Chapter 2

Geometry of Crystals

2-1 INTRODUCTION

Turning from the properties of x-rays, consider next the geometry and structure of crystals in order to discover what there is about crystals in general that enables them to diffract x-rays. Particular crystals of various kinds and how the very large number of crystals found in nature are classified into a relatively small number of groups must also be considered. The final sections of the chapter focus on the ways in which the orientation of lines and planes in crystals can be represented in terms of symbols or in graphical form.

Crystallography is a very broad subject and its origins precede the discovery of x-rays by many years. Only the more basic aspects are covered here: how atoms are arranged in some common crystals and how this arrangement determines the way in which a particular crystal diffracts x-rays. Readers who need a deeper knowledge of crystallography should consult such books as those by McKie and McKie [G.3], Borchardt-Ott [G.4], Sands [G.5] or Hammond [G.6].

2-2 LATTICES

A crystal may be defined as *a solid composed of atoms, ions or molecules arranged in a pattern periodic in three dimensions*. As such, crystals differ in a fundamental way from gases and liquids because the atomic, ionic or molecular arrangements in the latter do not posses the essential requirement of periodicity. Many solids are crystalline; if they are not single-crystals they consist of many contiguous crystals, i.e., they are polycrystalline. Not all solids are crystalline, however; some are *amorphous*, like glass, and do not have any regular interior arrangement of atoms, ions or molecules. There is, in fact, no essential difference between an amorphous solid and a liquid, and the former is often termed an "undercooled liquid." It is important to emphasize that not only are the atom, ion or molecule positions repetitious but also that there are certain symmetry relationships in their arrangement.

In thinking about crystals it is often convenient to ignore the actual atoms, ions, or molecules and to focus on the geometry of periodic arrays. The crystal is then represented as a *lattice*, that is, a three-dimensional array of points (*lattice points*), each of which has identical surroundings. As mathematical constructs, lattices are infinite in extent whereas crystals are not. In practical terms, most crystals consist of enough atoms to render this distinction moot.

Consider first a one-dimensional lattice. The entire "space" is this line with zero thickness. The points of the lattice are separated by a lattice translation vector **a** whose length, the lattice parameter, is written as |a|, *a* or a_0 (Fig. 2-1a)[1]. Translation of **na** from a lattice point, where n is an integer, brings one to another lattice point. Planar or two-dimensional lattices consist of two non-collinear lattice vectors **a** and **b**. These vectors have length *a* and *b* and are separated by an angle γ (Fig. 2-1b). Any translation **na** + p**b**, where p as well as n are integers, returns one to an equivalent position within the lattice or planar mesh. If a third translation vector **c**, non-coplanar with **a** and **b**, operates on the mesh of Fig. 2-1b, a three-dimensional or space lattice results (Fig. 2-1c). Thus, the points of this lattice can be generated solely by applying (repeatedly) the three translation vectors.

Normally **a, b** and **c** are defined in a right-handed sense (if the index finger of the right hand points along **a** and the middle finger is bent to point along **b**, the thumb will point along **c**) The vectors **a, b** and **c** define a unit cell, that is a prism or parallelopiped volume. Stacking the unit cells face-to-face is, in fact, another way of generating a lattice and sometimes offers greater clarity than considering only the translation vectors. Unit cells can also be defined using the six scalar lattice parameters (the lengths of the three lattice translation vectors a_0, b_0 and c_0 and the three inter-axial angles α, between **b** and **c**, β, between **c** and **a**, and γ). Figure 2-2a shows the relationship between axes and angles which is easy to commit to memory using Table 2-1. It is important to emphasize that the unit cell (its faces and interior) completely defines the lattice. Adjacent unit cells touch, and eight unit cells share each vertex, four each edge and two each face. Thus, even though there are eight lattice points in the unit cell shown in Fig. 2-1c, each is shared by eight other unit cells, only one-eighth of each may be attributed to the particular unit cell pictured. Therefore, there is only one lattice point per unit cell, and this and other unit cells, chosen such that they contain only one lattice point, are termed *primitive*.

Translation of the boundaries of the unit cell shown in Fig. 2-1c by a vector of the type $\pm\mathbf{a}/2 \pm \mathbf{b}/2 \pm \mathbf{c}/2$ centers the unit cell on one of the lattice points (indicated by an open instead of solid sphere) and illustrates that the particular unit cell origin or shape one chooses depends on what is most convenient. In Fig. 2-2b the arrows show the shift of the unit cell corners from the setting in Fig. 2-1c, and two of the unit cell body diagonals indicate the relationship between the lattice point and the corners of the unit cells. The gray areas represent projections, along a lattice vector, of a unit cell face onto a plane parallel to that face and containing a plane of lattice points. As a further aid to the eye, the separations of nearest neighbor lattice points from the unit cell faces are indicated with heavy lines. Non-primitive unit cells of some lattices, for example, are employed to illustrate important

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[1] Vectors are here represented by boldface symbols. The same symbol in italics stands for the magnitude of the vector.

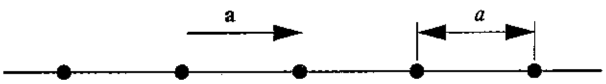


Figure 2-1 (a) One-dimensional lattice with parameter a.

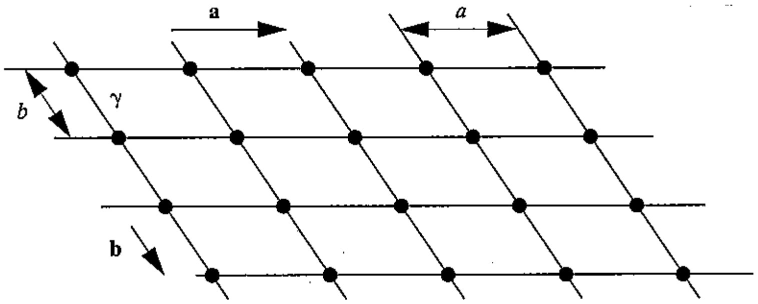


Figure 2-1 (b) Two-dimensional lattice with lattice translation vectors **a** and **b** and interaxial angle γ.

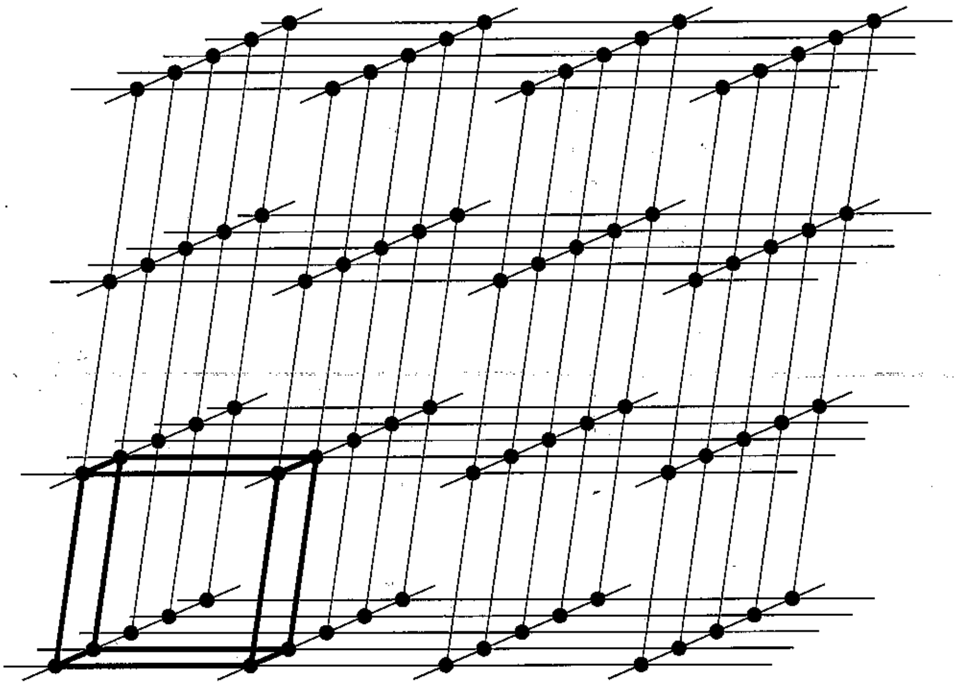


Figure 2-1 (c) Three-dimensional lattice with a primitive unit cell highlighted in bold. Lattice points are represented by the solid circles/spheres.

aspects of periodicity or symmetry. Once a particular unit cell or unit cell origin is defined, it must be consistently applied throughout the lattice.

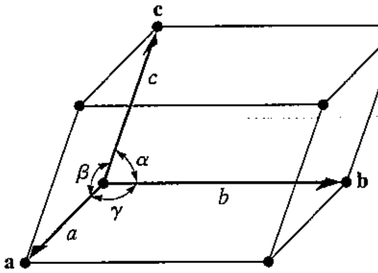


Figure 2-2 (a) Illustration of lattice vector and interaxial angle designations.

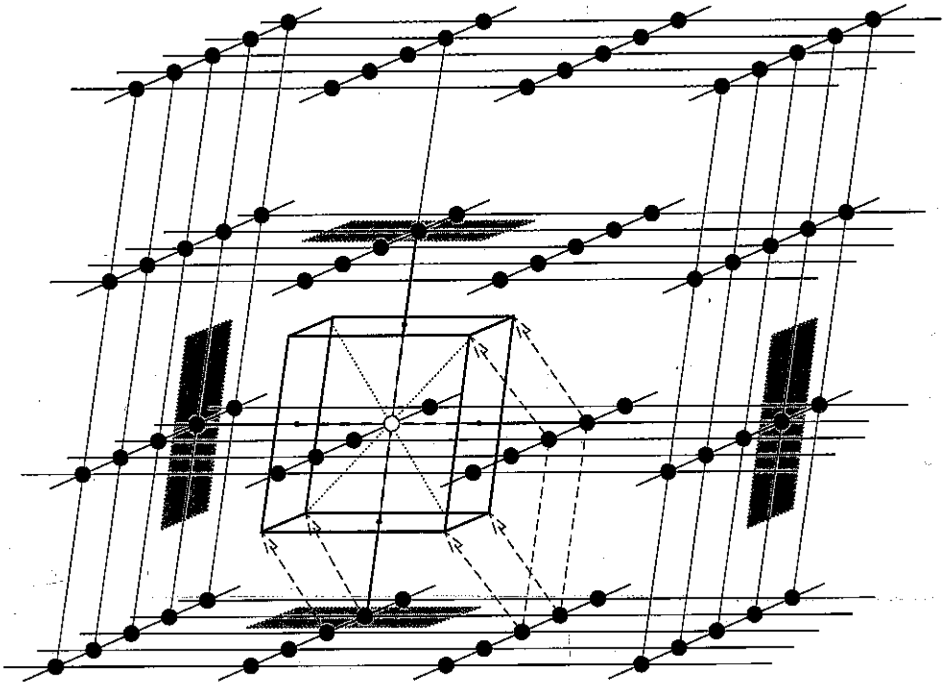


Figure 2-2 (b) Unit cells with the lattice points located at the cell corners and an alternative unit cell centered on one lattice point.

TABLE 2.1 DETERMINING WHICH INTER-AXIAL ANGLE IS BETWEEN WHICH PAIR OF AXES. THE ANGLE BETWEEN ANY TWO TRANSLATION VECTORS IS GIVEN BETWEEN THOSE VECTORS ON THE LINE BELOW.

Axis	**a**		**b**		**c**		**a**
Inter-axial Angle		γ		α		β	

A different notation for the lattice vectors uses $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$ in place of **a**, **b** and **c**, respectively. While use of $\mathbf{a}_1$ may seem somewhat more abstract than necessary, this notation can be much more convenient (see Section 2-4 and Chap. 3-5). One or the other of these notations will be used in this book, and what aspects of periodicity are being emphasized will determine which will be used.

2-3 DESIGNATION OF POINTS, LINES, AND PLANES

Every point within the lattice is uniquely defined with respect to the origin of the lattice by position vector $\mathbf{r} = u'\mathbf{a} + v'\mathbf{b} + w'\mathbf{c}$. If the origin of the lattice lies on a lattice point and if u', v' and w' are integers, the point located by $\mathbf{r}$ must be a lattice point and its coordinates are written simply as an ordered triplet $u'v'w'$. Points in space which are not lattice points have non-integer values of u', v' or w', and it is possible to write $\mathbf{r}$ as the sum of integer multiples n, p and q of the lattice vectors plus fractions u,v and w of the translation vectors:

$$\mathbf{r} = (n + u)\,\mathbf{a} + (p + v)\,\mathbf{b} + (q + w)\,\mathbf{c}. \tag{2-1}$$

Rearranging terms yields

$$\mathbf{r} = (n\mathbf{a} + p\mathbf{b} + q\mathbf{c}) + (u\mathbf{a} + v\mathbf{b} + w\mathbf{c}), \tag{2-2}$$

i.e., a vector between lattice points or between corners of equivalent unit cells plus a vector from the corner of a unit cell to a point within the unit cell at position uvw relative to the corner of that unit cell.

The direction of any line in a lattice may be described by first drawing a line through the origin parallel to the given line and then giving the coordinates of any point on the line through the origin. Let the line pass through the origin of the unit cell and any point having coordinates $u'\ v'\ w'$, where these numbers are not necessarily integral. (This line will also pass through the points $2u'\ 2v'\ 2w'$, $3u'\ 3v'\ 3w'$, etc.) Then $[uvw]$, written in square brackets, are the *indices* of the direction of the line. They are also the indices of any line parallel to the given line, since the lattice is infinite and the origin may be taken at any point. Whatever the values of u', v', w', they are always converted to a set of smallest integers by multiplication or division throughout: thus, $[\frac{1}{2}\,\frac{1}{2}\,1]$, [112], and [224] all represent the same direction, but [112] is the preferred form. Negative indices are written with a bar over the number, e.g., $[\bar{u}vw]$. Direction indices are illustrated in Fig. 2-3. Note how one can mentally shift the origin, to avoid using the adjacent unit cell, in finding a direction like [120].

Directions related by symmetry are called *directions of a form*, and a set of these are represented by the indices of one of them enclosed in angular brackets: for example, the four body diagonals of a cube, [111], $[1\,\bar{1}\,1]$, $[\bar{1}\,\bar{1}\,1]$, and $[\bar{1}\,1\,1]$, may all be represented by the symbol <111>.

The orientation of planes in a lattice may also be represented symbolically, according to a system popularized by the English crystallographer Miller [2.1]. In the general case, the given plane will be tilted with respect to the crystallographic axes, and, since these axes form a convenient frame of reference, the orientation of the plane might be described by giving the actual distances, measured from the ori-

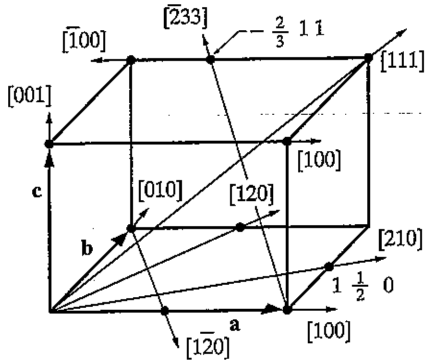
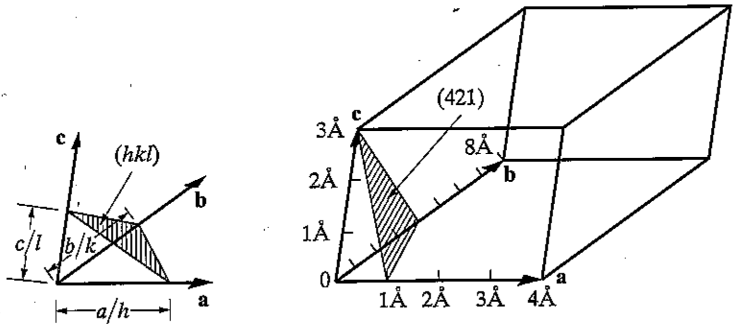


Figure 2-3 Indices of directions.

gin, at which it intercepts the three axes. Better still, by expressing these distances as fractions of the axial lengths, the numbers become are independent of the particular axial lengths involved in the given lattice. But a difficulty then arises when the given plane is parallel to a certain crystallographic axis, because such a plane does not intercept that axis, i.e., its "intercept" can only be described as "infinity." To avoid the introduction of infinity into the description of plane orientation, the reciprocal of the fractional intercept is used, this reciprocal being zero when the plane and axis are parallel. A workable symbolism results for the orientation of a plane in a lattice, the *Miller indices*, which are defined as *the reciprocals of the fractional intercepts which the plane makes with the crystallographic axes*. For example, if the Miller indices of a plane are (*hkl*), written in parentheses, then the plane makes fractional intercepts of $1/h$, $1/k$, $1/l$ with the axes, and, if the axial lengths are a, b, c, the plane makes actual intercepts of a/h, b/k, c/l, as shown in Fig. 2-4(a). Parallel to any plane in any lattice, there is a whole set of parallel equidistant planes, one of which passes through the origin; the Miller indices (*hkl*) usually refer to that plane in the set which is nearest the origin, although they may be taken as referring to any other plane in the set or to the whole set taken together.



