Elementary Crystallography for X-Ray Diffraction

(prepared by James R. Connolly, for EPS400-001, Introduction to X-Ray Powder Diffraction, Spring 2007

Introduction

Crystallography originated as the science of the study of macroscopic crystal forms, and the term "crystal" has been traditionally defined in terms of the structure and symmetry of these forms. With the advent of the x-ray diffraction, the science has become primarily concerned with the study of atomic arrangements in crystalline materials, and the definition of a crystal has become that of Buerger (1956): "a region of matter within which the atoms are arranged in a three-dimensional translationally periodic pattern." This orderly arrangement in a crystalline material is known as the crystal structure. X-ray crystallography is concerned with discovering and describing this structure.

There is no way around it – effective application of x-ray diffraction as an analytical tool in geology and materials science necessitates a basic understanding crystallography. The purpose of this section is to provide that background. The material here is anything but comprehensive. Crystallography is taught as a significant part of most Mineralogy courses, and multi-course sequences in crystallography are taught in many physics, geology and materials science graduate programs. What is presented here is skeletal treatment that is hopefully substantial enough to make sense of your diffraction data. The XRD Resource page (http://epswww.unm.edu/xrd/resources.htm) provides links to resources that students are encouraged to use to learn more.

The aspects of crystallography most important to the understanding and basic interpretation of XRD data are:

- conventions of lattice description, unit cells, lattice planes, d-spacing and Miller indices,
- crystal structure and symmetry elements,
- the reciprocal lattice (covered in a separate document)

How all of this is used in your x-ray diffraction work will be discussed over the course next few weeks. Details of crystal chemistry, atomic and molecular bonds, and descriptive crystallography will not be discussed; these topics are important in many advanced XRD studies, including structure refinements, particle size and shape analysis and other advanced techniques. In class we will use the animations on the CD-ROM tutorial from Klein (2002) to illustrate these concepts. This program will be available on our department network so it can be used by the class for self-study from the student workstations in our computer lab (Northrop Hall Rm. 209). I have borrowed freely from several sources to assemble this material, including Nuffield (1966), Klein (2002), and Jenkins and Snyder (1996).

Description of the Crystal Structure

A crystal structure is like a three-dimensional wallpaper design in that it is an endless repetition of some motif (i.e., a group of atoms or molecules). The process of creating the motif involves point-group operations (rotation, reflection, and inversion) that define it. The process of creating the wallpaper involves translation (with or without rotation or reflection) to create the complete structure (which we call the lattice). Real-world crystalline structures may be simple lattice structures, or combinations of lattices to make complex crystalline molecules. As long as the structure is repetitive, its structure may be discovered with the application of x-ray diffraction.

Lattice Notation

Klein (2002) defines a lattice as "an imaginary pattern of points (or nodes) in which every point (node) has an environment that is identical to that of any other point (node) in the pattern. A lattice has no specific origin, as it can be shifted parallel to itself."

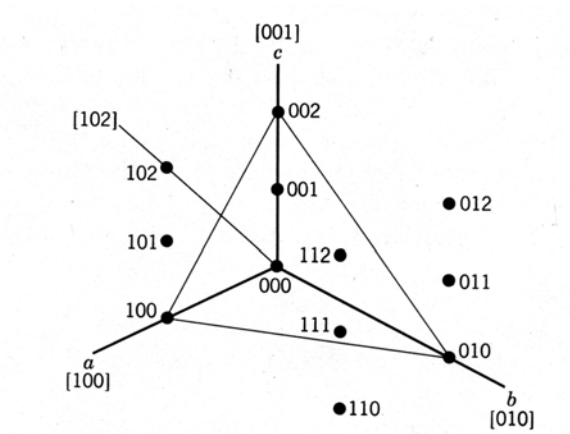

Fig. 1-5. Notation of lattice points, rows, and planes.

The figure at left (Fig 1-5) shows a method of notating lattice points, rows, and planes on the basis of the crystal coordinate systems. A point in the lattice is chosen at the origin and defined as 000. The *a*, *b* and *c* axes define the ***directions*** within the crystal structure with the angular relations defined by the particular crystal system.[1]

Lattice points are specified without brackets – 100, 101, 102, etc. 100 is thus a point one unit along the *a* axis, 002 is a point two units along the *c* axis, and 101 is a point one unit along *a* and one unit along *c*.

