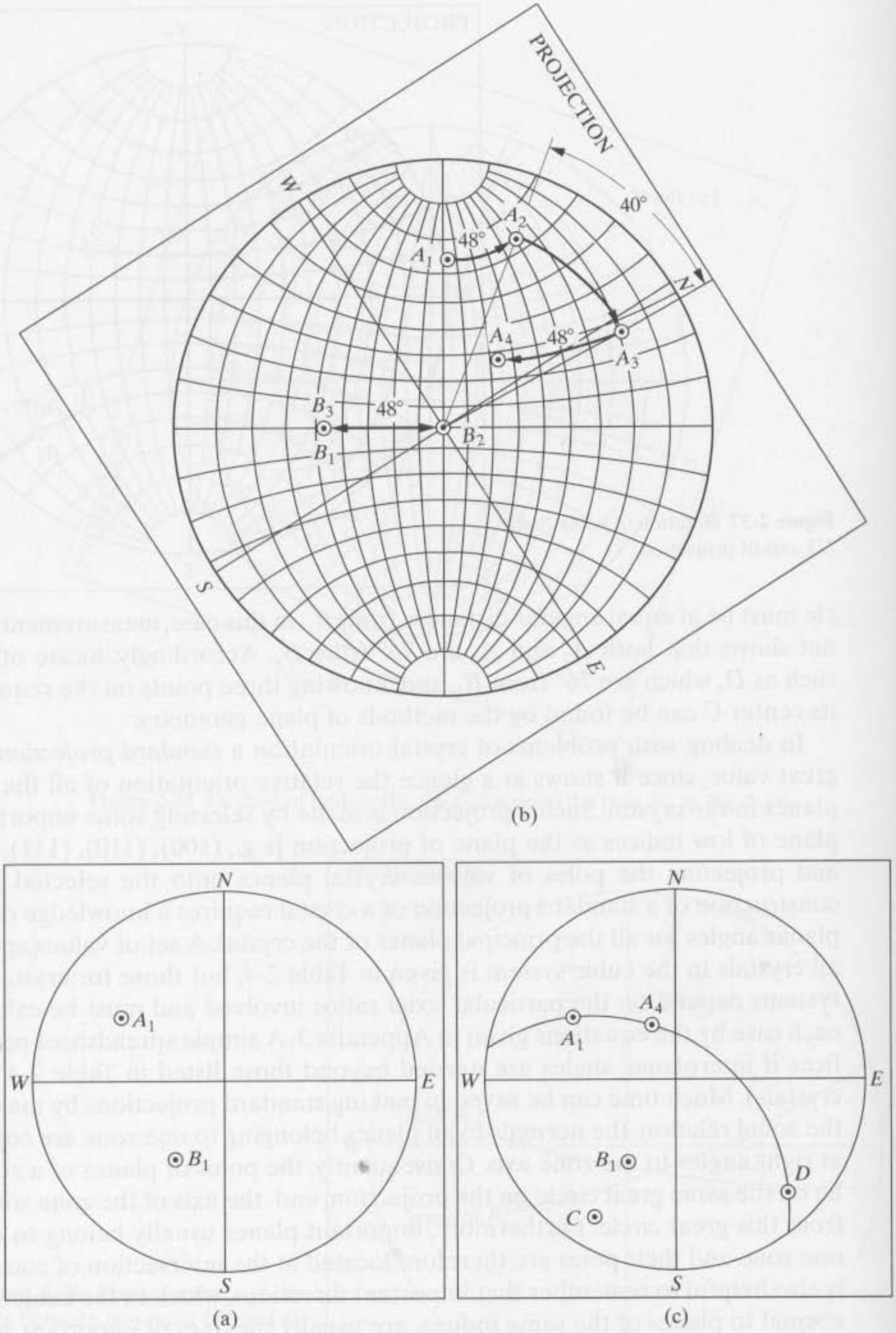

Figure 2-38 Rotation of a pole about an inclined axis.