(a)

(b)

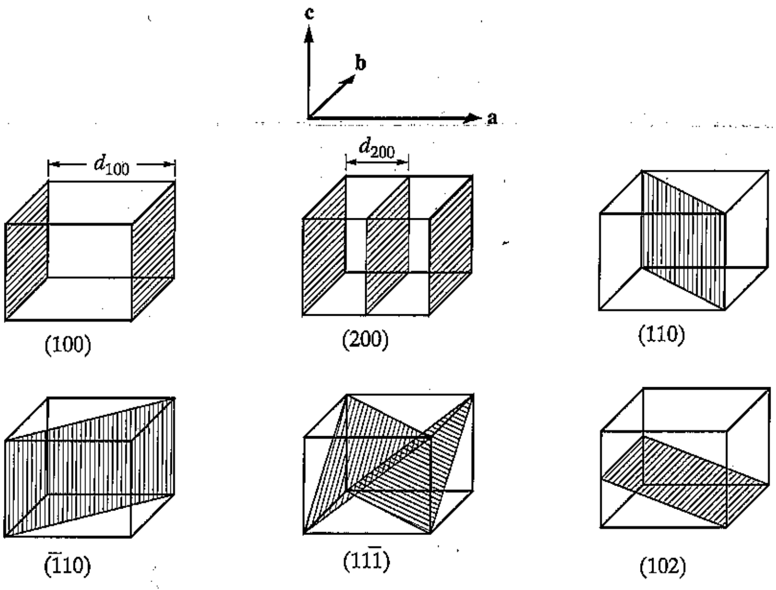
Figure 2-4 Plane designation by Miller indices.

Determining the Miller indices of the plane shown in Fig. 2-4(b) requires the following steps.

Axial lengths	4Å	8Å	3Å
Intercept lengths	1Å	4Å	3Å
Fractional intercepts	1/4	1/2	1
Miller indices	4	2	1

As stated earlier, if a plane is parallel to a given axis, its fractional intercept on that axis is taken as infinity and the corresponding Miller index is zero. If a plane cuts a negative axis, the corresponding index is negative and is written with a bar over it. Planes whose indices are the negatives of one another are parallel and lie on opposite sides of the origin, e.g., ($\bar{2}10$) and ($2\bar{1}0$). The planes (*nh nk nl*) are parallel to the planes (*hkl*) and have 1/*n*th the spacing. The same plane may belong to two different sets, the Miller indices of one set being multiples of those of the other; thus the same plane belongs to the (210) set and the (420) set, and, in fact, the planes of the (210) set form every second plane in the (420) set. In the cubic crystal system it is convenient to remember that a direction [*hkl*] is always perpendicular to a plane (*hkl*) of the same indices, but this is not generally true in other crystal systems. Further familiarity with Miller indices can be gained from a study of Fig. 2-5.

The various sets of planes in a lattice have various values of interplanar spacing. The planes of large spacing have low indices and pass through a high density of lat-



(100) (200) (110)

($\bar{1}10$) ($11\bar{1}$) (102)

Figure 2-5 Miller indices of lattice planes. The distance *d* is the plane spacing.

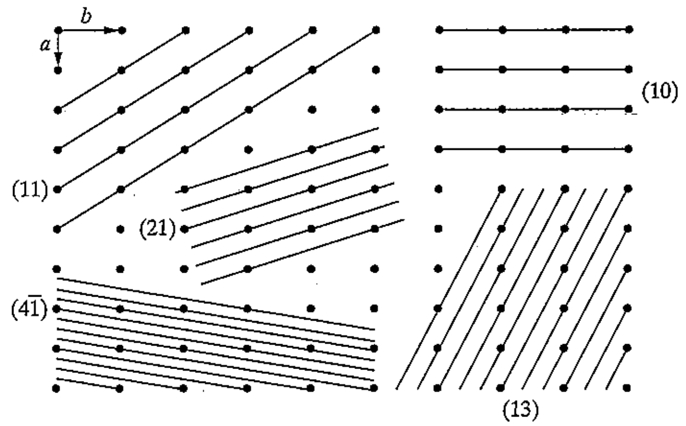


Figure 2-6 Two-dimensional lattice, showing that lines of lowest indices have the greatest spacing and the greatest density of lattice points.

tice points, whereas the reverse is true of planes of small spacing. Figure 2-6 illustrates this for a two-dimensional lattice, and it is equally true in three dimensions. The interplanar spacing d_{hkl}, measured at right angles to the planes, is a function both of the plane indices (*hkl*) and the lattice constants ($a, b, c, \alpha, \beta, \gamma$).

2-4 RECIPROCAL LATTICE

Vectors $\mathbf{a}_i$ (i.e., **a**, **b**, and **c**) define the basis vectors of a three-dimensional lattice. This *direct space* lattice, however, is not the only way that the periodicity and symmetry of a given arrangement of lattice points can be represented. As introduced by J. Willard Gibbs [2.2], a reciprocal lattice $\mathbf{b}_i$ (i.e., a lattice in *reciprocal space*) can be defined for every direct space lattice $\mathbf{a}_i$ by

$$\mathbf{b}_1 = \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3},$$

$$\mathbf{b}_2 = \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3} \qquad \text{and}$$

$$\mathbf{b}_3 = \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3}. \tag{2-3}$$

The cyclic permutation of the indices in the numerator insures that a right-handed reciprocal lattice is obtained. Strictly speaking, the denominator should be written using the same permutation of indices as the numerator, but this vector product is the volume of the unit cell of the direct space lattice and this volume is the same regardless of the order in which the $\mathbf{a}_i$ are multiplied.[2] One should note that the units of the reciprocal lattice are Å^{-1} and not Å.

The physical significance of the reciprocal lattice in diffraction is due to Ewald [2.3] and not to Gibbs. The reciprocal lattice has several important properties. First, the cross-product in the numerator means that $\mathbf{b}_1$ is perpendicular to $\mathbf{a}_2$ and $\mathbf{a}_3$, that $\mathbf{b}_2$ is perpendicular to $\mathbf{a}_3$ and $\mathbf{a}_1$ and that $\mathbf{b}_3$ is perpendicular to $\mathbf{a}_1$ and $\mathbf{a}_2$. This relationship means that the reciprocal lattice has the property of orthonormality, i.e.,

$$\mathbf{a}_i \cdot \mathbf{b}_j = \delta_{ij}, \tag{2-4}$$

where δ_{ij} is the Kroenecker delta and equals 0 if $i \neq j$ and 1 if $i = j$. It can be shown that the volume of the reciprocal lattice unit cell is the reciprocal of the volume of the direct space unit cell. Second, a vector $\mathbf{H}_{hkl}$ drawn from the origin of reciprocal space to any point in reciprocal space having coordinates h,k,l is perpendicular to the plane in direct space whose Miller indices are *hkl*. The length H_{hkl} of the reciprocal lattice vector $\mathbf{H}_{hkl} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$ equals the reciprocal of the periodicity of (hkl), i.e., $H_{hkl} = 1/d_{hkl}$.

Two examples of direct space lattices and the corresponding reciprocal space lattices appear in Figure 2-7. Sometimes drawings of the lattices are shown superimposed, but it is best to place the direct space and reciprocal space lattices side-by-side in order to avoid confusion in terms of units, etc. Note that the axes of each pair of lattices are shown in the correct alignment: $\mathbf{b}_2$ is perpendicular to both $\mathbf{a}_3$ and $\mathbf{a}_1$, etc. Also, in both cases, axes $\mathbf{a}_3$ are perpendicular to $\mathbf{a}_1$ and $\mathbf{a}_2$ and to the plane of the paper. The corresponding reciprocal lattices also have $\mathbf{b}_3$ perpendicular to the sheet of paper, and the *hk*0 plane of the reciprocal lattice is shown. In the case of the cubic lattice, $\mathbf{b}_1$ is parallel to $\mathbf{a}_1$ but for the hexagonal lattice $\mathbf{b}_1$ is not parallel to $\mathbf{a}_1$. Several planes in the direct space lattices are indicated along with their Miller indices. In the cubic lattice (110) and (210) are shown, and one can see that the reciprocal lattice vectors $\mathbf{H}_{110}$ and $\mathbf{H}_{210}$ are perpendicular to the corresponding planes. Similarly, in the hexagonal lattice, one can see that $\mathbf{H}_{120}$ is perpendicular to (120) and $\mathbf{H}_{110}$ is perpendicular to (110). Comparing the direct space vector [120] with the orientation of (120) in the drawing of hexagonal lattice demonstrates what should always be remembered: the direct space vector [*hkl*] in non-cubic systems will not necessarily be perpendicular to (*hkl*). One can also demonstrate by direct measurement that the lengths of the reciprocal lattice vectors are equal to the inverse of the spacing between corresponding planes.

In crystallographic terms, all that is needed to uniquely identify a set of parallel lattice planes (*hkl*) is their orientation and their periodicity. These are given by the normal to the planes (a single direction) and the spacing between the planes (d_{hkl}). A single lattice point in reciprocal space, defined by vector $\mathbf{H}_{hkl}$, is sufficient, therefore, to represent the infinite series of physical direct space planes. In other words,

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[2] If the notation **a**, **b** and **c** is used for the direct space vectors, then **a***, **b*** and **c*** are used for the corresponding reciprocal space vectors.

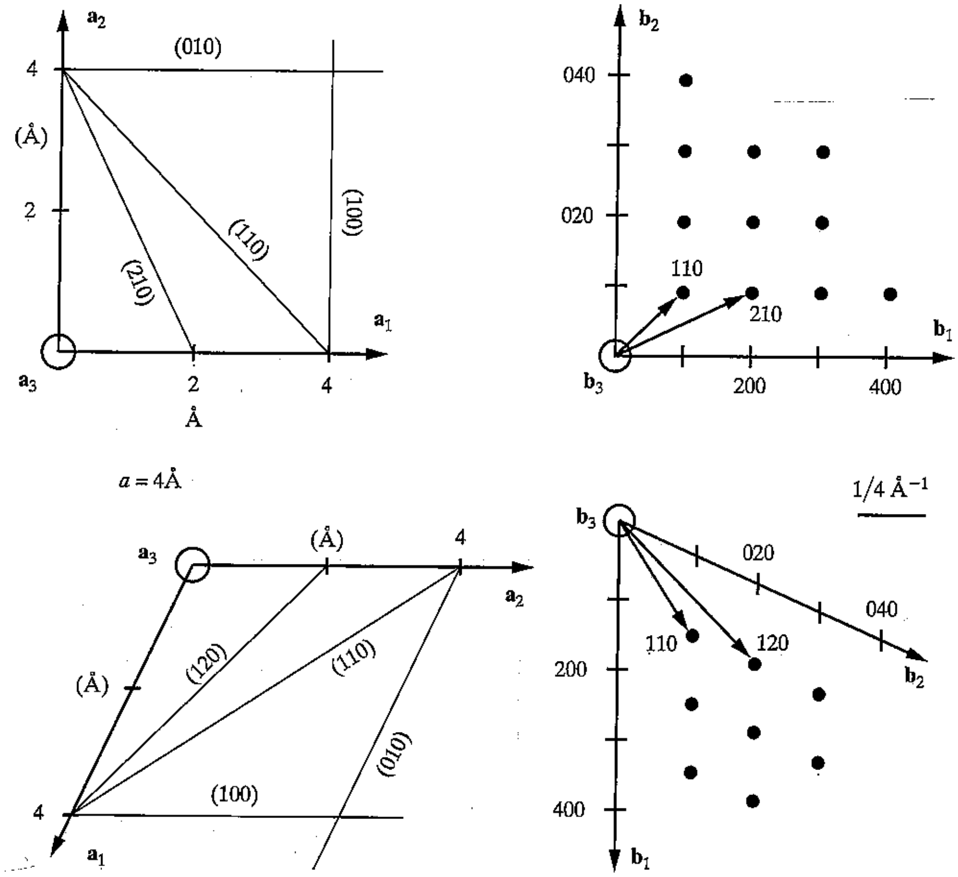


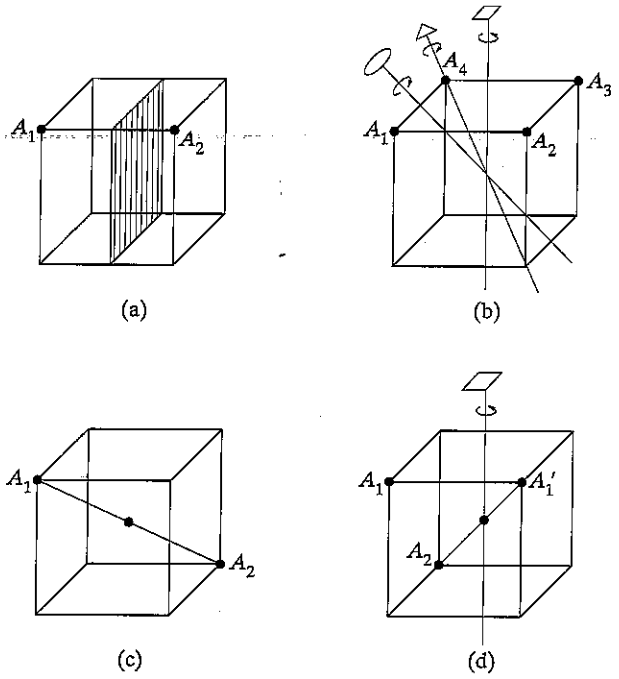
Figure 2-7 Illustration of crystal lattices (left side) and corresponding reciprocal lattices (right side) for a cubic system (top) and an hexagonal system (bottom).

the transformation from direct space to reciprocal space maps all direct space planes (*hkl*) onto a single point (i.e., the reciprocal lattice point with coordinates *h,k,l*). Note that the symmetry which is present in direct space appears in reciprocal space. As will be seen in the following two chapters, the reciprocal lattice representation of a crystal is a powerful tool for understanding diffraction.

2-5 SYMMETRY

One type of repetition, lattice translation, underlies the periodicity of one-, two- and three- dimensional nets. As mentioned in Sec. 2-2, the surroundings of each lattice point are identical, not only in kind but also in orientation. Symmetry is the second type of repetition required to define the periodicity of two-dimensional patterns seen in wallpaper or of three-dimensional assemblies of atoms, ions or molecules comprising crystals. The various symmetry operators act to change the orientation of the repeated features or *motifs* which populate a lattice. These operators are required to describe repeating patterns which are more complex than those generated through the simple repetition of lattice translations. For simplicity, the symmetry elements used in crystallography will be introduced distinct from lattices and only later will be incorporated into lattices to produce crystal structures.

Before considering how symmetry is incorporated in lattices, it is necessary to investigate how the symmetry elements operate on their surroundings. If a certain object is at a certain position relative to the symmetry element, the type of symmetry element dictates where to look to find an object identical, except for orientation, to the first. Alternatively, a body or structure is said to be symmetrical when its component parts are arranged in such balance, so to speak, that certain operations can be performed on the body which will bring it into coincidence with itself. For example, if a body is symmetrical with respect to a plane passing through it, then reflection of either half of the body across the *mirror plane* will produce a body coinciding with the other half. Thus a cube has several planes of symmetry, one of which is shown in Fig. 2-8(a). Points A_1 and A_2 in Fig. 2-8(a) must be identical because of the mirror plane through the center of the cube; they are related by reflection.



(a) (b) (c) (d)

Figure 2-8 Some symmetry elements of a cube. (a) Reflection plane. A_1 becomes $A_{2.}$ (b) Rotation axes. 4-fold axis: A_1 becomes A_2; 3-fold axis: A_1 becomes A_2; 2-fold axis: A_1 becomes $A_{4.}$ (c) inversion center. A_1 becomes A_2. (d) Rotation-inversion axis, 4-fold axis: A_1 becomes A'_2; inversion center: A'_1 becomes $A2$.

There are in all four macroscopic[3] symmetry operations or elements: *reflection, rotation, inversion* and *roto-inversion*. A body has n-fold rotational symmetry about an axis if a rotation of $360°/n$ brings it into self-coincidence. Thus a cube has a 4-fold axis normal to each face, a 3-fold axis along each body diagonal, and 2-fold axes joining the center of opposite edges. Some of these are shown in Fig. 2-8 where the small plane figures (square, triangle, and ellipse) designate the various axes. In Fig. 2-8(b), points A_1, A_2, A_3, and A_4 are related by the four-fold rotation axis (Fig. 2-8(b)) while points A_1 and A_4 are also related by the two-fold axis inclined with respect to the four-fold axis. In general, rotation axes may be 1-, 2-, 3-, 4- or 6-fold. Multiple 1-fold axes are present in all objects, and these are normally not shown while a 5-fold axis or one of higher degree than 6 are impossible, in the sense that unit cells having such symmetry cannot be made to fill space without leaving gaps.

A body has an inversion center if corresponding points of the body are located at equal distances from the center on a line drawn through the center. A body having an inversion center will come into coincidence with itself if every point in the body is inverted, or "reflected," in the inversion center. A cube has such a center at the intersection of body diagonals [Fig. 2-8(c)]. Finally, a body may have a rotation-inversion axis, either 1-, 2-, 3-, 4- or 6-fold. If it has an n-fold rotation-inversion axis, it can be brought into coincidence with itself by a rotation of $360°/n$ about the axis followed by an inversion in a center lying on the axis. Figure 2-8(d) illustrates the operation of a 4-fold rotation-inversion axis on a cube.

Consider next all of the positions and orientations an object or motif must take due to the operation of various symmetry elements (Fig. 2-9). The motif must appear even more frequently if, for example as in Fig. 2-9(g) and (h), two symmetry operators operate through the same point. The combined operation of a two-fold axis lying within a mirror plane "produces" a second mirror plane, perpendicular to the first mirror and also containing the two-fold axis (i.e., horizontal in Fig. 2-9(g)). When a four-fold axis lies within a single mirror plane as shown in Fig. 2-9(h) symmetry requires a total of eight identical motifs (in various orientations) and four mirror planes to be present.

The different symmetry operations acting through a point are termed *point groups*. In two-dimensions there are ten point groups which can be included in lattices. In three-dimensions, the number of point groups increases to thirty-two: unlike in two-dimensions, inversion centers are no longer equivalent to two-fold axes, and combinations such as mirrors perpendicular to rotation axes are possible.[4]

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[3] So called to distinguish them from certain microscopic symmetry operations which are not of concern here. The macroscopic elements can be deduced from the angles between faces of a well-developed crystal, without any knowledge of the atomic arrangement inside the crystal. The microscopic symmetry elements, on the other hand, depend entirely on atom arrangement, and their presence cannot be inferred from the external development of the crystal.