Lattice planes are defined in terms of the **Miller indices**, which are ***defined as the reciprocals of the intercepts of the planes on the coordinate axes cleared of fractions***. In Fig. 1-5, the plane shown intercepts *a* at 100, *b* at 010 and *c* at 002. The Miller index of the plane is thus calculated as 1/1(*a*), 1/1(*b*), 1/2(*c*), and reduced to integers as 2*a*,2*b*,1*c*. Miller indices are by convention given in parentheses, i.e., (221). If the calculations result in indices with a common factor (i.e., (442)) the index is reduced to the simplest set of integers (221). This means that a Miller index refers to a ***family*** of parallel lattice planes defined by a fixed translation distance (defined as ***d***) in a direction perpendicular to the plane. If directions are negative along the lattice, a bar is placed over the negative direction, i.e. (2 $\bar{2}$ 1)

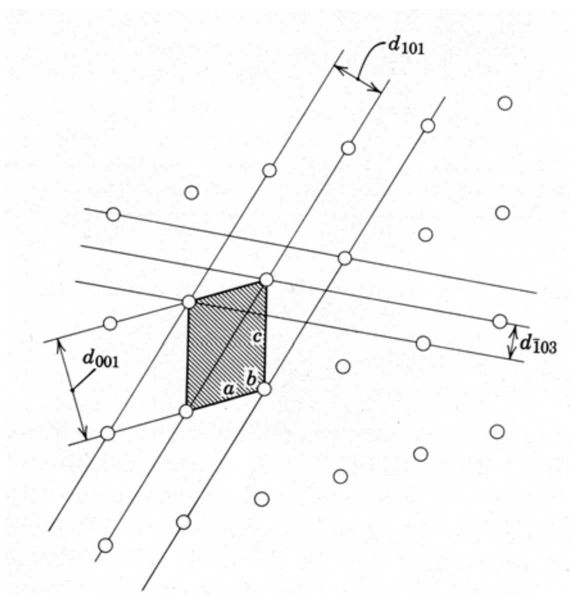

Fig. 1-7. Interplanar spacings.

Families of planes related by the symmetry of the crystal system are enclosed in braces { }. Thus, in the tetragonal system {110} refers to

[1] Note that the angular relations between the coordinate axes are not necessarily orthogonal but are dependent on the particular crystal system. The angular relations in the different crystal systems are discussed below.

the four planes (110), ($\bar{1}$10), ($\bar{1}\,\bar{1}$0) and (1$\bar{1}$0). Because of the high symmetry in the cubic system, {110} refers to twelve planes. ***As an exercise, write the Miller indices of all of these planes.***

Spacing of Lattice Planes: The perpendicular distance separating each lattice plane in a stack is denoted by the letter *d*. Figure 1-7 shows several lattice planes and the associated *d* spacings. In *a* and *c* are in the plane of the paper, and *b* is perpendicular to the plane of the page. The notation shown for the *d* spacing and the relationship to the particular lattice plane (i.e., d_{001}, d_{101}, d_{103}) with the Miller index for the particular plane shown in the subscript (but usually without parentheses) are standard notation used in crystallography and x-ray diffraction.

The values of *d* spacings in terms of the geometry of the different crystal systems are shown in Table 1-2 below (from Nuffield, 1966). The crystal systems (discussed in the next section) are listed in order of decreasing symmetry. The calculations are increasingly complex as symmetry decreases. Crystal structure calculations are relatively simple for the cubic system, and can be done with a good calculator for the tetragonal and orthorhombic system. In actual practice, these calculations are usually done with the aid of specialized computer programs specifically written for this purpose.

Table 1-2. Values of the Interplanar Spacing (d_{hkl}) in the Six Crystal Systems

System	d_{hkl}
Cubic	$\left[\frac{1}{a^2}(h^2+k^2+l^2)\right]^{-1/2}$
Tetragonal	$\left[\frac{h^2+k^2}{a^2}+\frac{l^2}{c^2}\right]^{-1/2}$
Orthorhombic	$\left[\frac{h^2}{a^2}+\frac{k^2}{b^2}+\frac{l^2}{c^2}\right]^{-1/2}$
Hexagonal	$\left[\frac{4}{3a^2}(h^2+hk+k^2)+\frac{l^2}{c^2}\right]^{-1/2}$ hexagonal indexing
	$\left[\frac{1}{a^2}\frac{(h^2+k^2+l^2)\sin^2\alpha+2(hk+kl+lh)(\cos^2\alpha-\cos\alpha)}{1-2\cos^3\alpha+3\cos^2\alpha}\right]^{-1/2}$ rhombohedral indexing
Monoclinic	$\left[\frac{\frac{h^2}{a^2}+\frac{l^2}{c^2}-\frac{2hl\cos\beta}{ac}}{\sin^2\beta}+\frac{k^2}{b^2}\right]^{-1/2}$
Triclinic	$\left[\frac{\frac{h^2}{a^2}\sin^2\alpha+\frac{k^2}{b^2}\sin^2\beta+\frac{l^2}{c^2}\sin^2\gamma+\frac{2hk}{ab}(\cos\alpha\cos\beta-\cos\gamma)+\frac{2kl}{bc}(\cos\beta\cos\gamma-\cos\alpha)+\frac{2lh}{ca}(\cos\gamma\cos\alpha-\cos\beta)}{1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma}\right]^{-1/2}$

Symmetry

The repetition of the arrangement of atoms (or motif) in a crystal structure is what produces the diffraction pattern, thus a large part of X-ray crystallography is discerning the motif by "solving" the diffraction pattern. If there is no repetition (as in truly amorphous materials) there is no diffraction pattern. Repetition of the motif in a lattice defines its symmetry.