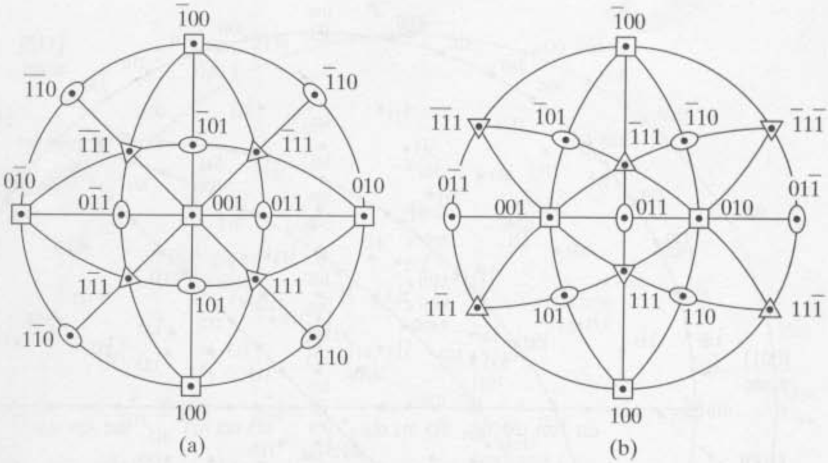

Figure 2-39 Standard projections of cubic crystals, (a) on (001) and (b) on (011).

the {100} cube poles follows immediately from Fig. 2-28. To locate the {110} poles first note from Table 2-4 that they must lie at 45° from {100} poles, which are themselves 90° apart. In this way (011) is found for example, on the great circle joining (001) and (010) and at 45° from each. After all the {110} poles are plotted, the {111} poles are found at the intersection of zone circles. Inspection of a crystal model or drawing or use of the zone relation given by Eq. (2-6) will show that (111), for example, belongs to both the zone $[\bar{1}01]$ and the zone $[0\bar{1}1]$. The pole of (111) is thus located at the intersection of the zone circle through $(0\bar{1}0)$, (101), and (010) and the zone circle through $(\bar{1}00)$, (011), and (100). This location may be checked by measurement of its angular distance from (010) or (100), which should be 54.7°. The (011) standard projection shown in Fig. 2-39(b) is plotted in the same manner. Alternatively, it may be constructed by rotating all the poles in the (001) projection 45° to the left about the *NS* axis of the projection, since this operation will bring the (011) pole to the center. In both of these projections symmetry symbols have been given each pole in conformity with Fig. 2-8(b), and it will be noted that the projection itself has the symmetry of the axis perpendicular to its plane, Figs. 2-39(a) and (b) having 4-fold and 2-fold symmetry, respectively.

Figure 2-40 is a standard (001) projection of a cubic crystal with considerably more detail and a few important zones indicated. A standard (0001) projection of a hexagonal crystal (zinc) is given in Fig. 2-41.

It is sometimes necessary to determine the *Miller indices of a given pole* on a crystal projection, for example the pole *A* in Fig. 2-42(a), which applies to a cubic crystal. If a detailed standard projection is available, the projection with the unknown pole can be superimposed on it and its indices will be disclosed by its coincidence with one of the known poles on the standard. Alternatively, the method illustrated in Fig. 2-42 may be used. The pole *A* defines a direction in space, normal to the plane (*hkl*) whose indices are required, and this direction makes angles