[4] Texts such as that of Schwartz and Cohen [G.7] and those on crystallography [G.3-G.6] illustrate this topic in considerably greater detail.

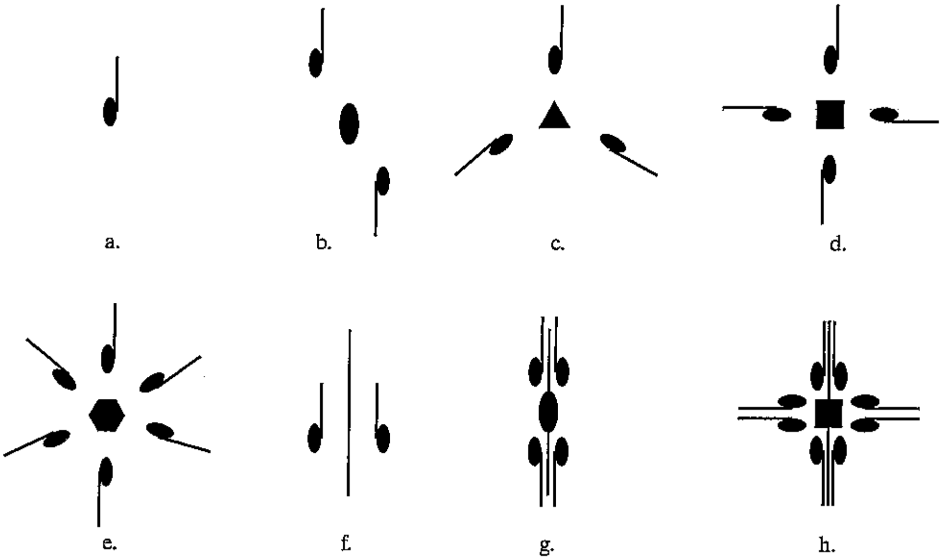


Figure 2-9 Symmetry operators for crystallography; the point group designations are in quotations. (a)-(h) are 1-fold axis "1", two-fold axis "2", three-fold axis "3", four-fold axis "4", six-fold axis "6", mirror plane "m", mirror plus two-fold axis "2m", mirror plus four-fold axis "4m", respectively.

It is important to emphasize that symmetry elements operate throughout space. The discussion thus far has concentrated on direct space, but all the principles described also apply in reciprocal space.

2-6 CRYSTAL SYSTEMS

In defining a lattice with three non-coplanar lattice vectors, units cells of various shapes can result, depending on the length and orientation of the vectors. For example, if the vectors **a**, **b**, **c** are of equal length and at right angles to one another, or **a** = **b** = **c** and $\alpha = \beta = \gamma = 90°$, the unit cell is cubic. Giving special values to the axial lengths and angles, produces unit cells of various shapes and therefore various kinds of point lattices, since the points of the lattice are located at the primitive unit cell corners. It turns out that only seven different kinds of cells are necessary to include all the possible point lattices. These correspond to the seven *crystal systems* into which all crystals can be classified. These systems are listed in Table 2-2. (Some writers consider the rhombohedral system as a subdivision of the hexagonal, thus reducing the number of crystal systems to six.)

Seven different point lattices can be obtained simply by putting points at the corners of the unit cells of the seven crystal systems. However, there are other arrangements of points which fulfill the requirements of a point lattice, namely, that each lattice point have identical surroundings. The French crystallographer Bravais worked on this problem and in 1848 demonstrated that there are fourteen possible

TABLE 2.2 CRYSTAL SYSTEMS AND BRAVAIS LATTICES

(The symbol ≠ means that equity is not required by symmetry. Accidental equality may occur, as shown by an example in Sec. 2-4.)

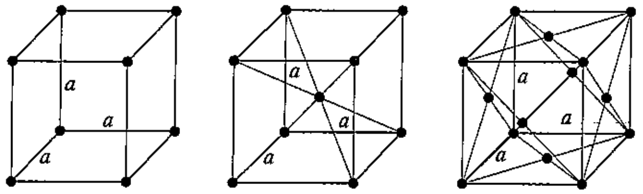
System	Axial lengths and angles	Bravais lattice	Lattice symbol
Cubic	Three equal axes at right angles $a = b = c, \quad \alpha = \beta = \gamma = 90°$	Simple Body-centered Face-centered	P I F
Tetragonal	Three axes at right angles, two equal $a = b \neq c, \quad \alpha = \beta = \gamma = 90°$	Simple Body-centered	P I
Orthorhombic	Three unequal axes at right angles $a \neq b \neq c, \quad \alpha = \beta = \gamma = 90°$	Simple Body-centered Base-centered Face-centered	P I C F
Rhombohedral*	Three equal axes, equally inclined $a = b = c, \quad \alpha = \beta = \gamma \neq 90°$	Simple	R
Hexagonal	Two equal coplanar axes at 120°, third axis at right angles $a = b \neq c, \quad \alpha = \beta = 90° \quad (\gamma = 120°)$	Simple	P
Monoclinic	Three unequal axes, one pair not at right angles $a \neq b \neq c, \quad \alpha = \gamma = 90° \neq \beta$	Simple Base-centered	P C
Triclinic	Three unequal axes, unequally inclined and none at right angles $a \neq b \neq c, \quad (\alpha \neq \beta \neq \gamma \neq 90°)$	Simple	P

* Also called trigonal.

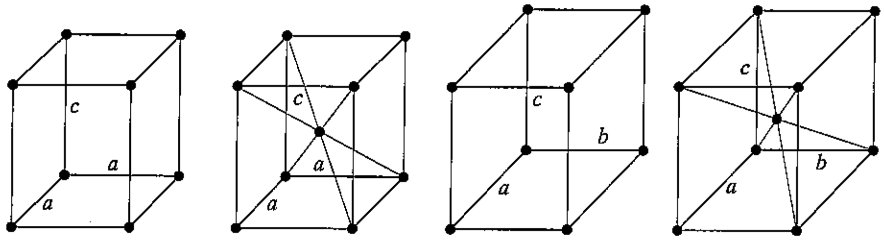
point lattices and no more [2.4]; this important result is commemorated by the use of the terms *Bravais lattice* and *point lattice* as synonymous. For example, if a point is placed at the center of each cell of a cubic point lattice, the new array of points also forms a point lattice. Similarly, another point lattice can be based on a cubic unit cell having lattice points at each corner and in the center of each face.

The fourteen Bravais lattices are described in Table 2-2 and illustrated in Fig. 2-10. Some unit cells are *simple*, or *primitive*, cells (symbol P or R), and some are *non-primitive* cells (any other symbol): primitive cells have only one lattice point per cell while nonprimitive have more than one. A lattice point in the interior of a cell "belongs" to that cell, while one in a cell face is shared by two cells and one at a corner is shared by eight. The number of lattice points per cell is therefore given by

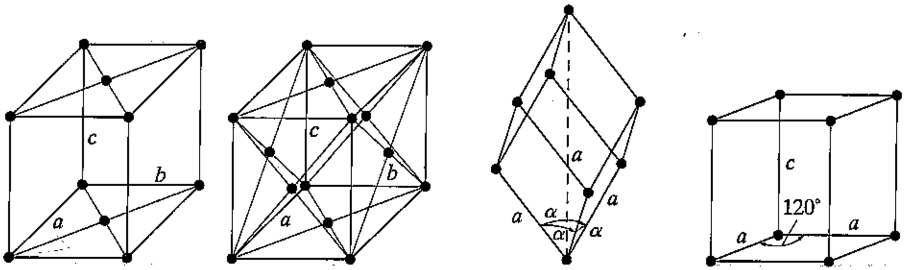
$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}, \tag{2-5}$$



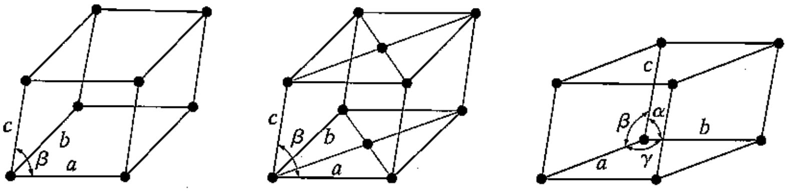
SIMPLE CUBIC (*P*) BODY-CENTERED CUBIC (*I*) FACE-CENTERED CUBIC (*F*)



SIMPLE TETRAGONAL (*P*) BODY-CENTERED TETRAGONAL (*I*) SIMPLE ORTHORHOMBIC (*P*) BODY-CENTERED ORTHORHOMBIC (*I*)



BASE-CENTERED ORTHORHOMBIC (*C*) FACE-CENTERED ORTHORHOMBIC (*F*) RHOMBOHEDRAL (*R*) HEXAGONAL (*P*)



SIMPLE MONOCLINIC (*P*) BASE-CENTERED MONOCLINIC (*C*) TRICLINIC (*P*)

Figure 2-10 The fourteen Bravais lattices.

where N_i = number of interior points, N_f = number of points on faces, and N_C = number of points on corners. Any cell containing lattice points on the corners only is therefore primitive, while one containing additional points in the interior or on faces is nonprimitive. The symbols *F* and *I* refer to face-centered and body-centered cells, respectively, while *A*, *B*, and *C* refer to base-centered cells, centered on one pair of opposite faces *A*, *B*, or *C*. (The *A* face is the face defined by the *b* and *c* axes, etc.) The symbol *R* is used especially for the rhombohedral system. In Fig. 2-10, axes of equal length in a particular system are given the same symbol to indicate their equality, e.g., the cubic axes are all marked *a*, the two equal tetragonal axes are marked *a* and the third one *c*, etc.

At first glance, the list of Bravais lattices in Table 2-2 appears incomplete. Why not, for example, a base-centered tetragonal lattice? The full lines in Fig. 2-11 delineate such a cell, centered on the *C* face, but the same array of lattice points can be referred to the simple tetragonal cell shown by dashed lines, so that the base-centered arrangement of points is not a new lattice. However, the base-centered cell is a perfectly good unit cell and may be used rather than the simple cell. Choice of one or the other has certain consequences, which are described later (Problem 4-3).

The lattice points in a nonprimitive unit cell can be extended through space by repeated applications of the unit-cell vectors a, b, c just like those of a primitive cell. The lattice points associated with a unit cell can be translated one by one or as a group. In either case, equivalent lattice points in adjacent unit cells are separated by one of the vectors **a**, **b**, **c**, wherever these points happen to be located in the cell (Fig. 2-12).

Now, the possession of a certain minimum set of symmetry elements is a fundamental property of each crystal system, and one system is distinguished from another just as much by its symmetry elements as by the values of its axial lengths

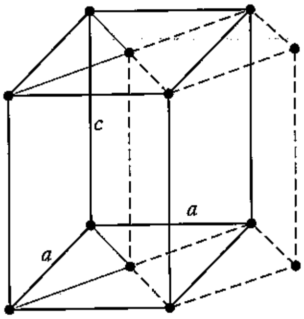


Figure 2-11 Relation of tetragonal *C* lattice (full lines) to tetragonal *P* lattice (dashed lines).

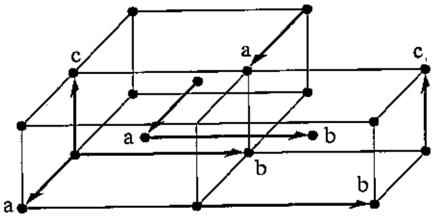


Figure 2-12 Extension of lattice points through space by the unit cell vectors **a**, **b**, **c**.

and angles. In fact, *these are interdependent.* For example, the existence of 4-fold rotation axes normal to the faces of a cubic cell *requires* that the cell edges be equal in length and at 90° to one another. On the other hand, a tetragonal cell has only one 4-fold axis, and this symmetry requires that only two cell edges be equal, namely, the two that are at right angles to the rotation axis.

The minimum number of symmetry elements possessed by each crystal system is listed in Table 2-3. Some crystals may possess more than the minimum symmetry elements required by the system to which they belong, but none may have less. The existence of certain symmetry elements often implies the existence of others. For example, a crystal with three 4-fold rotation axes necessarily has, in addition, four 3-fold axes and falls in the cubic system. The converse is not true; there are cubic lattices which do not have three four-fold axes (see the unit cell of AuBe shown in Fig. 2-23).

Symmetry operations apply not only to the unit cells shown in Fig. 2-10, considered merely as geometric shapes, but also to the point lattices associated with them. The latter condition rules out the possibility that the cubic system, for example, could include a base-centered point lattice, since such an array of points would not have the minimum set of symmetry elements required by the cubic system, namely four 3-fold rotation axes. Such a lattice would be classified in the tetragonal system, which has no 3-fold axes and in which accidental equality of the a and c axes is allowed.

Crystals in the rhombohedral (trigonal) system can be referred to either a rhombohedral or a hexagonal lattice. Appendix 4 gives the relation between these two lattices and the transformation equations which allow the Miller indices of a plane (see Sec. 2-8) to be expressed in terms of either set of axes.

2-7 PRIMITIVE AND NONPRIMITIVE CELLS

In any point lattice a unit cell may be chosen in an infinite number of ways and may contain one or more lattice points per cell. It is important to note that unit cells do not "exist" as such in a lattice: they are a mental construct and can accordingly be chosen for utility. The conventional cells shown in Fig. 2-10 are convenient and conform to the symmetry elements of the lattice.

TABLE 2.3 SYMMETRY ELEMENTS

System	Minimum symmetry elements
Cubic	Four 3-fold rotation axes
Tetragonal	One 4-fold rotation (or rotation - inversion) axis
Orthorhombic	Three perpendicular 2-fold rotation (or rotation - inversion) axes
Rhombohedral	One 3-fold rotation (or rotation - inversion) axis
Hexagonal	One 6-fold rotation (or rotation - inversion) axis
Monoclinic	One 2-fold rotation (or rotation - inversion) axis
Triclinic	None

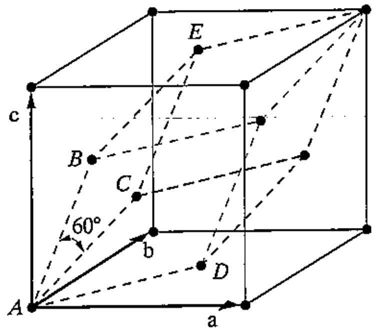


Figure 2-13 Face-centered cubic point lattice referred to cubic and rhombohedral cells.

Any of the fourteen Bravais lattices may be referred to a primitive unit cell. For example, the face-centered cubic lattice shown in Fig. 2-13 may be referred to the primitive cell indicated by dashed lines. The latter cell is rhombohedral, its axial angle α is 60°, and each of its axes is $1/\sqrt{2}$ times the length of the axes of the cubic cell. Each cubic cell has four lattice points associated with it, each rhombohedral cell has one, and the former has, correspondingly, four times the volume of the latter. Nevertheless, it is usually more convenient to use the cubic cell rather than the rhombohedral one because the former immediately suggests the cubic symmetry which the lattice actually possesses. Similarly, the other centered non-primitive cells listed in Table 2-2 are preferred to the primitive cells possible in their respective lattices.

Why then do the centered lattices appear in the list of the fourteen Bravais lattices? If the two cells in Fig. 2-13 describe the same set of lattice points, as they do, why not eliminate the cubic cell and let the rhombohedral cell serve instead? The answer is that this cell is a *particular* rhombohedral cell with an axial angle α of 60°. In the general rhombohedral lattice no restriction is placed on the angle α; the result is a lattice of points with a single 3-fold symmetry axis. When α becomes equal to 60°, the lattice has four 3-fold axes, and this symmetry places it in the cubic system. The general rhombohedral cell is still needed.

If nonprimitive lattice cells are used, the vector from the origin to any point in the lattice will now have components which are nonintegral multiples of the unit-cell vectors **a**, **b**, **c**. The position of any lattice point in a cell may be given in terms of its *coordinates*; if the vector from the origin of the unit cell to the given point has components $x\mathbf{a}$, $y\mathbf{b}$, $z\mathbf{c}$, where x, y, and z are fractions, then the coordinates of the point are $x\ y\ z$. Thus, point A in Fig. 2-13, taken as the origin, has coordinates 0 0 0 while points B, C, and D, when referred to cubic axes, have coordinates $0\,\frac{1}{2}\,\frac{1}{2}$, $\frac{1}{2}\,0\,\frac{1}{2}$, and $\frac{1}{2}\,\frac{1}{2}\,0$, respectively. Point E has coordinates $\frac{1}{2}\,\frac{1}{2}\,1$ and is equivalent to point D, being separated from it by the vector **c**. The coordinates of equivalent points in different unit cells can always be made identical by the addition or subtraction of a set of integral coördinates: in this case, subtraction of 0 0 1 from $\frac{1}{2}\,\frac{1}{2}\,1$ (the coordinates of E) gives $\frac{1}{2}\,\frac{1}{2}\,0$ (the coordinates of D).