A symmetry operation may be thought of as moving a shape-object in such a way that after the movement, the object appears exactly the same as it did before the movement.

An alternative way to view symmetry is as a series of replication operations on one surface of a shape-object by which the entire object may be generated. Crystal structures are defined based on the symmetry operations used to replicate (or create) the structure.

All symmetry operations may be defined by several basic movement operations described below:

Rotation (Symbols used: **1,2,3,4,6.** Indicates the number of times the form is replicated during one 360° rotation. As an example, in 4-fold rotation, it takes four rotational movements of the form to return to the original position, and the form is identically repeated at each of the four rotational stages.)[2]

Reflection (Symbol used: **m**. Form is replicated by mirror reflection across a plane.)

Inversion (Symbol used: ***i***. Form is replicated by projection of all points through a point of inversion; this point defines a center of symmetry.)

Rotation-Inversion (Symbol used: $\bar{\mathbf{1}}$ for single rotation/inversion. May be combined with rotational operations, i.e., $\bar{\mathbf{3}}$ = 3-fold rotation w. inversions at each rotation.)

Translation (A lateral movement which replicates the form along a linear axis)

In general, rotation, reflection and inversion operations generate a variety of unique arrangements of lattice points (i.e., a shape structure) in three dimensions. These translation-free symmetry operations are called ***point-group elements***.

Translations are used to generate a lattice from that shape structure. The translations include a simple linear translation, a linear translation combined with mirror operation (glide plane), or a translation combined with a rotational operation (screw axis). A large number of 3-dimensional structures (the 230 Space Groups) are generated by these translations acting on the 32 point groups as discussed in the next section.

The repetitive nature of crystal structures results in the presence of stacks of planar arrays of atoms. Repeating, equidistant planar elements (d-spacings) are present in all crystals. The measurement of these d-spacings and the variations in intensity of the diffractions caused by them can be used to uniquely "fingerprint" the crystal studied. This is the basis of x-ray crystallography.

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[2] It is noted that "5" is omitted from the list. Although a pentagon shape may be replicated by a 5-fold rotation, crystalline structures that occur in nature cannot meet the rotation criteria by 5-fold rotation. There are some synthetic materials that do show this kind of symmetry, however they do not display 3-dimensional translational symmetry and are referred to as "quasicrystals" (Pecharsky and Zavalij, 2003).

Classification and Crystal Structure

The repetition of the atomic-molecular motif in a lattice is what defines the crystal structure. This section begins with the five possible planar lattices, the Bravais lattices developed from them in three dimensions, the point-groups derived by non-translation symmetry operations, and the 230 possible space groups derived by translations of the point groups. The development is, at best, incomplete. For a more comprehensive discussion, the reader is referred to Klein (2002) or Nuffield (1966). For a detailed and rigorous treatment, the reader is referred to Donald Bloss (1971) *"Crystallography and Crystal Chemistry: An Introduction"*.

Lattices and Crystal Systems

There are five planar translation lattices defined by possible angular and length relations between the two-dimensional coordinate systems, shown in Fig. 1-3 (from Nuffield, 1966).

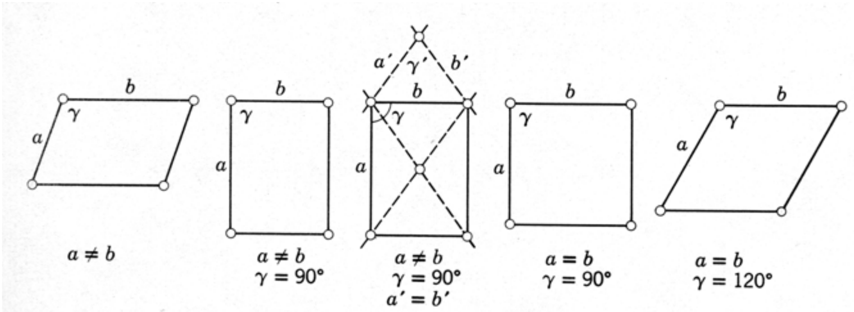

Fig. 1-3. The five plane lattices.