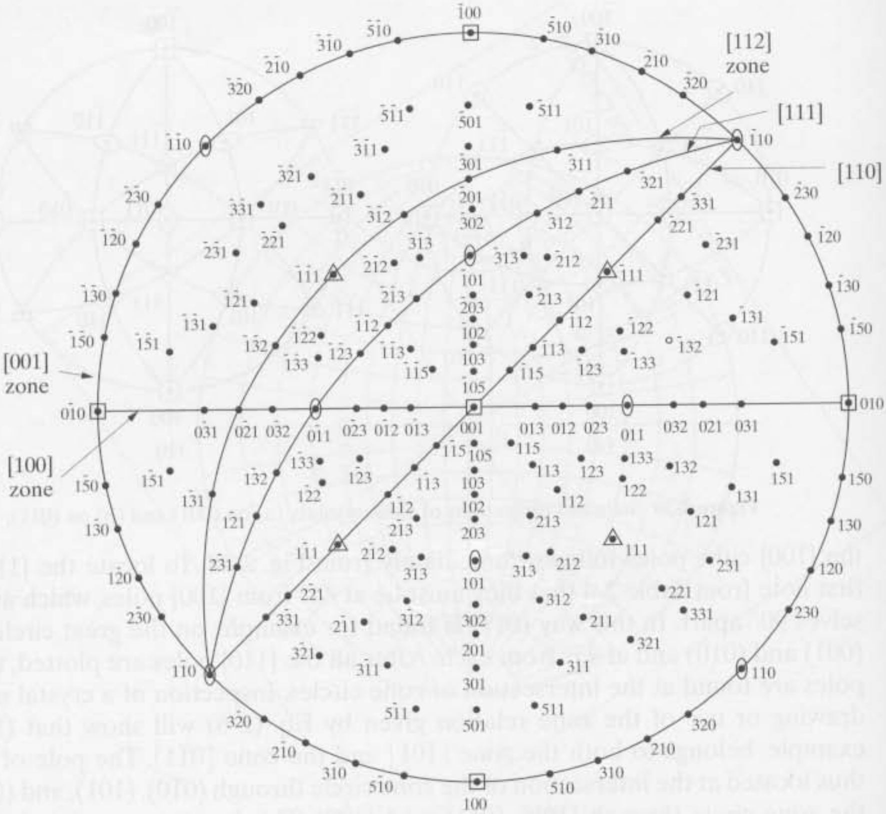

Figure 2-40 Standard (001) projection of a cubic crystal, after Barrett [1.7].

ρ, σ, τ with the coordinate axes **a**, **b**, **c**. These angles are measured on the projection as shown in (a). Let the perpendicular distance between the origin and the (hkl) plane nearest the origin be d [Fig. 2-42(b)], and let the direction cosines of the line A be $p, q\ r$. Therefore

$$p = \cos\rho = \frac{d}{a/h}, \qquad \mathrm{q} = \cos\sigma = \frac{d}{b/k}, \qquad \mathrm{r} = \cos\tau = \frac{d}{c/l},$$

$$h{:}k{:}l = pa{:}qb{:}rc. \tag{2-13}$$

For the cubic system the simple result is that the Miller indices required are in the same ratio as the direction cosines.

The lattice reorientation caused by *twinning* can be shown clearly on the stereographic projection. In Fig. 2-43 the open symbols are the {100} poles of a cubic crystal projected on the (001) plane. If this crystal is FCC, then one of its possible twin

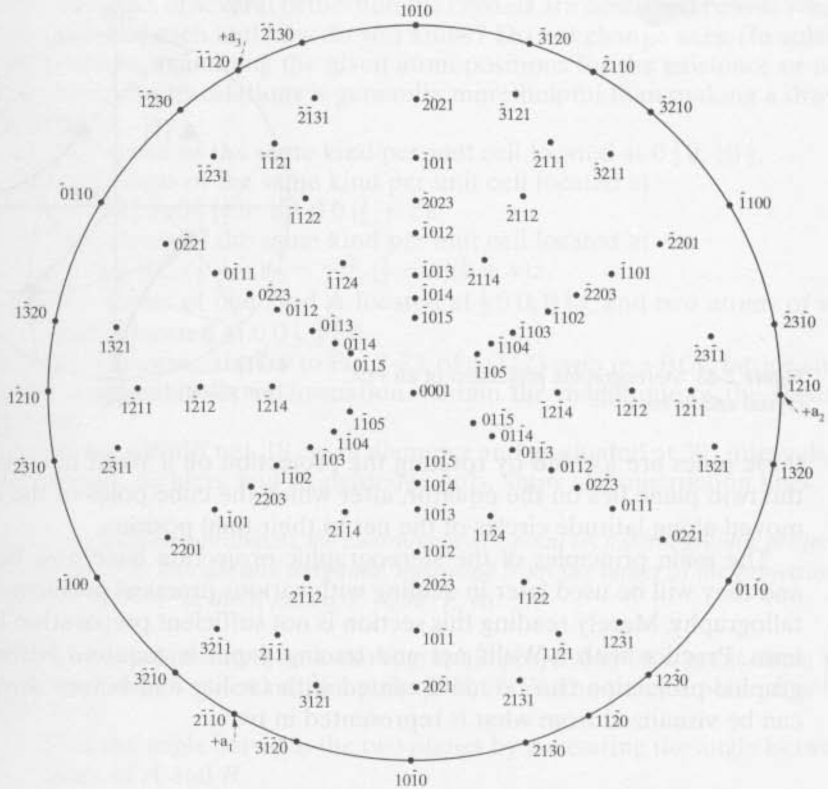

Figure 2-41 Standard (0001) projection for zinc (hexagonal, $c/a = 1.86$) [1.7]