Note that the coordinates of a body-centered point, for example, are always $\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}$ no matter whether the unit cell is cubic, tetragonal, or orthorhombic, and whatever its size. The coordinates of a point position, such as $\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}$, may also be regarded as an operator which, when "applied" to a point at the origin, will move or translate it to the position $\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}$, the final position being obtained by simple addition of the operator $\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}$ and the original position 0 0 0. In this sense, the vectors between 000 and all body-centered positions in the eight adjacent unit cells, i.e., $\langle\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}\rangle$ are called the "body-centering translations," since they will produce the two point positions characteristic of a body-centered cell when applied to a point at the origin. Similarly, the four point positions characteristic of a face-centered cell, namely, 0 0 0, $0\,\frac{1}{2}\,\frac{1}{2}$, $\frac{1}{2}\,0\,\frac{1}{2}$ and $\frac{1}{2}\,\frac{1}{2}\,0$, are related by the face-centering translations $\langle\frac{1}{2}\,\frac{1}{2}\,0\rangle$. The base-centering translations depend on which pair of opposite faces are centered; if centered on the *C* face, for example, the equivalent positions are 0 0 0, $\frac{1}{2}\,\frac{1}{2}\,0$ and the C-face centering translations are $[\frac{1}{2}\,\frac{1}{2}\,0]$ not $[0\,\frac{1}{2}\,\frac{1}{2}]$ nor $[\frac{1}{2}\,0\,\frac{1}{2}]$. These centering translations, summarized below, should be memorized:

$$\text{body–centering} = \langle\tfrac{1}{2}\,\tfrac{1}{2}\,\tfrac{1}{2}\rangle$$

$$\text{face–centering} = \langle\tfrac{1}{2}\,\tfrac{1}{2}\,0\rangle$$

$$\text{base–centering} = [\tfrac{1}{2}\,\tfrac{1}{2}\,0] \text{ or } [\tfrac{1}{2}\,0\,\tfrac{1}{2}] \text{ or } [0\,\tfrac{1}{2}\,\tfrac{1}{2}]$$

Normally one writes "000 + body-centering translation", "000 + face-centering translation" or "000 + base-centering translation" when discussing unit cells with only one atom per lattice point (i.e., Nb, Ni, Cu). Other unit cells have more than one atom per unit lattice point. Silicon, for example, has a face-centered cubic Bravais lattice with atoms at 000 and $\frac{1}{4}\,\frac{1}{4}\,\frac{1}{4}$ plus face centering translations, for a total of four lattice points but eight atoms per unit cell. More complex molecular crystals, typical of substances found in biological systems, have large numbers of atoms of different types per lattice point.

Note that the indices of a plane or direction are meaningless unless the orientation of the unit-cell axes is given. This means that the indices of a particular lattice plane depend on the unit cell chosen. For example, consider the right-hand vertical plane of the cell shown by full lines in Fig. 2-11; the indices of this plane are of the form {100} for the base-centered cell and {110} for the simple cell.

In any crystal system there are sets of equivalent lattice planes related by symmetry. These are called *planes of a form* or a *family of planes,* and the indices of any one plane, enclosed in braces {*hkl*}, stand for the whole set. In general, planes of a form have the same spacing but different Miller indices. For example, the faces of a cube, (100), (010), ($\bar{1}$00), (0$\bar{1}$0), (001), and (00$\bar{1}$), are planes of the form {100}, since all of them may be generated from any one by operation of the 4-fold rotation axes perpendicular to the cube faces. In the tetragonal system, however, only the planes (100), (010), ($\bar{1}$00), and (0$\bar{1}$0) belong to the form {100}; the other two planes, (001) and $(00\bar{1})$, belong to the different form $\{001\}$; the first four planes mentioned are related by a 4-fold axis and the last two by a 2-fold axis.[5]

Planes of a zone are planes which are all parallel to one line, called the *zone axis*, and the zone, i.e., the set of planes, is specified by giving the indices of the zone axis. Such planes may have quite different indices and spacings, the only requirement being that they are parallel to a single line. Figure 2-14 shows some examples. If the axis of a zone has indices $[uvw]$, then any plane belongs to that zone whose indices (hkl) satisfy the relation

$$hu + kv + lw = 0. \tag{2-6}$$

(A proof of this relation is given in Sec. 3 of Appendix.) Any two nonparallel planes are planes of a zone since they are both parallel to their line of intersection. If their indices are $(h_1k_1l_1)$ and $(h_2k_2l_2)$, then the indices of their zone axis $[uvw]$ are given by $[h_1k_1l_1] \times [h_2k_2l_2]$, that is,

$$\begin{aligned} u &= k_1l_2 - k_2l_1, \\ v &= l_1h_2 - l_2h_1, \\ w &= h_1k_2 - h_2k_1. \end{aligned} \tag{2-7}$$

Before turning to the special system of indexing for hexagonal crystal systems, it is important to revisit the topic of interplanar spacings d_{hkl} for $\{hkl\}$. The exact relation depends on the crystal system involved and for the cubic system takes on the relatively simple form

$$\text{(Cubic)} \qquad d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}. \tag{2-8}$$

In the tetragonal system the spacing equation naturally involves both a and c since these are not generally equal:

$$\text{(Tetragonal)}\ d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2(a^2/c^2)}}. \tag{2-9}$$

Interplanar spacing equations for all systems are given in Appendix 3. In the cubic system, it is important to remember that $[hkl]$ is perpendicular to (hkl). It is equally important never to forget that for all other crystal systems $[hkl]$ generally is not perpendicular to (hkl).

---

[5] Certain important crystal planes are often referred to by name without any mention of their Miller indices. Thus, planes of the form $\{111\}$ in the cubic system are often called octahedral planes, since these are the bounding planes of an octahedron. In the hexagonal system, the (0001) plane is called the basal plane, planes of the form $\{10\bar{1}0\}$ are called prismatic planes, and planes of the form $\{10\bar{1}1\}$ are called pyramidal planes.

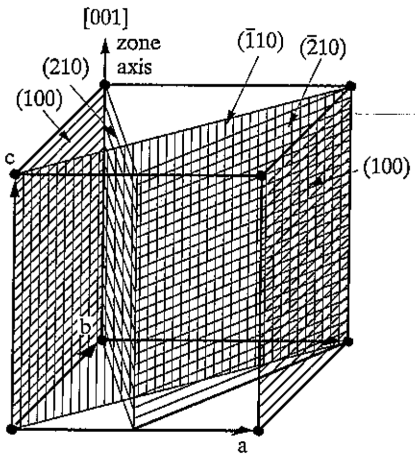


Figure 2-14 All shaded planes in the cubic lattice shown are planes of the zone {001}.

2-8 INDEXING IN THE HEXAGONAL SYSTEM

A slightly different system of plane indexing is used in the hexagonal system. The unit cell of a hexagonal lattice is defined by two equal and coplanar vectors $\mathbf{a}_1$ and $\mathbf{a}_2$, at 120° to one another, and a third axis **c** at right angles [Fig. 2-15(a)]. The complete lattice is constructed, as usual, by repeated translations of the points at the unit cell corners by the vectors $\mathbf{a}_1$, $\mathbf{a}_2$, **c**. Some of the points so generated are shown in the figure, at the ends of dashed lines, in order to exhibit the hexagonal symmetry of the lattice, which has a 6-fold rotation axis parallel to **c**. The third axis $\mathbf{a}_3$, lying in the basal plane of the hexagonal prism, is so symmetrically related to $\mathbf{a}_1$ and $\mathbf{a}_2$

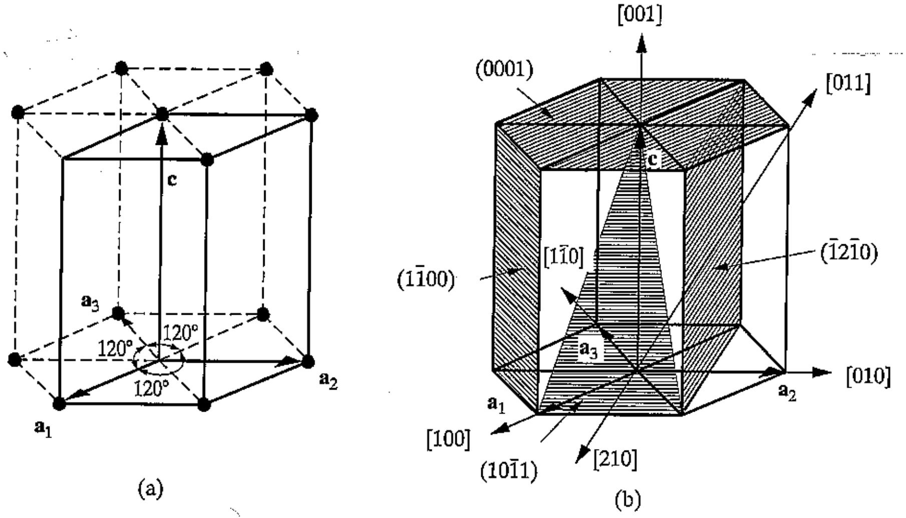


Figure 2-15 (a) The hexagonal unit cell (heavy lines) and (b) indices of planes and directions.

that it is often used in conjunction with the other two. Thus the indices of a plane in the hexagonal system, called Miller-Bravais indices, refer to *four* axes and are written $(hkil)$. The index i is the reciprocal of the fractional intercept on the $\mathbf{a}_3$ axis. Since the intercepts of a plane on $\mathbf{a}_1$ and $\mathbf{a}_2$ determine its intercept on $\mathbf{a}_3$, the value of i depends on the values of h and k. The relation is

$$h + k = -i. \tag{2-10}$$

Since i is determined by h and k, it is sometimes replaced by a dot and the plane symbol written $(hk \cdot l)$ Sometimes even the dot is omitted. However, this usage defeats the purpose for which Miller-Bravais indices were devised, namely, to give similar indices to similar planes. For example, the side planes of the hexagonal prism in Fig. 2-15(b) are all similar and symmetrically located, and their relationship is clearly shown in their full Miller-Bravais symbols: $(10\bar{1}0)$, $(01\bar{1}0)$, $(\bar{1}100)$, $(\bar{1}010)$, $(0\bar{1}10)$, $(1\bar{1}00)$. On the other hand, the abbreviated symbols of these planes, $(10 \cdot 0)$, $(01 \cdot 0)$, $(\bar{1}1 \cdot 0)$, $(\bar{1}0 \cdot 0)$, $(0\bar{1} \cdot 0)$, $(1\bar{1} \cdot 0)$ do not immediately suggest this relationship.

Directions in a hexagonal lattice are best expressed in terms of the *three* basic vectors $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{c}$. Figure 2-15(b) shows several examples of both plane and direction indices. Another system, involving four indices, is sometimes used to designate directions. The required direction is broken up into four component vectors, parallel to $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$, and $\mathbf{c}$ and so chosen that the third index is the negative of the sum of the first two. Then, if $[UVW]$ are the indices of a direction referred to three axes and $[uvtw]$ the four-axis indices, the two are related as follows:

$$\begin{aligned}
U &= u - t & u &= (2U - V)/3 \\
V &= v - t & v &= (2V - U)/3 \\
W &= w & t &= -(u + v) = -(U + V)/3 \\
& & w &= W.
\end{aligned} \tag{2-11}$$

Thus, $[100]$ becomes $[2\bar{1}\bar{1}0]$, $[210]$ becomes $[10\bar{1}0]$, etc.

2-9 CRYSTAL STRUCTURE

So far discussion focused on topics from the field of *mathematical (geometrical) crystallography* and barely acknowledged actual crystals and the atoms of which they are composed. In fact, all of the above was well known long before the discovery of x-ray diffraction, i.e., long before there was any certain knowledge of the interior arrangements of atoms in crystals.

It is now time to describe the structure of some actual crystals and to relate this structure to the point lattices, crystal systems, and symmetry elements discussed above. The cardinal principle of crystal structure is that *the atoms of a crystal are set in space in some fixed relation to the points of a Bravais lattice.* It follows from this that the atoms of a crystal will be arranged periodically in three dimensions and that this arrangement of atoms will exhibit many of the properties of a Bravais lattice, in particular many of its symmetry elements.

The features associated with each lattice point are termed the *basis* of the lattice, and this applies to one- and two-dimensional lattices as well as three-dimensional crystal structures. Figure 2-16 shows three different bases for a one-dimensional lattice; the vertical dashed lines mark the end of the unit cells. The basis for lattice (b) is a single dot-dash, with the dot to the right of the dash, that for (c) is a dash-dot dot-dash combination and that for (d) is a dash-dot dash-dot combination. The symmetry in Fig. 2-16(c) can be represented by mirrors (solid vertical lines in the figure) or by 2-fold rotation axes perpendicular to the page. Note that the mirror at "O" (or the 2-fold axis at "O" in the alternate version) acts throughout the entire one-dimensional space: the features at A and B appear at A' and B'.

The term *space group* defines the entire spatial arrangement of a crystal system, that is, translation (i.e., the vectors which define the size and shape of the unit cell)

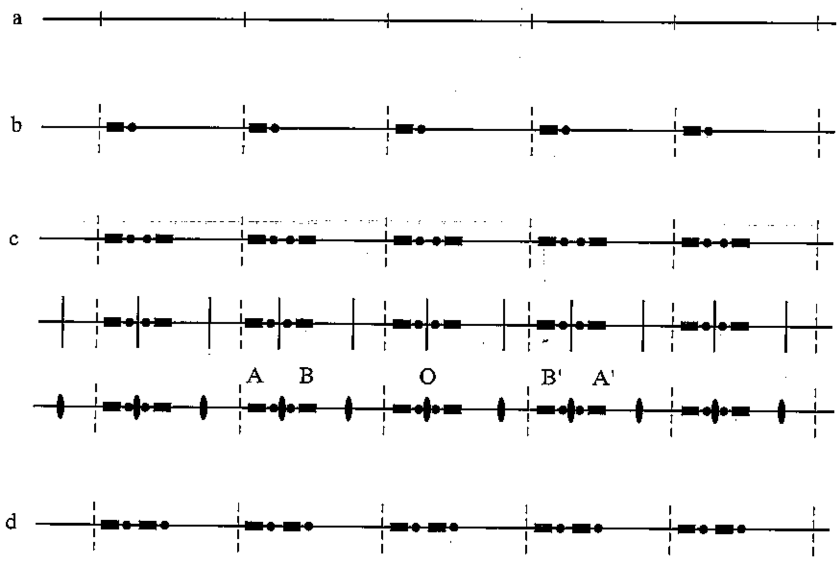


Figure 2-16 (a) One dimensional lattice with unit cells marked by vertical bars. (b) One-dimensional lattice populated with a "dash-dot" motif and showing one-fold symmetry. The borders of the unit cells are indicated by the vertical dashed lines. (c) Three representations of the same one-dimensional lattice populated with the dash-dot motif. The top line shows only the dash-dot motifs and unit cell boundaries. The middle lattice shows where mirror planes occur in the lattice (vertical bars) while the bottom lattice includes two-fold axes. (d) One-dimensional lattice with a basis consisting of two dash-dot motifs.

combined with the symmetry elements acting through a point (i.e., the point group) specify the space group. There are two point groups and two space groups for one-dimensional lattices, 17 space groups in two-dimensions and 230 unique space groups in three-dimensions. Thus, the combination of symmetry elements with different lattice types (not all symmetry element combinations nor lattice types have been covered here, see [G.3-G.6] for more details) dictate that three-dimensional crystals cannot have any atomic arrangement, only one of the 230 possibilities cataloged in Volume A of the International Tables for Crystallography [G.1]. Instead, different crystals have different bases ranging from single atoms to thousands or millions of atoms.

The simplest crystals imaginable are those formed by placing atoms of the same kind *on* the points of a Bravais lattice. Not all such crystals exist but many metals crystallize in this simple fashion, and Fig. 2-17 shows two common metal structures based on the body-centered cubic (BCC) and face-centered cubic (FCC) lattices. The former has two atoms per unit cell and the latter four.

The next degree of complexity is encountered when two or more atoms of the same kind are "associated with" each point of a Bravais lattice, as exemplified by the hexagonal close-packed (HCP) structure common to many metals. This structure is simple hexagonal and is illustrated in Fig. 2-18. There are two atoms per unit cell, as shown in (a), one at 0 0 0 and the other at $\frac{2}{3}\frac{1}{3}\frac{1}{2}$ (or at $\frac{1}{3}\frac{2}{3}\frac{1}{2}$, which is an equivalent position). Figure 2-18(b) shows the same structure with the origin of the unit cell shifted so that the point 1 0 0 in the new cell is midway between the atoms at 100 and $\frac{2}{3}\frac{1}{3}\frac{1}{2}$ in (a), the nine atoms shown in (a) corresponding to the nine atoms marked with an X in (b). The "association" of pairs of atoms with the points of a simple hexagonal Bravais lattice is suggested by the dashed lines in (b). Note, however, that the atoms of a close-packed hexagonal structure do not themselves form a point lattice, the surroundings of an atom at 000 being different from those of an atom at $\frac{2}{3}\frac{1}{3}\frac{1}{2}$. Figure 2-18 (c) shows still another representation of the HCP structure: the three atoms in the interior of the hexagonal prism are directly above the centers of alternate triangles in the base and, if repeated through space by the vectors $\mathbf{a}_1$ and $\mathbf{a}_2$, would also form a hexagonal array just like the atoms in the layers above and below.