When translated in three dimensions, the plane lattices define an assemblage of points in space. By selection of different groups of points in two dimensions, and "copying" that group in the third dimension, we can produce the fourteen space lattices shown on page 7 (Fig. 5.63 from Klein, 2002). These lattices are called the Bravais lattices after Auguste Bravais (1811-1863) who was the first to show that they were unique. The CD-ROM tutorial (Klein, 2002) includes an animated derivation of ten of the fourteen space lattices from the plane lattices (Module 3 – Generation of 10 Bravais lattices).

The six crystal systems (table on following page) are defined by relationships between unit cell edge lengths and the angles between those edges. The combination of centering and relationship between the angles between lattice directions and axis length define the 14 lattice types within the 6 crystal systems. In the primitive lattice (P) all atoms in the lattice are at the corners. In the body centered lattices (I) there is an additional atom at the center of the lattice. There are two types of face centering, one in which the atoms are centered on a pair of opposing plane lattices (C) and another in which an atom is centered on each face (F). ***It is important to note that the choice of the planar replication unit and the direction of that replication in three dimensions that determines the character of the lattice.***

System	Type	Edge - Angle Relations	Symmetry
Triclinic	P	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$	$\bar{1}$
Monoclinic	P (b = twofold axis) C	$a \neq b \neq c$ $\alpha = \gamma = 90° \neq \beta$	2/m
	P (c = twofold axis) C	$a \neq b \neq c$ $\alpha \neq \beta = 90° \neq \gamma$	
Orthorhombic	P C (or A, B) I F	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$	mmm
Tetragonal	P I	$a_1 = a_2 \neq c$ $\alpha = \beta = \gamma = 90°$	4/mmm
Hexagonal	R P	$a_1 = a_2 \neq c$ $\alpha = \beta = 90°, \gamma = 120°$	$\bar{3}$ m 6/mmm
Cubic	P I F	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90°$	m3m

(Please note that in this simplified chart, the symmetry notations are ***not*** inclusive, and represent simplified "Laue Group" symmetry for the crystal class. Later graphics and tables expand upon the symmetry possibilities available in the different systems.)

Fig. 5.63 (on following page, from Klein, 2002) shows the 14 unique Bravais lattices. These are defined by translation of the two-dimensional lattices in the third dimension combined with placement of presence atoms in addition to those at the lattice corners (P). These atoms can be body-centered (I) or face-centered (F) in the lattice.