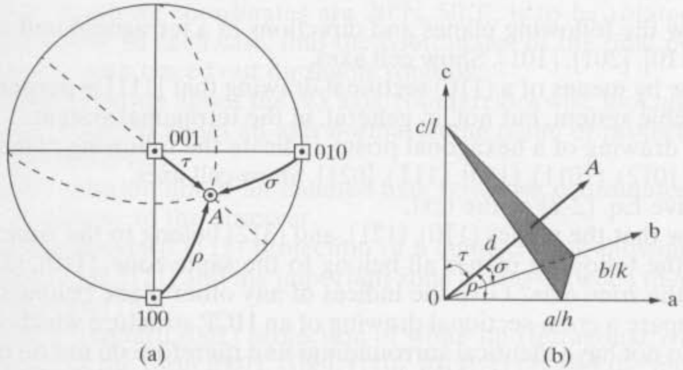

Figure 2-42 Determination of the Miller indices of a pole.

planes is $(\bar{1}\bar{1}1)$, represented on the projection both by its pole and its trace. The cube poles of the twin formed by reflection in this plane are shown as solid symbols;

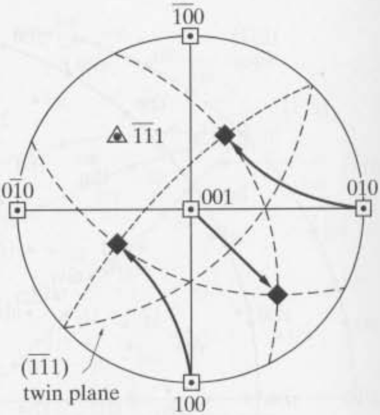

Figure 2-43 Stereographic projection of an FCC crystal and its twin.

these poles are located by rotating the projection on a Wulff net until the pole of the twin plane lies on the equator, after which the cube poles of the crystal can be moved along latitude circles of the net to their final position.

The main principles of the stereographic projection have now been presented and they will be used later in dealing with various practical problems in x-ray crystallography. Merely reading this section is not sufficient preparation for such problems. Practice with a Wulff net and tracing paper is required before the stereographic projection can be manipulated with facility and before three dimensions can be visualized from what is represented in two.

PROBLEMS

2-1 Draw the following planes and directions in a tetragonal unit cell: (001), (011), (113), [110], [201], [$\bar{1}$01]. Show cell axes.
2-2 Show by means of a (1$\bar{1}$0) sectional drawing that [111] is perpendicular to (111) in the cubic system, but not, in general, in the tetragonal system.
2-3 In a drawing of a hexagonal prism, indicate the following planes and directions ($1\bar{2}10$), ($10\bar{1}2$), ($\bar{1}011$), [110], [$11\bar{1}$], [021]. Show cell axes.
2-4 Derive Eq. (2-2) of the text.
2-5 Show that the planes (1$\bar{1}$0), (1$\bar{2}$1), and ($\bar{3}$12) belong to the zone [111].
2-6 Do the following planes all belong to the same zone: ($\bar{1}$10), ($\bar{3}$11), ($\bar{1}\bar{3}$2)? If so, what is the zone axis? Give the indices of any other plane belonging to this zone.
***2-7** Prepare a cross-sectional drawing of an HCP structure which will show that all atoms do not have identical surroundings and therefore do not lie on a point lattice.
2-8 Show that c/a for hexagonal close packing of spheres is 1.633.
2-9 Show that the HCP structure (with c/a = 1.633) and the FCC structure are equally close-packed, and that the BCC structure is less closely packed than either of the former.