The HCP structure is so called because it is one of the two ways in which spheres can be packed together in space with the greatest possible density and still have a periodic arrangement. Such an arrangement of spheres in contact is shown in Fig. 2-18(d) and appears to have first been noted by Kepler [2.5], who is better known

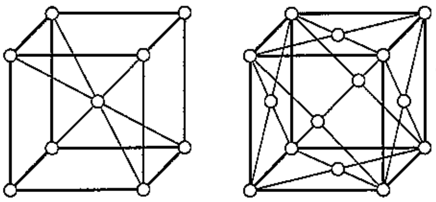
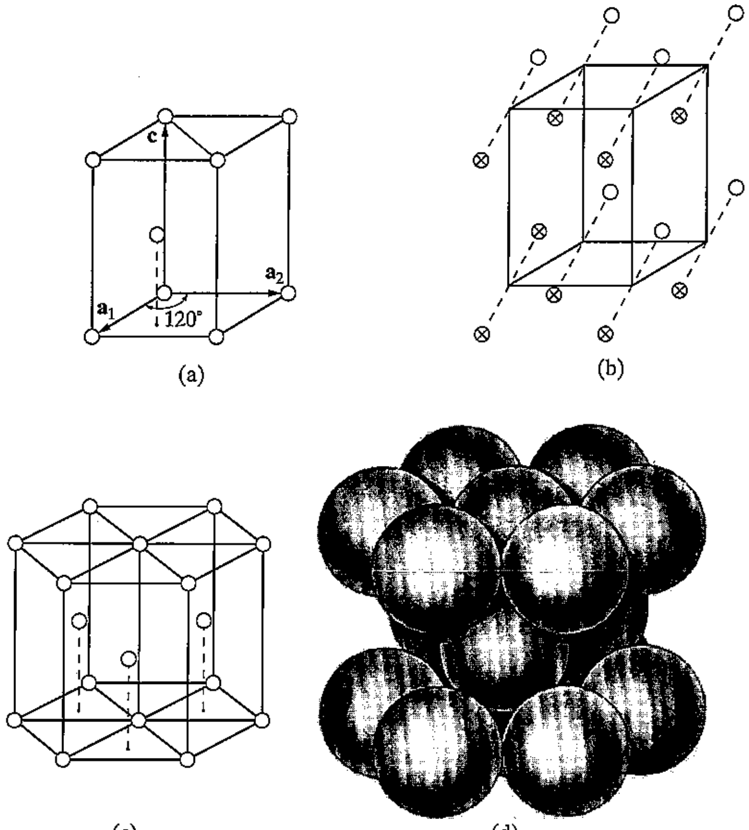

BCC FCC

Figure 2-17 Structures of some common metals. Body-centered cubic: α-Fe, Cr, Mo, V, etc.: face-centered cubic: γ-Fe, Cu, Pb, Ni, etc.

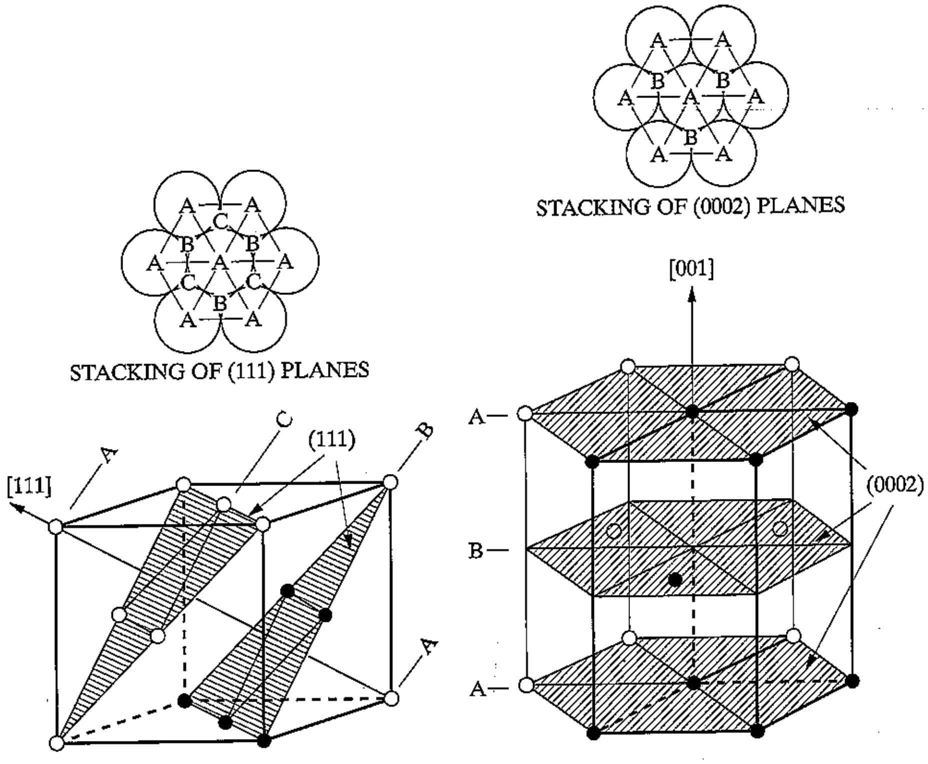


(a) (b) (c) (d)

Figure 2-18 The hexagonal close-packed structure, shared by Zn, Mg, Be, αTi, etc.

for his work in astronomy. If these spheres are regarded as atoms, then the resulting picture of an HCP metal is much closer to physical reality than is the relatively open structure suggested by the drawing of Fig. 2-18(c), and this is true, generally, of all crystals. On the other hand, it may be shown that the ratio of c to a in an HCP structure formed of spheres in contact is 1.633 whereas the c/a ratio of metals having this structure varies from about 1.58 (Be) to 1.89 (Cd). As there is no reason to suppose that the atoms in these crystals are not in contact, it follows that they must be ellipsoidal in shape rather than spherical.

The FCC structure is an equally close-packed arrangement. Its relation to the HCP structure is not immediately obvious, but Fig. 2-19 shows that the atoms on the (111) planes of the FCC structure are arranged in a hexagonal pattern just like the atoms on the (0002) planes of the HCP structure. The only difference between the two structures is the way in which these hexagonal sheets of atoms are arranged above one another. In an HCP metal, the atoms in the second layer are above the hollows in the first layer and the atoms in the third layer are above the atoms in the



FACE-CENTERED CUBIC

HEXAGONAL CLOSE-PACKED

Figure 2-19 Comparison of FCC and HCP structures. The black atoms in the FCC drawing delineate half a hexagon, which is completed on the same plane extended into the next unit cell below (not shown).

first layer, so that the layer stacking sequence can be summarized as *A B A B A B* .... The first two atom layers of an FCC metal are put down in the same way, but the atoms of the third layer are so placed in the hollows of the second layer that not until the fourth layer does a position repeat. FCC stacking therefore has the sequence *A B C A B C* ... . These stacking schemes are indicated in the plan views shown in Fig. 2-19.

Another example of the "association" of more than one atom with each point of a Bravais lattice is given by uranium. The structure of the form stable at room temperature, α-uranium, is illustrated in Fig. 2-20 by plan and elevation drawings. In such drawings, the height, of an atom (expressed as a fraction of the axial length) above the plane of the drawing (which includes the origin of the unit cell and two of the cell axes) is given by the numbers marked on each atom. The Bravais lattice is base-centered orthorhombic, centered on the C face, and Fig. 2-20 shows how the atoms occur in pairs through the structure, each pair associated with a lattice point. There are four atoms per unit cell, located at $0\,y\,\frac{1}{4}$, $0\,\bar{y}\,\frac{3}{4}$, $\frac{1}{2}(\frac{1}{2}+y)\frac{1}{4}$, and $\frac{1}{2}(\frac{1}{2}-y)\frac{3}{4}$.

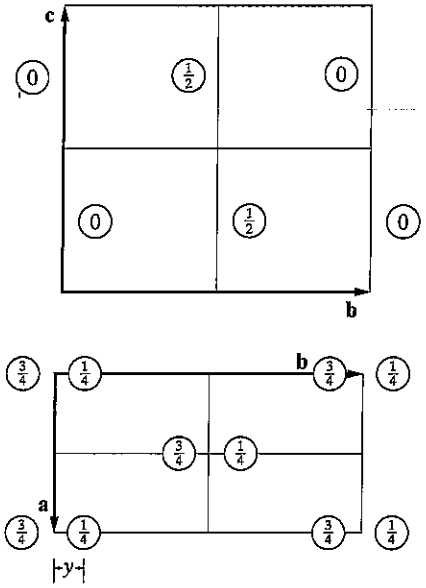


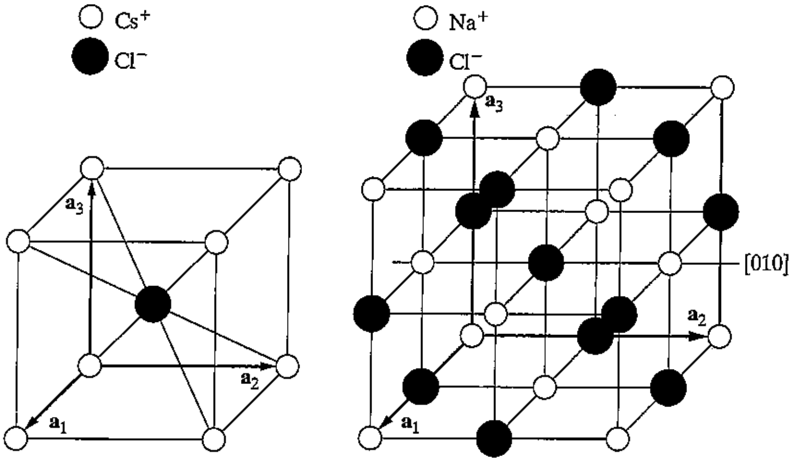
Figure 2-20 The structure of α-uranium, after Jacob and Warren [2.6].

Here is an example of a variable parameter y in the atomic coordinates. Crystals often contain such variable parameters, which may have any fractional value without destroying any of the symmetry elements of the structure. A quite different substance might have exactly the same structure as uranium except for slightly different values of a, b, c, and y. For uranium y is 0.105 ± 0.005.

Turning to the crystal structure of *compounds* of unlike atoms, structures are built on the skeleton of a Bravais lattice but that certain other rules must be obeyed, precisely because there are unlike atoms present. Consider, for example, a crystal of A_xB_y which might be an ordinary chemical compound, an intermediate phase of relatively fixed composition in some alloy system, or an ordered solid solution. Then the arrangement of atoms in A_xB_y must satisfy the following conditions:

1. Body-, face-, or base-centering translations, if present, must begin and end on atoms of the same kind. For example, if the structure is based on a body-centered Bravais lattice, then it must be possible to go from an A atom, say, to *another* A atom by the translation $\frac{1}{2}\frac{1}{2}\frac{1}{2}$
2. The set of A atoms in the crystal and the set of B atoms must separately possess the same symmetry elements as the crystal as a whole, since in fact they make up the crystal. In particular, the operation of any symmetry element present must bring a given atom, A for example, into coincidence with another atom of the same kind, namely A.

Consider the structures of a few common crystals in light of the above requirements. Figure 2-21 illustrates the unit cells of two ionic compounds, CsCl and NaCl. These structures, both cubic, are common to many other crystals and, wherever they



(a) CsCl (b) NaCl

Figure 2-21 The structures of (a) CsCl (common to CsBr, NiAl, ordered β-brass, ordered CuPd, etc.) and (b) NaCl (common to KCl, CaSe, PbTe, etc.).

occur, are referred to as the "CsCl structure" and the "NaCl structure." In considering a crystal structure, one of the most important things to determine is its Bravais lattice, since that is the basic framework on which the crystal is built and because, as Chap. 4 demonstrates, it has a profound effect on the way in which that crystal diffracts x-rays.

What is the Bravais lattice of CsCl? Figure 2-21 (a) shows that the unit cell contains two atoms, ions really, since this compound is completely ionized even in the solid state: a cesium ion at 000 and a chlorine ion at $\frac{1}{2}\frac{1}{2}\frac{1}{2}$. The Bravais lattice is obviously not face-centered, but the body-centering translation $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ connects two atoms. However, these are unlike atoms and the lattice is therefore *not* body-centered. It is, by elimination, simple cubic. If one wishes, one may think of both ions, the cesium at 000 and the chlorine at $\frac{1}{2}\frac{1}{2}\frac{1}{2}$, as being associated with the lattice point at 0 0 0. It is not possible, however, to associate any one cesium ion with any particular chlorine ion and refer to them as a CsCl molecule; the term "molecule" therefore has no real physical significance in such a crystal, and the same is true of most inorganic compounds and alloys.

Close inspection of Fig. 2-21(b) will show that the unit cell of NaCl contains 8 ions, located as follows:

$$4\ \text{Na}^+\ \text{at}\quad 0\ 0\ 0,\quad \tfrac{1}{2}\ \tfrac{1}{2}\ 0,\quad \tfrac{1}{2}\ 0\ \tfrac{1}{2},\quad \text{and}\quad 0\ \tfrac{1}{2}\ \tfrac{1}{2};$$

$$4\ \text{Cl}^-\ \text{at}\quad \tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2},\quad 0\ 0\ \tfrac{1}{2},\quad 0\ \tfrac{1}{2}\ 0,\quad \text{and}\quad \tfrac{1}{2}\ 0\ 0$$

The sodium ions are clearly face-centered, and the face-centering translations [000] and $\langle\frac{1}{2}\frac{1}{2}\frac{1}{2}\rangle$, when applied to the chlorine ion at $\frac{1}{2}\frac{1}{2}\frac{1}{2}$, will reproduce all the chlorine-ion positions. The Bravais lattice of NaCl is therefore face-centered cubic. The ion positions, incidentally, may be written in summary form as:

$$4 \quad \text{Na}^+ \quad \text{at} \quad 0\ 0\ 0 \quad + \quad \text{face–centering translations.}$$

$$4 \quad \text{Cl}^- \quad \text{at} \quad \tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2} \quad + \quad \text{face–centering translations.}$$

Note also that in these, as in all other structures, the operation of any symmetry element possessed by the lattice must bring similar atoms or ions into coincidence. For example, in Fig. 2-21(b), 90° rotation about the 4-fold [010] rotation axis shown brings the chlorine ion at $0\ 1\ \frac{1}{2}$ into coincidence with the chlorine ion at $\frac{1}{2}\ 1\ 1$, the sodium ion at 0 1 1 with the sodium ion at 1 1 1, etc

Elements and compounds often have closely similar structures. Figure 2-22 shows the unit cells of diamond and the zinc-blende form of ZnS. Both are face-centered cubic. Diamond has 8 atoms per unit cell, located at

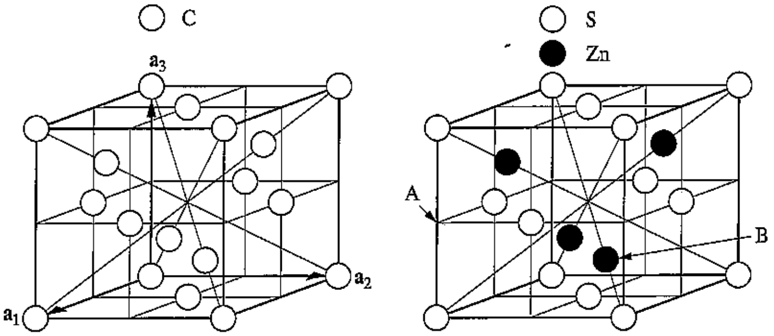
$$0\ 0\ 0 \quad + \quad \text{face–centering translations.}$$

$$\tfrac{1}{4}\ \tfrac{1}{4}\ \tfrac{1}{4} \quad + \quad \text{face–centering translations.}$$

In other words, a "molecule" of two atoms is associated with each of the face-centered lattice points. The atom positions in zinc blende are identical with these, but the first set of positions is now occupied by one kind of atom (S) and the other by a different kind (Zn).

Note that diamond and a metal like copper have quite dissimilar structures, although both are based on a face-centered cubic Bravais lattice. To distinguish between these two, the terms "diamond cubic" and "face-centered cubic" are usually used. The industrially important semiconductor, silicon has the diamond cubic structure.

Instead of referring to a structure by name, such as the "NaCl structure," one can use the designations introduced years ago in *Strukturbericht* [G.8]. These consist of



(a) Diamond (b) Zinc blend

Figure 2-22 The structures of (a) diamond (common to Si, Ge, and gray Sn) and (b) the zinc-blende form of ZnS (common to HgS, CuI, AlSb, BeSe, etc.).

a letter and a number: the letter A indicates an element, B an AB compound, C an AB_2 compound, etc. The structure of copper, for example, is called the A1 structure, α–Fe is A2, zinc is A3, diamond is A4, NaCl is B1, etc. A full list is given by Pearson [G.9, Vol. 1, p. 85].

Some rather complex crystals can be built on a cubic lattice. For example, the ferrites, which are magnetic and are used in recording tapes, computer floppy disks and in hard drives, have the formula $MO \cdot Fe_2O_3$, where M is a divalent metal ion like Mn, Ni, Fe, Co, etc. Their structure is related to that of the mineral spinel. The Bravais lattice of the ferrites is face-centered cubic, and the unit cell contains 8 "molecules" or a total of $8 \times 7 = 56$ ions. There are therefore 56/4 or 14 ions associated with each lattice point.

The number of atoms per unit cell in any crystal is partially dependent on its Bravais lattice. For example, the number of atoms per unit cell in a crystal based on a body-centered lattice must be a multiple of 2, since there must be, for any atom in the cell, a corresponding atom of the same kind at a translation of $\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}$ from the first. The number of atoms per cell in a base-centered lattice must also be a multiple of 2, as a result of the base-centering translations. Similarly, the number of atoms per cell in a face-centered lattice must be a multiple of 4.

The reverse of these propositions is not true. It would be a mistake to assume, for example, that if the number of atoms per cell is a multiple of 4, then the lattice is necessarily face-centered. The unit cell of the intermediate phase AuBe, for example (Fig. 2-23), contains 8 atoms and yet it is based on a simple cubic Bravais lattice. The atoms are located as follows:

4 Au at

$$u\;\;u\;\;u,\quad (\tfrac{1}{2}+u)(\tfrac{1}{2}-u)\bar{u},\quad \bar{u}(\tfrac{1}{2}+u)(\tfrac{1}{2}-u),\quad (\tfrac{1}{2}-u)\bar{u}(\tfrac{1}{2}+u),$$

4 Be at

$$w\;\;w\;\;w,\quad (\tfrac{1}{2}+w)(\tfrac{1}{2}-w)\bar{w},\quad \bar{w}(\tfrac{1}{2}+w)(\tfrac{1}{2}-w),\quad (\tfrac{1}{2}-w)\bar{w}(\tfrac{1}{2}+w),$$

where $u = 0.100$ and $w = 0.406$, each ± 0.005. If the parameter u is put equal to zero, the atomic coordinates of the gold atoms become those of a face-centered cubic cell. The structure of AuBe may therefore be regarded as distorted face-centered cubic, in which the presence of the beryllium atoms has forced the gold atoms out of their original positions by a distance $\pm u$, $\pm u$, $\pm u$. These translations are all in directions of the form <111>, i.e., parallel to body diagonals of the cube, and are shown as dotted lines in Fig. 2-23. The three-fold axes characteristic of cubic Bravais lattices remain, but four-fold axes are not present due to the distortion. Thus, this structure is an example of a cubic crystal system without set of three perpendicular four-fold axes.