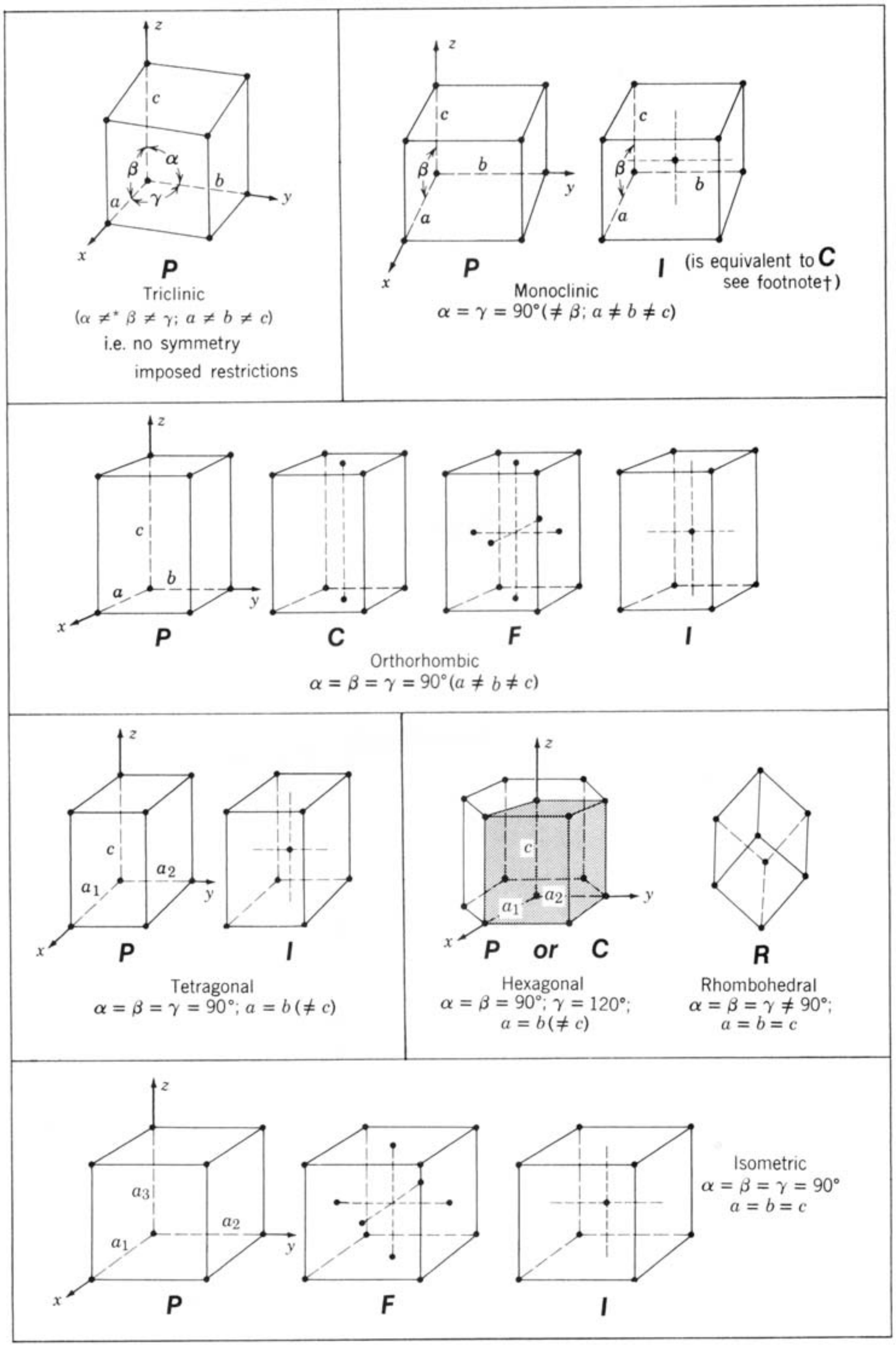

Table 5.9 from Klein, 2002 (below) presents another way of cross-referencing the distribution of the 14 Bravais Lattices among the six crystal systems that the reader might find helpful.

TABLE 5.9 Description of Space Lattice Types and Distribution of the 14 Bravais Lattices Among the Six Crystal Systems

Name and Symbol	Location of Nonorigin Nodes	Multiplicity of Cell
Primitive (*P*)	. . . .	1
Side-centered (*A*)	Centered on A face (100)	2
(*B*)	Centered on B face (010)	2
(*C*)	Centered on *C* face (001)	2
Face-centered (*F*)	Centered on all faces	4
Body-centered (*I*)	An extra lattice point at center of cell	2
Rhombohedral (*R*)	A primitive rhombohedral cell	1

Primitive (*P*) in each of the 6 crystal systems	= 6
Body-centered (*I*) in monoclinic, orthorhombic, tetragonal, and isometric	= 4
Side-centered (*A* = *B* = *C*) in orthorhombic	= 1
Face-centered (*F*) in orthorhombic and isometric	= 2
Rhombohedral (*R*) in hexagonal	= 1
	Total = 14

Figure 1-8 (from Nuffield, 1966) below describes diagrammatically (as spherical projections) the translation-free symmetry operations by which the 32 point-groups are generated from the 14 Bravais lattices. On the diagrams small dots represent upper hemisphere projections, open circles represent lower hemisphere projections. The upper row shows mirror operations (***m***), the middle row shows 1-fold through 6-fold rotational operations (**1**,**2**,**3**,**4**,**6**), and the bottom row shows rotation-inversion operations ($\bar{\mathbf{1}}$,$\bar{\mathbf{2}}$,$\bar{\mathbf{3}}$,$\bar{\mathbf{4}}$,$\bar{\mathbf{6}}$).