It should now be apparent that the term "simple," when applied to a Bravais lattice, is used in a very special, technical sense and that some very complex structures can be built up on a "simple" lattice. In fact, they may contain more than a hundred atoms per unit cell. The only workable definition of a simple lattice is a negative

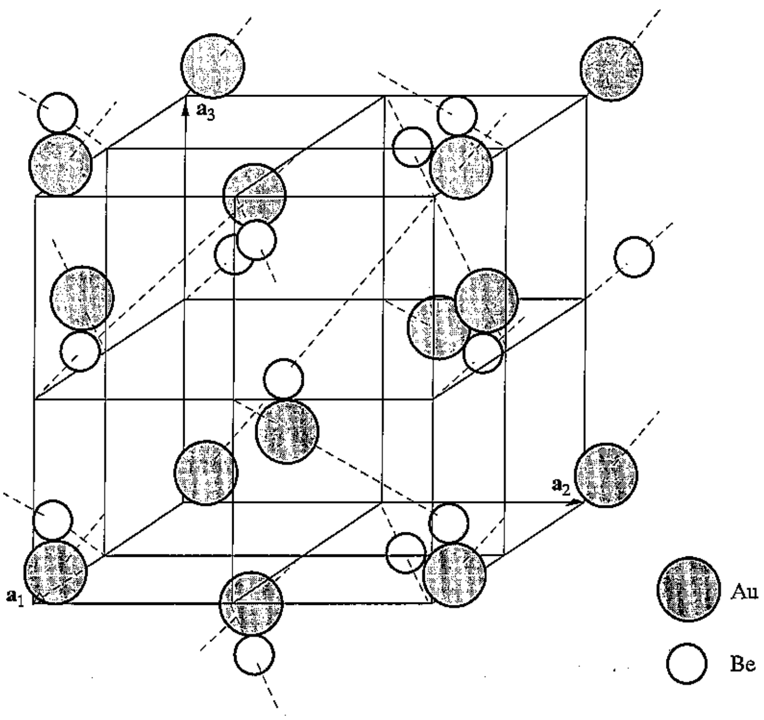
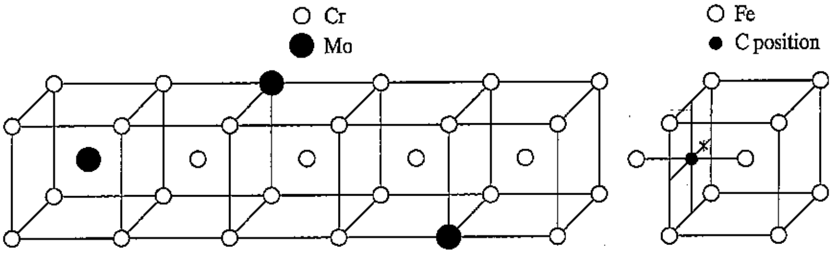


Figure 2-23 The structure of AuBe, shared by FeSi, NiSi, CoSi, MnSi, etc. It is known as the FeSi structure [2.7].

one: a given lattice is simple if it is neither body-, base-, nor face-centered; these latter possibilities can be ruled out by showing that the set of atomic positions does not contain the body-, base-, or face-centering translations. There is no rule governing the allowable number of atoms per cell in a simple lattice: this number may take on any one of the values 1, 2, 3, 4, 5, etc., although not in every crystal system and not every higher integer is permitted. Incidentally, not every theoretical possibility known to mathematical crystallography is realized in nature; for example, no known element crystallizes with a simple hexagonal lattice containing one atom per unit cell.

There is another way of arranging unlike atoms on a point lattice besides those considered so far and that is exemplified by the structure of *solid solutions*. These solutions are of two types, substitutional and interstitial; in the former, solute atoms substitute for, or replace, solvent atoms on the lattice of the solvent, while in the latter, solute atoms fit into the interstices of the solvent lattice. The interesting feature of these structures is that the solute atoms are distributed more or less at random. For example, consider a 10 atomic percent solution of molybdenum in chromium, which has a BCC structure. The molybdenum atoms can occupy either the corner or body-centered positions of the cube in a random, irregular manner, and a small portion of the crystal might have the appearance of Fig. 2-24(a). Five adjoining unit



(a) (b)

Figure 2-24 Structure of solid solutions: (a) Mo in Cr (substitutional); (b) C in α-Fe (interstitial).

cells are shown there, with a total of 29 atoms, 3 of which are molybdenum. This section of the crystal therefore contains somewhat more than 10 atomic percent molybdenum, but the next five cells would probably contain somewhat less. Such a structure does not obey the ordinary rules of crystallography: for example, the right-hand cell of the group shown does not have cubic symmetry, and one finds throughout the structure that the translation given by one of the unit cell vectors may begin on an atom of one kind and end on an atom of another kind. All that can be said of this structure is that it is BCC *on the average*, and experimentally it displays the x-ray diffraction effects proper to a BCC lattice. This is not surprising since the x-ray beam used to examine the crystal is so large compared to the size of a unit cell that it observes, so to speak, millions of unit cells at the same time and so obtains only an average "picture" of the structure.

The above remarks apply equally well to interstitial solid solutions. These form whenever the solute atom is small enough to fit into the solvent lattice without causing too much distortion. Ferrite, the solid solution of carbon in α–iron, is a good example.[6] In the unit cell shown in Fig. 2-24(b), there are two kinds of "holes" in the lattice: one at $\frac{1}{2}0\frac{1}{2}$ (marked ●) and equivalent positions in the centers of the cube faces and edges, and one at $\frac{1}{4}0\frac{1}{2}$ (marked ×) and equivalent positions. All the evidence at hand points to the fact that the carbon atoms in ferrite are located in the holes at $\frac{1}{2}0\frac{1}{2}$ and equivalent positions. On the average, however, no more than about 1 of these positions in 500 unit cells is occupied, since the maximum solubility of carbon in ferrite is only about 0.1 atomic percent.

Still another type of structure worth noting is that of *ordered solid solutions*. As described above, a typical substitutional solid solution has solute atoms distributed more or less at random on the lattice points of the solvent.[7] On the other hand, there are solutions in which this is true only at elevated temperatures; when cooled

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[6] Note the double meaning of the word *ferrite*: (1) metallurgical, for the metallic solid solution mentioned above, and (2) ceramic or mineralogical, for the oxide MO · Fe_2O_3 previously described.

[7] Of course, when the solution becomes concentrated, there is no real distinction between "solvent" and "solute." There is only one lattice, with two or more kinds of atoms distributed on it.

to lower temperatures, the solute atoms take up an orderly, periodic arrangement while still remaining on the lattice points of the solvent. The solid solution is then said to be *ordered* and to possess a *superlattice*. The alloy $AuCu_3$ is a classic example: at high temperatures the copper and gold atoms are located more or less at random on face-centered cubic lattice sites, while at low temperature the gold atoms occupy only the cube corner positions and the copper atoms only the face-centered positions. In its temperature range of stability then, an ordered solid solution resembles a chemical compound, with atoms of one kind on one set of lattice sites and atoms of a different kind on another set. But an ordered solid solution is a "half-hearted compound" because, when heated, it disorders before it melts; a real compound, like NaCl, remains ordered right up to the melting point. Crystallographically, the structures of the disordered and ordered solid solutions are quite different; disordered $AuCu_3$ is, on the average, face-centered cubic while the ordered form is simple cubic. Such structures will be discussed more fully in Chap. 10.

2-10 ATOM SIZES AND COORDINATION

When two or more unlike atoms unite to form a chemical compound, intermediate phase, or solid solution, the kind of structure formed is dependent, in part, on the relative sizes of the atoms involved. But what is meant by the size of an atom? To regard an atom as something like a billiard ball with a sharply defined bounding surface is surely an oversimplification, since electron density decreases gradually at the "surface" of the atom and that there is a small but finite probability of finding an electron at quite large distances from the nucleus. One, not entirely satisfactory, way of defining atomic size lies in considering a crystal as a collection of rigid spheres in contact. The size of an atom, then, is given by the distance of closest approach of atom centers in a crystal of the element, and this distance can be calculated from the lattice parameters.

For example, the lattice parameter a of α–iron is 2.87 Å, and in a BCC lattice the atoms are in contact only along the diagonals of the unit cube. The diameter of an iron atom is therefore equal to one half the length of the cube diagonal, or $(\sqrt{3}/2)a = 2.48\text{Å}$. The following formulas give the distance of closest approach in the three common structures:

$$\text{BCC} = \frac{\sqrt{3}}{2}a,$$

$$\text{FCC} = \frac{\sqrt{2}}{2}\text{a},$$

$$\text{HCP} = a \quad \text{(between atoms in basal plane)},$$

$$= \sqrt{\frac{a^2}{3} + \frac{c^2}{4}} \left(\begin{array}{c} \text{between atom in basal plan} \\ \text{and neighbors above or below} \end{array} \right) \qquad (2\text{-}12)$$

Values of the distance of closest approach, together with the crystal structures and lattice parameters of the elements, are tabulated in Appendix 5.

To a first approximation, the size of an atom is a constant. In other words, an iron atom has about the same size whether it occurs in pure iron, an intermediate phase, or a solid solution. This is a very useful fact to remember when investigating unknown crystal structures, for it enables prediction of roughly how large a hole is necessary in a proposed structure to accommodate a given atom. More precisely, it is known that the size of an atom has a slight dependence on its *coordination number*, which is the number of nearest neighbors of the given atom and which depends on crystal structure. The coordination number of an atom in the FCC or HCP structures is 12, in BCC 8, and diamond cubic 4. The smaller the coordination number, the smaller the volume occupied by a given atom, and the approximate amount of contraction to be expected with decrease in coordination number is found to be:

Change in coordination	Size contraction, percent
12→8	3
12→6	3
12→4	12

This means, for example, that the diameter of an iron atom is greater if the iron is dissolved in FCC copper than if it exists in a crystal of BCC α-iron or is dissolved in BCC vanadium. If it were dissolved in copper, its diameter would be approximately 2.48/0.97, or 2.56 Å.

The size of an atom in a crystal also depends on whether its binding is ionic, covalent, metallic, or van der Waals, and on its state of ionization. The more electrons are removed from a neutral atom the smaller it becomes, as shown strikingly for iron, whose atoms and ions Fe, Fe^{++}, Fe^{+++} have diameters of 2.48, 1.66, and 1.34 Å, respectively.

The spatial arrangement of atoms about a given point is often described by words such as *octahedral* and *tetrahedral*. For example, in the NaCl structure of Fig. 2-21(b) the central Cl^- ion at $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ is said to be octahedrally surrounded by Na^+ ions, because the six Na^+ ions in the face-centered positions lie on the corners of an octahedron, a solid bounded by eight triangular sides. In the zinc blende structure of Fig. 2-22(b) the empty position marked *A* is octahedrally surrounded by sulphur atoms, of which only four are in the cell shown, and would be referred to as an octahedral hole in the structure. This group of atoms is shown separately in Fig. 2-25. In the same structure the Zn atom at $\frac{1}{4}\frac{1}{4}\frac{1}{4}$, marked *B* in Fig. 2-22(b), is surrounded by four S atoms at the corners of a tetrahedron, a solid bounded by four triangular sides (Fig. 2-25). In fact, all four of the Zn atoms in the unit cell have tetrahedral S surroundings. Also in the ZnS structure the reader can demonstrate, by sketching three cells adjacent to the one shown, that the hole at *A* is tetrahedrally surrounded by Zn atoms. Thus, the hole at *A* has both octahedral (s) and tetrahedral (Zn) surroundings, an unusual circumstance.

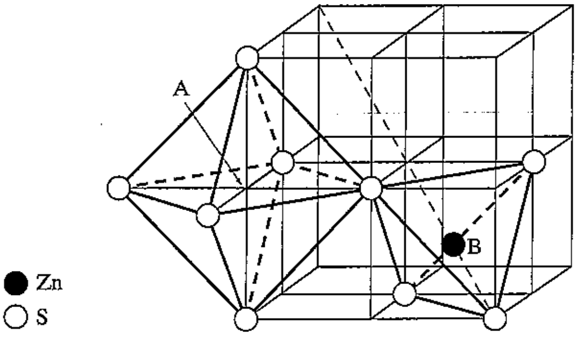


Figure 2-25 Portion of the zinc blend structure. Compare Figure 2-22(b). The hole at *A* has octahedral surroundings. The Zn atom at *B* has tetrahedral surroundings.

2-11 CRYSTAL SHAPE

The shape of crystals has been ignored thus far so that their internal structure could be emphasized. However, the shape of crystals is, to the layman, perhaps their most characteristic property, and nearly everyone is familiar with the beautifully developed flat faces exhibited by natural minerals or crystals artificially grown from a supersaturated salt solution. In fact, it was with a study of these faces and the angles between them that the science of crystallography began.

Nevertheless, the shape of crystals is really a secondary characteristic, since it depends on, and is a consequence of, the interior arrangement of atoms. Sometimes the external shape of a crystal is rather obviously related to its smallest building block, the unit cell, as in the little cubic grains of ordinary table salt (NaCl has a cubic lattice) or the six-sided prisms of natural quartz crystals (hexagonal lattice). In many other cases, however, the crystal and its unit cell have quite different shapes; gold, for example, has a cubic lattice, but natural gold crystals are octahedral in form, i.e., bounded by eight planes of the form {111}.

An important fact about crystal faces was known long before there was any knowledge of crystal interiors. It is expressed as the *law of rational indices*, which states that the indices of naturally developed crystal faces are always composed of small whole numbers, rarely exceeding 3 or 4. Thus, faces of the form {100}, {111}, $\{1\bar{1}00\}$, {210}, etc., are observed but not such faces as {510}, {719}, etc. Earlier discussion in this chapter concluded that planes of low indices have the largest density of lattice points, and it is a law of crystal growth that such planes develop at the expense of planes with high indices and few lattice points.

In materials work, however, crystals with well-developed faces are in the category of things heard of but rarely seen. They occur occasionally on the free surface of castings, in some electrodeposits, or under other conditions of no external constraint. Instead, a crystal is most usually a "grain," seen through a microscope in the company of many other grains on a polished section. If an isolated single crystal is encountered it will have been artificially grown either from the melt, and thus have the shape of the crucible in which it solidified, or by recrystallization, and thus have the shape of the starting material, whether sheet, rod, or wire.

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. 2-10. 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 $\ldots ABCABCABC\ldots$can become $\ldots ABCAB^{*}ABC\ldots$ or $\ldots ABCA^{*}CABCA\ldots$, 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 $\ldots ABABABAB\ldots$ can become $\ldots ABABA^{*}CBCBCB\ldots$ 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:

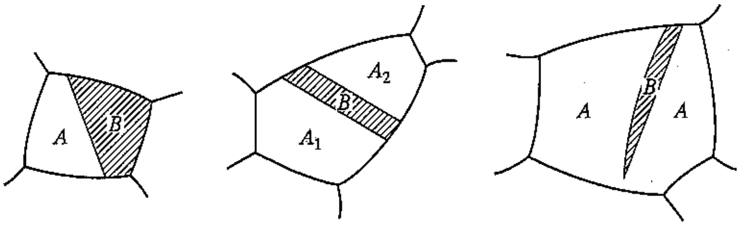
1. Annealing twins, such as occur in FCC metals and alloys (Cu, Ni, α–brass, Al, etc.), which have been cold-worked and then annealed to cause recrystallization.
2. Deformation twins, such as occur in deformed HCP metals (Zn, Mg, Be, etc.) and BCC metals (α–Fe, W, etc.).

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]



(a) (b) (c)

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 $ABCABC\ldots$ in an FCC crystal. If, however, a mistake should occur and this sequence become altered to $CBACBA\ldots$, 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
⟶	⟷	⟵

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.

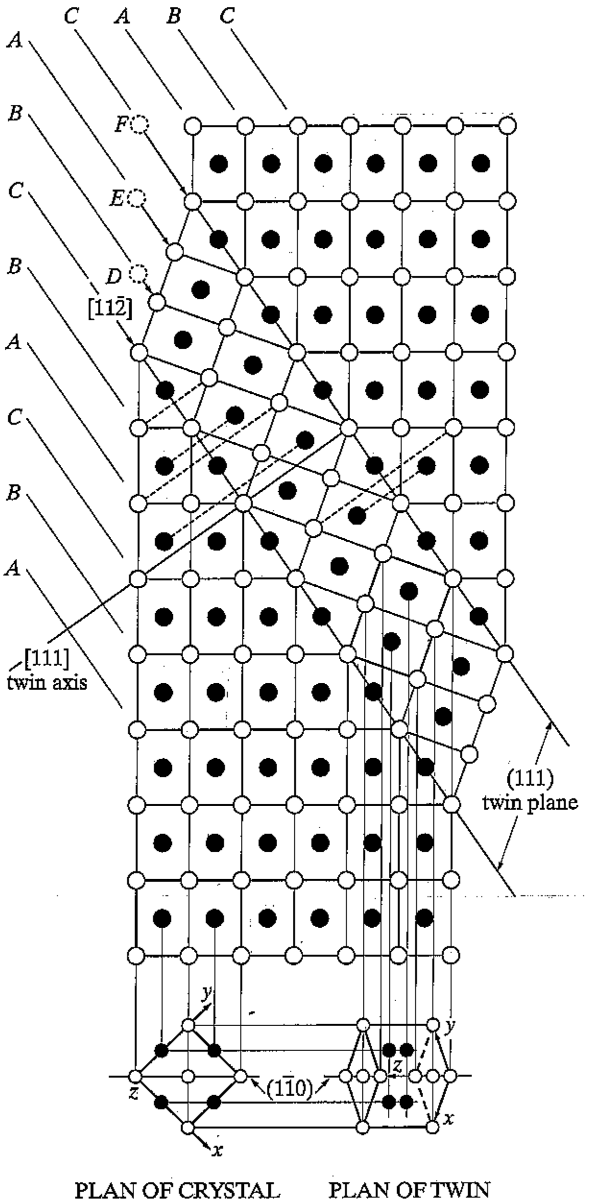


Figure 2-27. Twin band in FCC lattice. Plane of main drawing is (1$\bar{1}$0).

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 some one point within the crystal. If a refer-

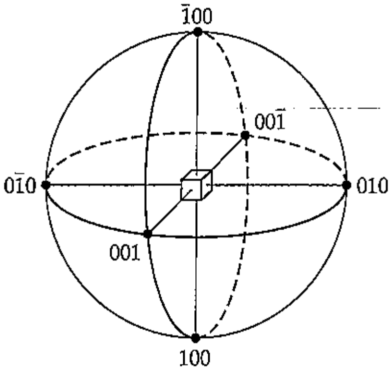


Figure 2-28 {100} poles of a cubic crystal.

ence 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.

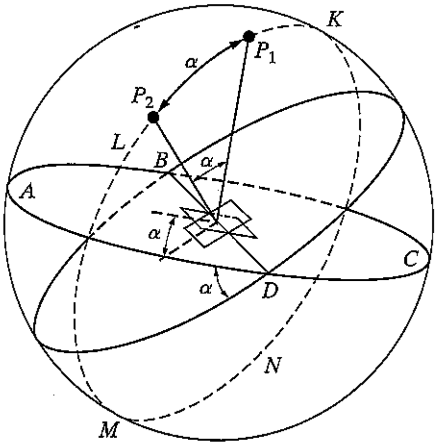


Figure 2-29 Angle between two planes.

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

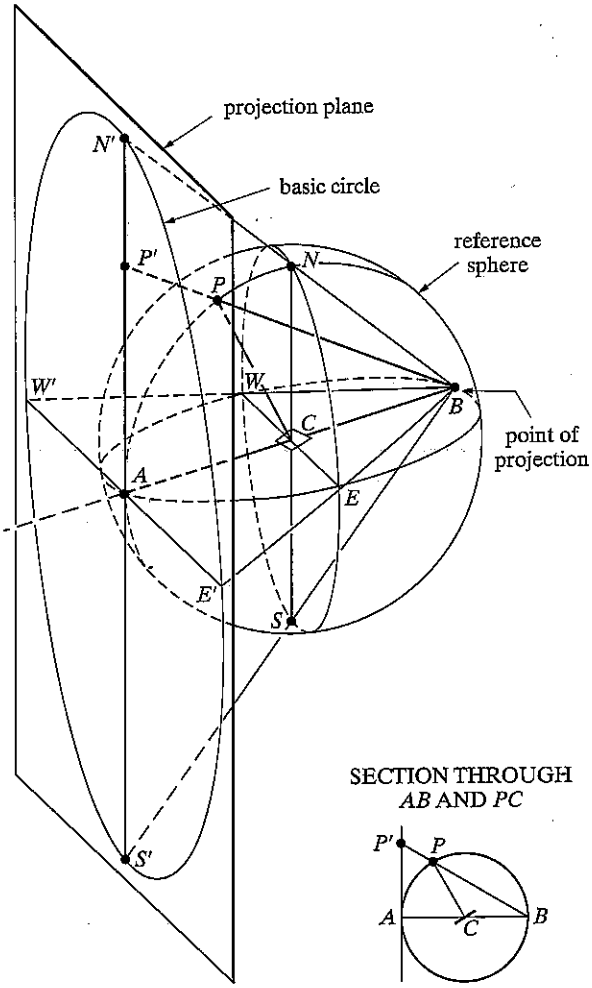


Figure 2-30 The stereographic projection

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 are $N'G'S'$. 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-

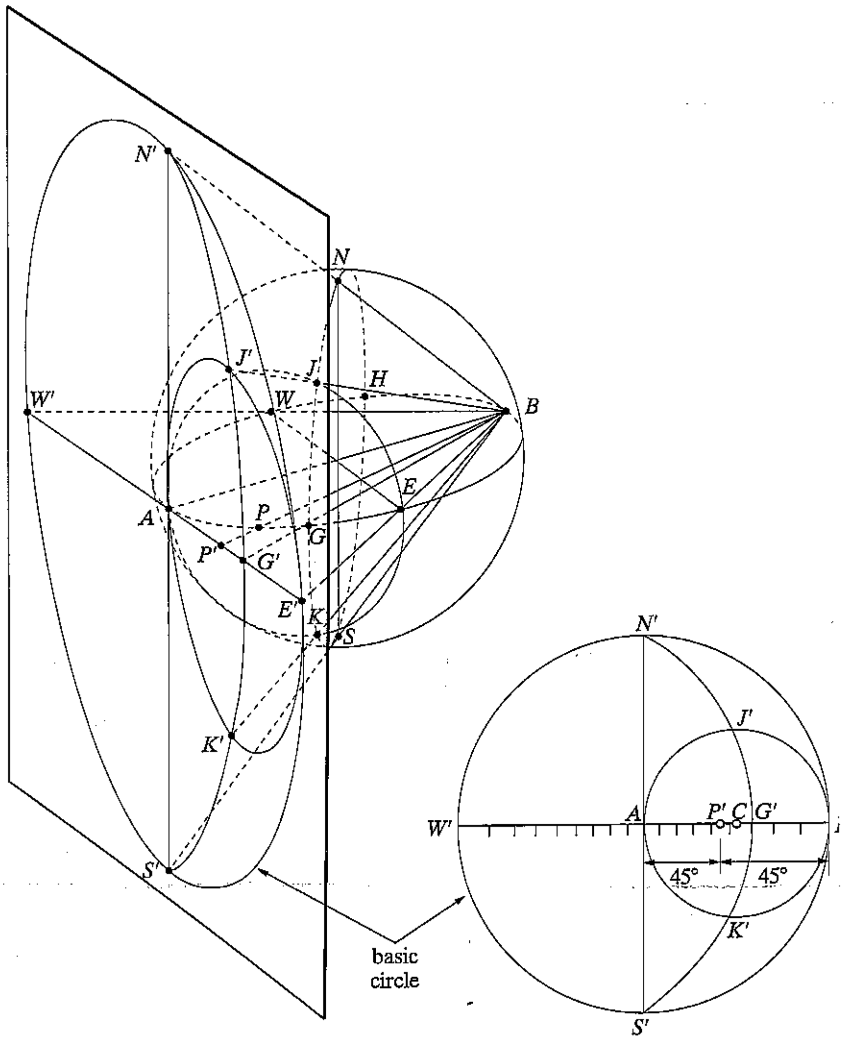


Figure 2-31 Stereographic projection of great and small circles.

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

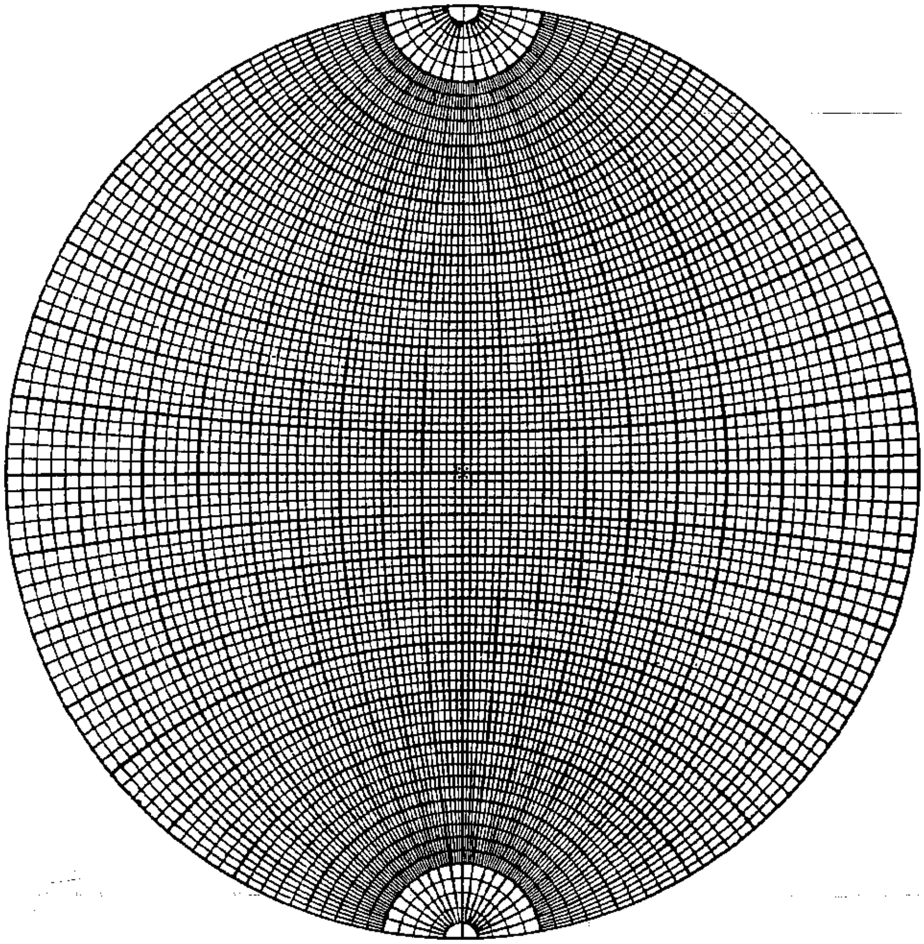


Figure 2-32 Wulff net drawn to 2° intervals.

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 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

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

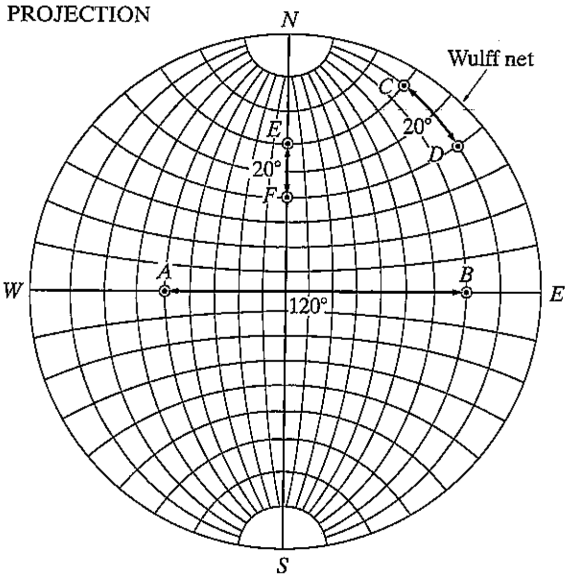


Figure 2-33 Stereographic projection superimposed on Wulff net for measurement of angle between poles. For illustrative purposes this net is graduated at 10° intervals..

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-

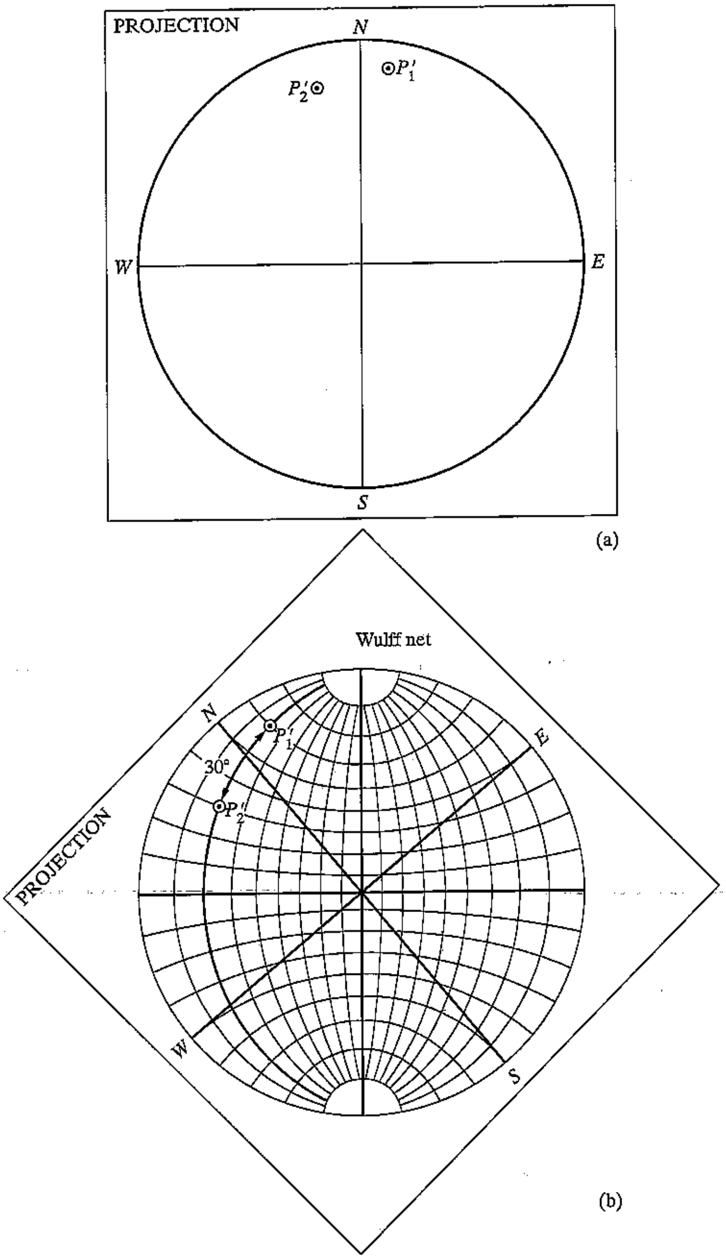


Figure 2-34 (a) Stereographic projection of poles P_1 and P_2 of Fig. 2-29. (b) Rotation of projection to put poles on same great circle of Wulff net. Angle between poles = 30°.

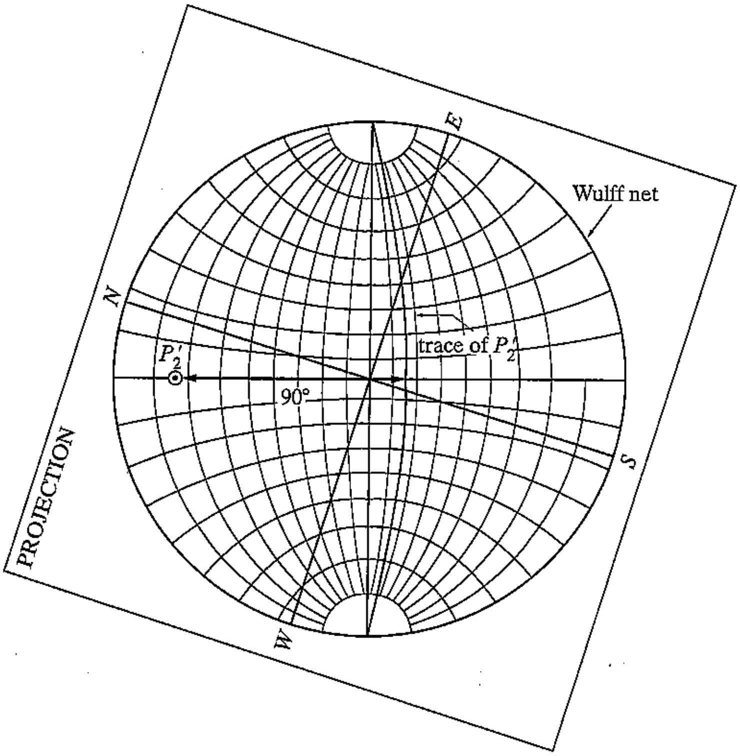


Figure 2-35 Method of finding the trace of a pole (the pole P'_2 in Fig. 2-34).

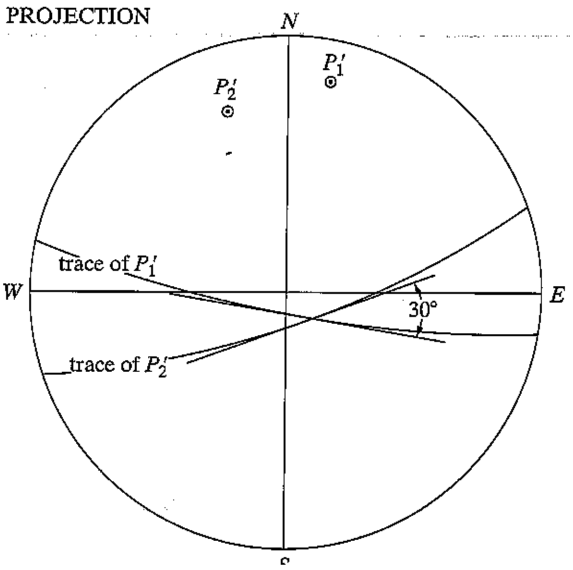


Figure 2-36 Measurement of an angle between two poles (P_1 and P_2 of Fig. 2-29) by measurement of the angle of intersection of the corresponding traces.