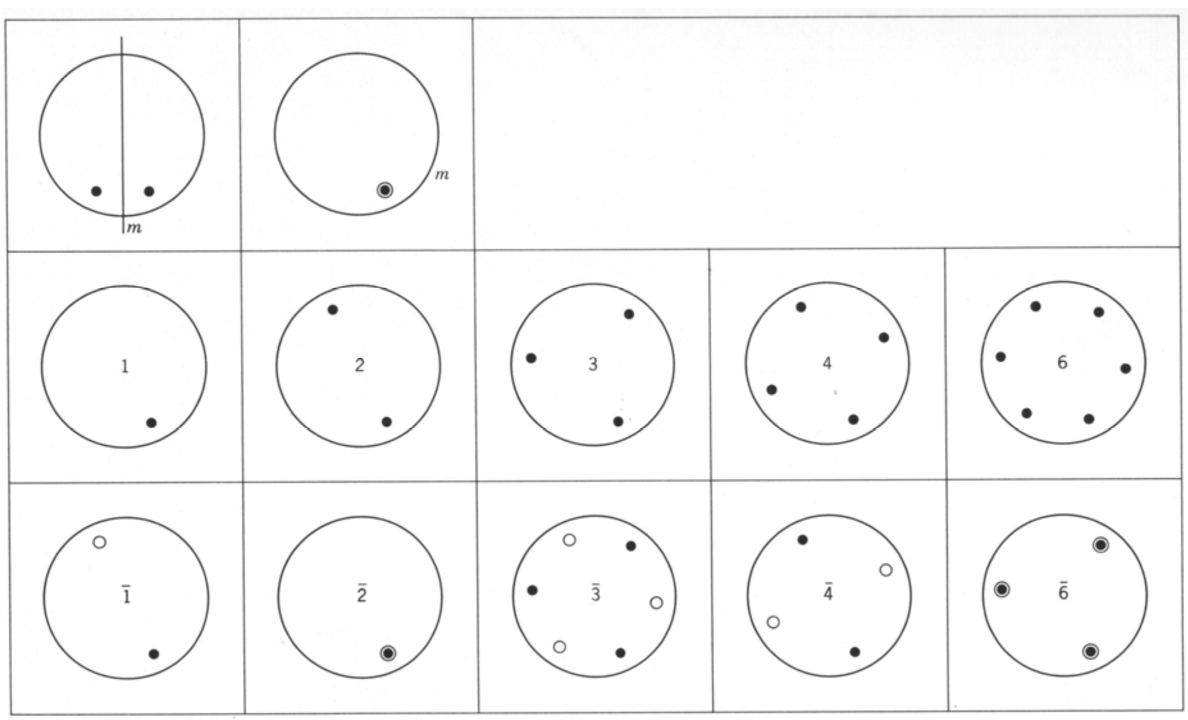

Fig. 1-8. The translation-free symmetry operations.

Note that **1** and $\bar{\mathbf{1}}$ represent the lowest symmetry conditions, 1-fold rotation and simple centrosymmetry (inversion through a center), respectively; this is the only symmetry in the triclinic system. It is also noted that $\bar{\mathbf{2}}$ is exactly equivalent to the mirror condition where the mirror plane is parallel with the page surface (found in the monoclinic system).

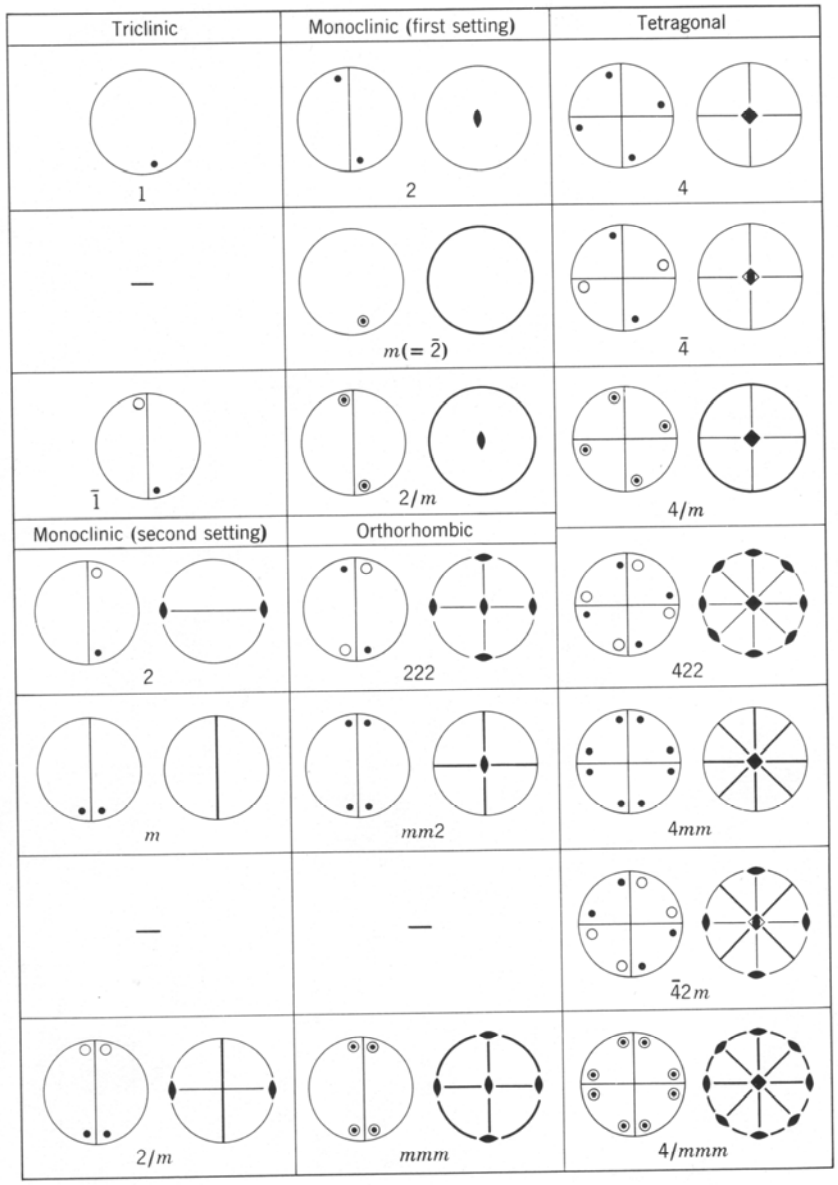

Fig. 1-9. The 32 point groups (after *International Tables for X-ray Crystallography*, **1**, Kynoch Press, Birmingham (1952)].