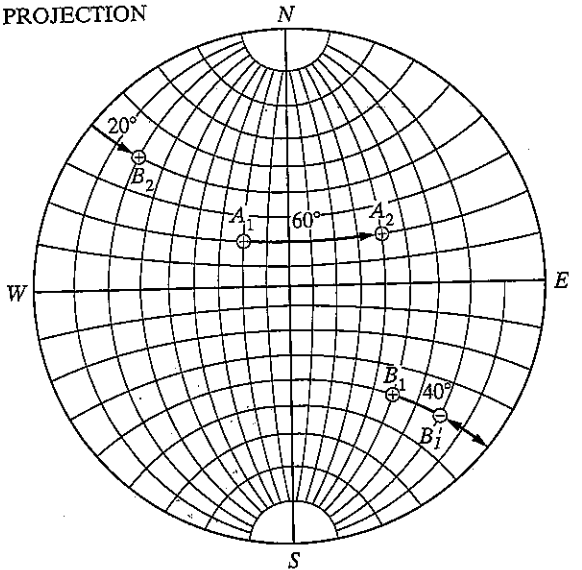


Figure 2-37 Rotation of poles about *NS* axis of projection.

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[TR 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

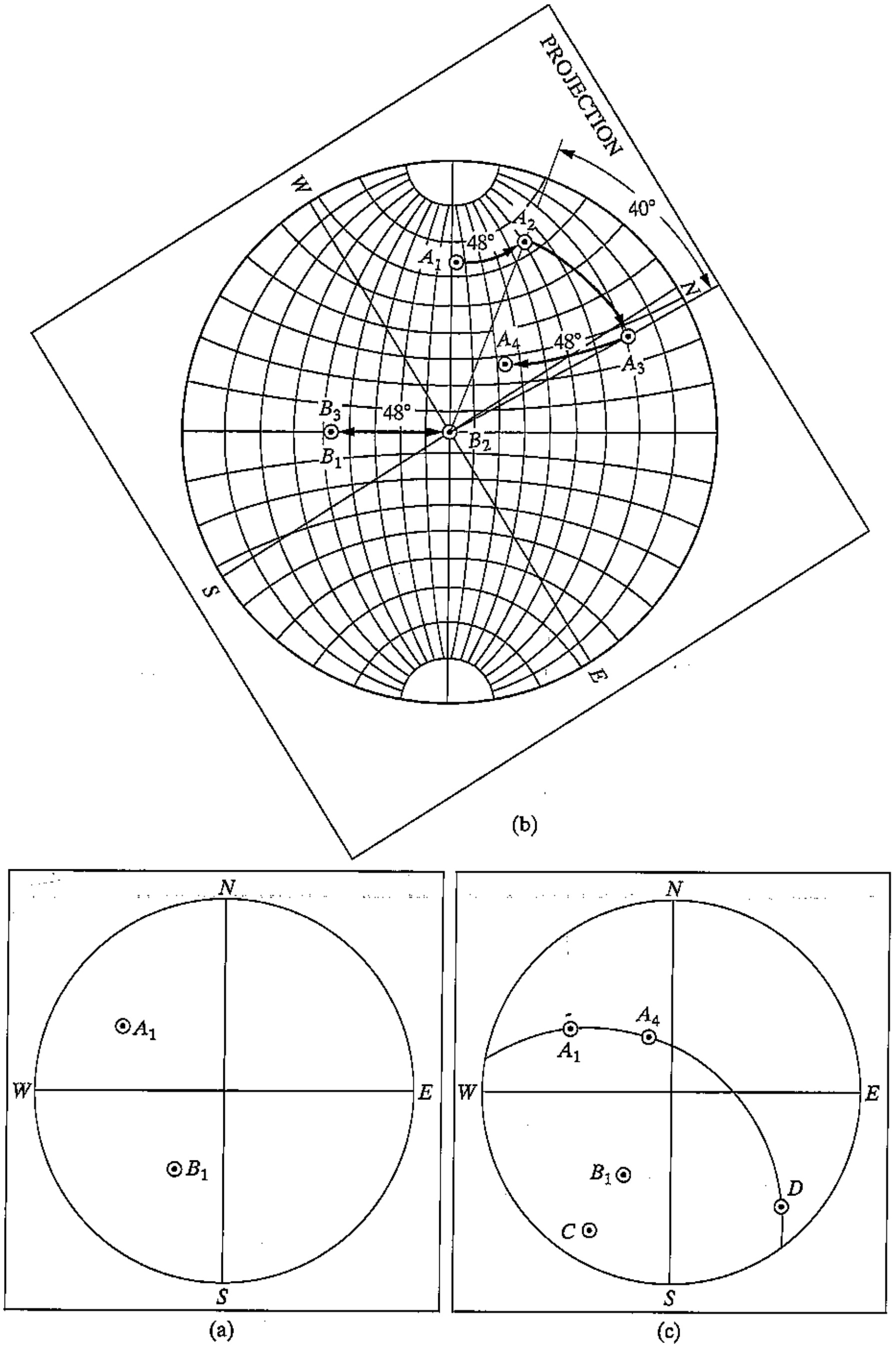
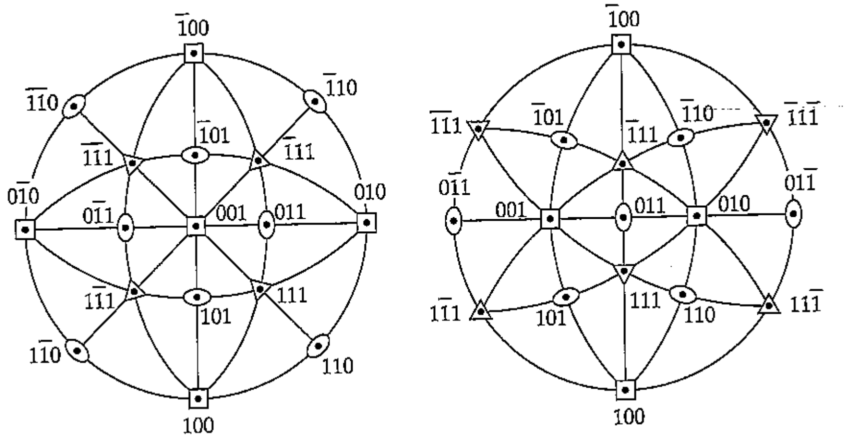


Figure 2-38 Rotation of a pole about an inclined axis.



(a) (b)

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

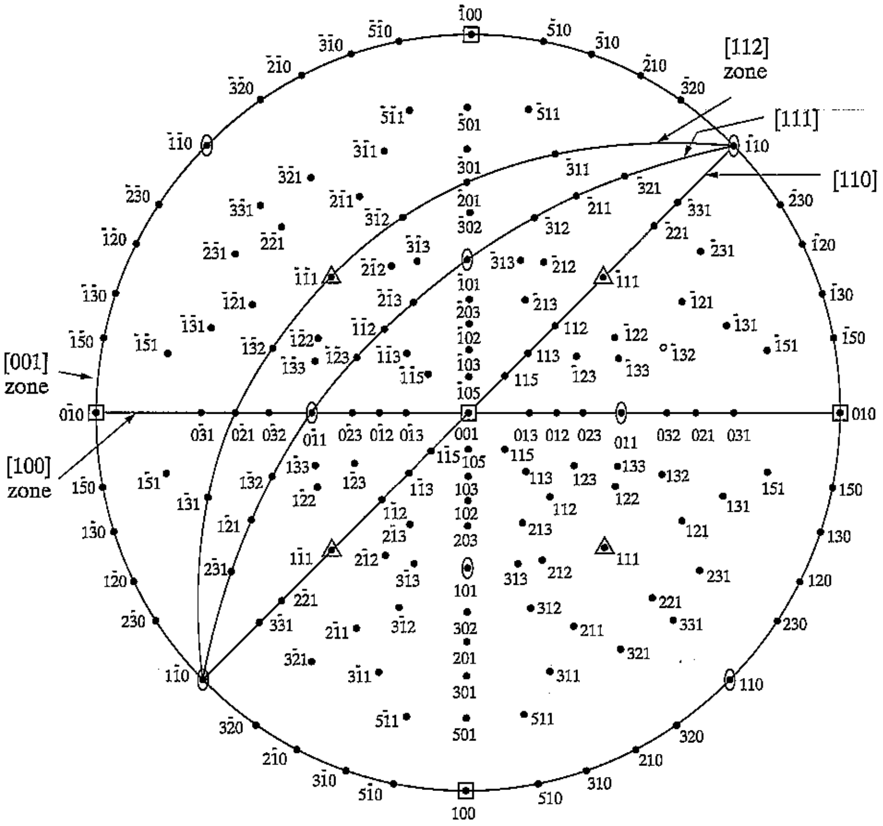


Figure 2-40 Standard (001) projection of a cubic crystal, after Barrett [1.7].

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

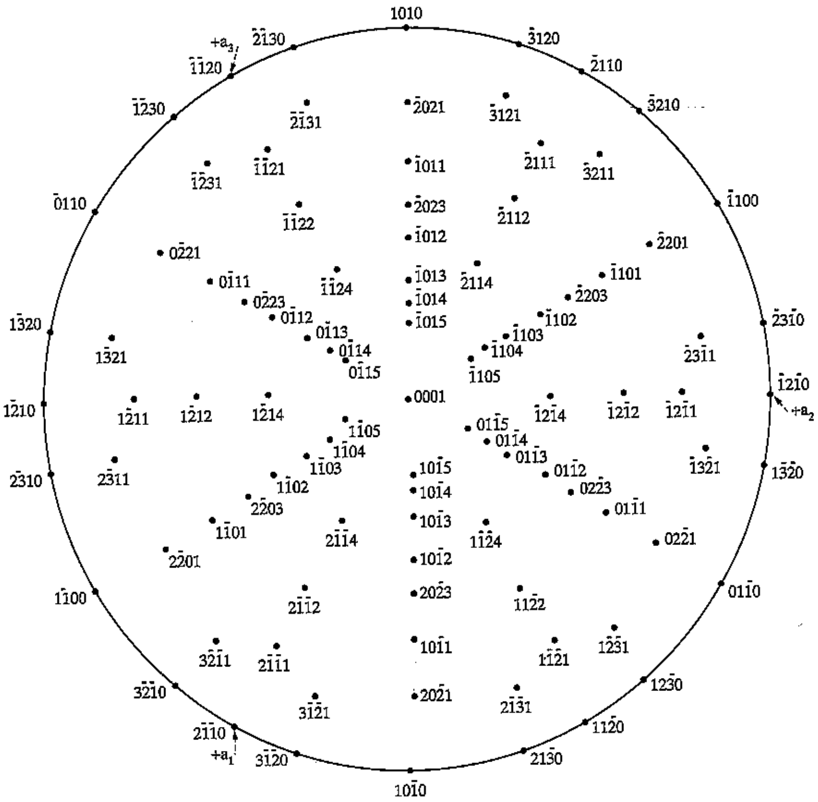
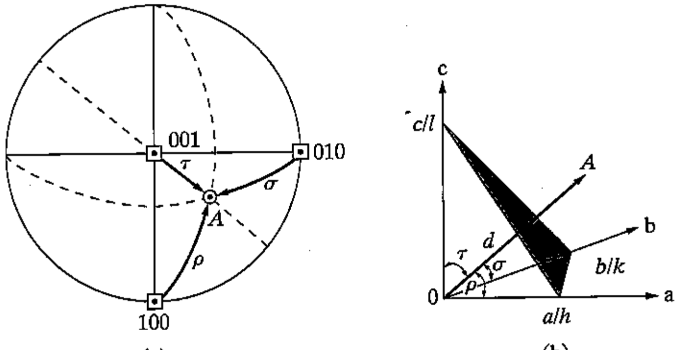


Figure 2-41 Standard (0001) projection for zinc (hexagonal, $c/a = 1.86$) [1.7]



(a) (b)

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;

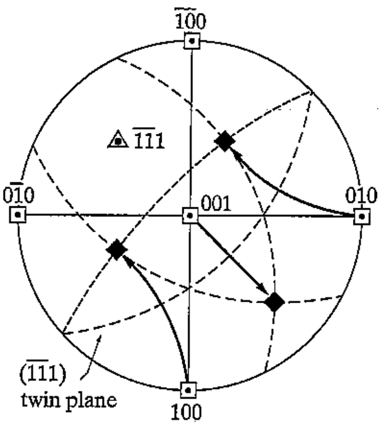


Figure 2-43 Stereographic projection of an FCC crystal and its twin.

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.

2-10 The unit cells of several orthorhombic crystals are described below. What is the Bravais lattice of each and how do you know? Do not change axes. (In solving this kind of problem, examining the given atom positions for the existence or nonexistence of centering translations is generally more helpful than making a drawing of the structure.)

a) Two atoms of the same kind per unit cell located at $0\,\tfrac{1}{2}\,0, \tfrac{1}{2}\,0\,\tfrac{1}{2}$.

b) Four atoms of the same kind per unit cell located at $0\,0\,z, 0\,\tfrac{1}{2}\,z, 0\,\tfrac{1}{2}\,(\tfrac{1}{2}+z),\ 0\,0\,(\tfrac{1}{2}+z)$.

c) Four atoms of the same kind per unit cell located at $x\,y\,z,\ \bar{x}\,\bar{y}\,z, (\tfrac{1}{2}+x)(\tfrac{1}{2}-y)\bar{z}, (\tfrac{1}{2}-x)(\tfrac{1}{2}+y)\bar{z}$.

d) Two atoms of one kind A located at $\tfrac{1}{2}\,0\,0, 0\,\tfrac{1}{2}\,\tfrac{1}{2}$; and two atoms of another kind B located at $0\,0\,\tfrac{1}{2}, \tfrac{1}{2}\,\tfrac{1}{2}\,0$.

***2-11** Make a drawing, similar to Fig. 2-23, of a (112) twin in a BCC lattice and show the shear responsible for its formation. Obtain the magnitude of the shear strain graphically.

2-12 Construct a Wulff net, 18 cm in diameter and graduated at 30° intervals, by the use of compass, dividers, and straightedge only. Show all construction lines.

In some of the following problems, the coordinates of a point on a stereographic projection are given in terms of its latitude and longitude, measured from the center of the projection. Thus, the N pole is 90° N, 0° E, the E pole is 0° N, 90° E, etc.

2-13 Plane A is represented on a stereographic projection by a great circle passing through the N and S poles and the point 0°N, 70°W. The pole of plane B is located at 30°N, 50°W.

a) Find the angle between the two planes by measuring the angle between the poles of A and B.

b) Draw the great circle of plane B and demonstrate that the stereographic projection is angle-true by measuring with a protractor the angle between the great circles of A and B.

***2-14** Pole A, whose coordinates are 20°N, 50°E, is to be rotated about the axes described below. In each case, find the coordinates of the final position of pole A and show the path traced out during its rotation.

a) 100° rotation about the *NS* axis, counterclockwise looking from *N* to *S*.

b) 60° rotation about an axis normal to the plane of projection, clockwise to the observer.

c) 60° rotation about an inclined axis B, whose coordinates are 10°S, 30°W, clockwise to the observer.

2-15 Draw a standard (111) projection of a cubic crystal, showing all poles of the form {100}, {110}, {111} and the important zone circles between them. Compare with Figs. 2-39(a) and (b).

2-16 Draw a standard (001) projection of white tin (tetragonal, $c/a = 0.545$), showing all poles of the form {001}, {100}, {110}, {011}, {111} and the important zone circles between them. Compare with Fig. 2-39(a).

2-17 Draw a standard (0001) projection of beryllium (hexagonal, $c/a = 1.57$), showing all poles of the form $\{2\bar{1}\bar{1}0\}$, $\{10\bar{1}0\}$, $\{2\bar{1}\bar{1}1\}$, $\{10\bar{1}1\}$ and the important zone circles between them. Compare with Fig. 2-40.

2-18 On a standard (001) projection of a cubic crystal, in the orientation of Fig. 2-36(a), the pole of a certain plane has coordinates 53.3°S, 26.6°E. What are its Miller indices? Verify your answer by comparison of measured angles with those given in Table 2-4.

***2-19** Duplicate the operations shown in Fig. 2-43 and thus find the locations of the cube poles of a $(\bar{1}\bar{1}1)$ reflection twin in a cubic crystal. What are their coordinates?

2-20 Show that the twin orientation found in Prob. 2-19 can also be obtained by

a) Reflection in a $\{112\}$ plane. Which one?
b) 180° rotation about a $\langle 111 \rangle$ axis. Which one?
c) 60° rotation about a $\langle 111 \rangle$ axis. Which one?

In (c), show the paths traced out by the cube poles during their rotation.

***2-21** Plot the great-circle route from Washington, D.C. (39°N, 77°W) to Moscow (56°N, 38°E).

a) What is the distance between the two cities? (Radius of the earth = 6360 km.)
b) What is the true bearing of an airplane flying from Washington to Moscow at the beginning, midpoint, and end of the trip? (The bearing is the angle measured clockwise from north to the flight direction. Thus east is 90° and west is 270°.)

2-22 Cellulose $(C_6H_{10}O_5)_x$ crystallizes as monoclinic crystals with lattice parameters $a = 7.87$ Å, $b = 10.31$ Å, $c = 10.13$ Å, and $\beta = 122°$.

a) Plot the lattice points for $(h0l)$, i.e., in direct space. Superimpose the lattice points of the adjacent $(h0l)$ on the first plot.
b) Plot the $h0l$ net of the reciprocal lattice (i.e., the reciprocal lattice plane containing reciprocal lattice points of the form $h0l$). Superimpose the points of the $(h1l)$ reciprocal lattice net onto the first plot.

2-23 Lutetium has a hexagonal structure with lattice parameters $a = 3.516$ Å and $c = 5.570$ Å. Plot the $h0l$ plane of the reciprocal lattice of this material.

2-24 Aluminum silicate (mullite) $Al_6Si_2O_{13}$ has an orthorhombic Bravais lattice and lattice parameters $a = 7.5456$ Å, $b = 7.6898$ Å and $c = 2.8842$ Å. Assuming that the Bravais lattice is simple orthorhombic, in one diagram plot the $h0l$ net of the reciprocal lattice, and in a second diagram plot the $0kl$ net of the reciprocal lattice.