(Figure is continued on next page)

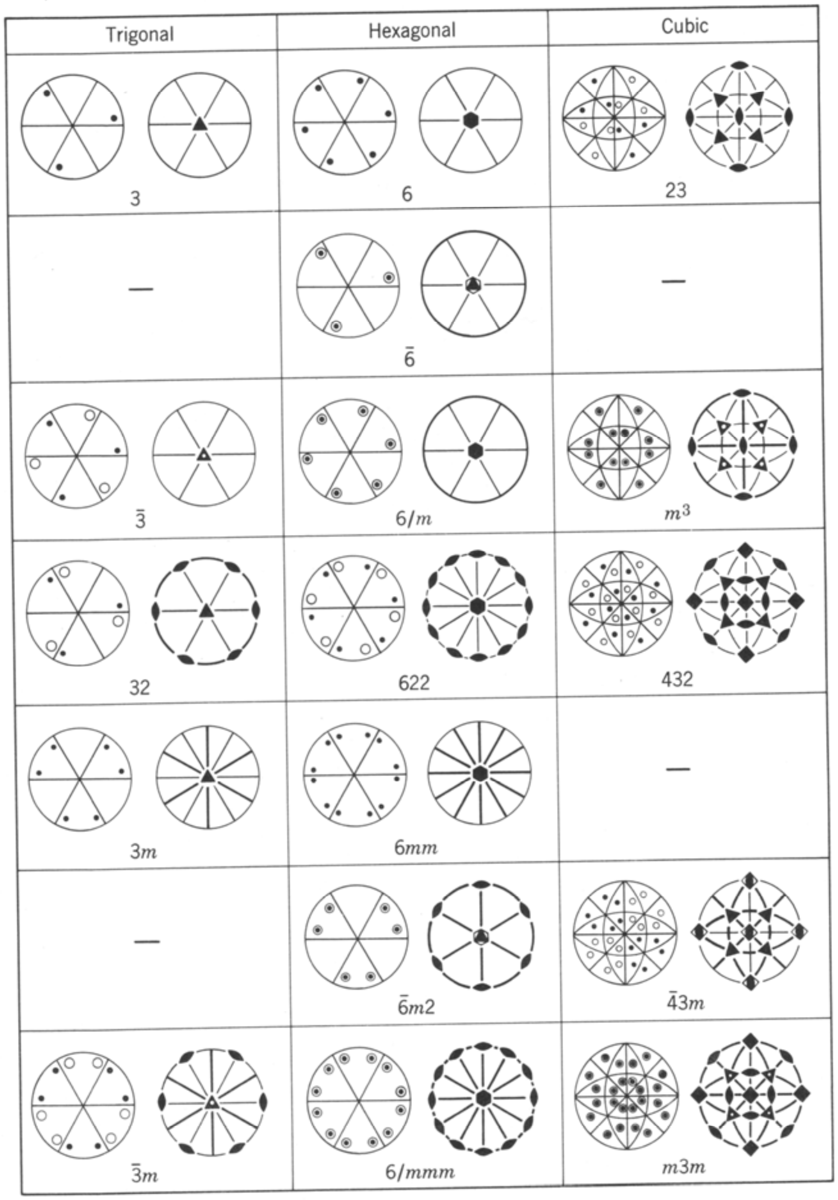

Fig. 1-9 (*Continued*).

Table 5.5 from Klein (2002) on the following page summarizes (and explains) the crystal classes as defined by their symmetry elements, including the standardized Hermann-Mauguin notation used in crystallographic notation. Some notation conventions:

- numbers indicate rotations (2-fold, 4-fold, etc.)
- multiple numbers indicate multiple rotations (usually parallel with axes; in higher symmetry systems rotations are around other symmetry directions)
- m indicates a mirror planes (multiple m = multiple mirror planes)
- /m following a number indicates rotation perpendicular to a mirror plane
- A bar over a number indicates a rotoinversion
- P (primitive), F (face centered), I (body centered), R (rhombohedral primitive), and side centered (A,B, or C) lattice types used with Space Group notation (Table 5.10)

TABLE 5.5 Characteristic Symmetry, and Relationships Between Crystal Axes and Symmetry Notation of Crystal Systems

Crystal Class	System	Characteristic Symmetry	Hermann–Mauguin Notation
1, $\bar{1}$	Triclinic	onefold (inversion or identity) symmetry only	Because of low symmetry, no crystallographic constraints.
2, *m*, 2/*m*	Monoclinic	one twofold rotation axis and/or mirror	The twofold axis is taken as the *b* axis, and the mirror (the *a–c* plane) is vertical (second setting).
222, *mm*2, 2/*m*2/*m*2/*m*	Orthorhombic	three mutually perpendicular directions about which there is binary symmetry (2 or *m*)	The symbols refer to the symmetry elements in the order *a*, *b*, *c*; twofold axes coincide with the crystallographic axes.
4, $\bar{4}$, 4/*m*, 422, 4*mm*, $\bar{4}$2*m*, 4/*m*2/*m*2/*m*	Tetragonal	one fourfold axis	The fourfold axis refers to the *c* axis; the second symbol (if present) refers to the axial directions (a_1 and a_2); the third symbol (if present) to directions at 45° to a_1 and a_2.
6, $\bar{6}$, 6/*m*, 622, 6*mm*, $\bar{6}$*m*2, 6/*m*2/*m*2/*m*, 3, $\bar{3}$, 32, 3*m*, $\bar{3}$2/*m*	Hexagonal*	one sixfold axis; one threefold axis	The first number refers to the *c* axis; the second and third symbols (if present) refer respectively to symmetry elements parallel to and perpendicular to the crystallographic axes a_1, a_2, and a_3.
23, 2/*m*$\bar{3}$, 432, $\bar{4}$3*m*, 4/*m*$\bar{3}$2/*m*	Isometric	four threefold axes each inclined at 54°44′ to the crystallographic axes (see Fig. 5.15)	The first number refers to the three crystallographic axes a_1, a_2, and a_3; the second number refers to four diagonal directions of 3-fold symmetry (between corners of a cube); the third number or symbol (if present) refers to six directions between the edges of a cube.

*The accepted orientation of the symmetry elements in two crystal classes of the hexagonal system is not straightforward. These are $\bar{6}$*m*2 and 3*m*. The location of the six- or threefold axis is unambiguous. However, the location of the next symmetry element is not obvious. In $\bar{6}$*m*2, the third entry (twofold rotation axes) coincides with the perpendiculars to a_1, a_2, and a_3; the *m*'s are coincident with these same directions. In 3*m* the *m*'s are located in directions perpendicular to a_1, a_2, and a_3.

Translation Operations

Direct translation (i.e., linear replication without rotation or reflection) enables the point group symmetry elements to replicate into a macroscopic crystalline structure but is not capable of adding unique symmetry to the structure and thus does not effect the variations which produce the Space Groups. Translational symmetry operations combine direct translation with rotation and/or reflection. These operations acting on the Bravais lattices and point groups produce the 230 Space Groups. The translational symmetry operations are:

Screw-axis: rotation about an axis combined with translation parallel to the axis. Screw axes are restricted by the translational periodicity of the crystals to repetitions at angular intervals of 180, 120, 90, and 60°, defining 2-fold, 3-fold, 4-fold and 6-fold axes, respectively. The subscript notation indicates the fraction of the total translation as the numerator of a fraction in which the main number is the denominator. Thus, 4_1 indicates 4-fold screw operation with ¼ the translation increment. 4_2 indicates 4-fold screw operation of a motif pair with ½ (i.e., 2/4) the translation increment.

Glide Plane: reflection across a plane combined with translation parallel to the plane. Glides are expressed as *a/2*, *b/2*, or *c/2* (increment x ½) when the glide is parallel to a crystallographic axis and the motif is repeated twice during in one translation increment. If the denominator is 4 (x ¼), the motif repeats 4 times during the increment. Diagonal glides occur, bisecting axis directions. Types are the diagonal (n) when the repeat increment is 2 or diamond (d) when the repeat increment is 4. Table 6.4 below from Klein (2002) summarizes the symbols used to represent the various mirror and glide planes.

TABLE 6.4 Symbols for Mirror and Glide Planes*

Symbol	Symmetry Plane	Graphic Symbol: Normal to Plane of Projection	Graphic Symbol: Parallel to Plane of Projection†	Nature of Glide Translation
m	Mirror		120°	None
a, *b*	Axial glide plane			*a*/2 along [100] or *b*/2 along [010]
c	Axial glide plane		None	*c*/2 along the *c* axis
n	Diagonal glide plane			*a*/2 + *b*/2; *a*/2 + *c*/2; *b*/2 + *c*/2; or *a*/2 + *b*/2 + *c*/2 (tetragonal and isometric)
d	Diamond glide plane			*a*/4 + *b*/4; *b*/4 + *c*/4; *a*/4 + *c*/4; or *a*/4 + *b*/4 + *c*/4 (tetragonal and isometric)

*From *International Tables for X-ray Crystallography*, 1969, v. 1, N. F. M. Henry and K. Lonsdale, eds.; Birmingham, England: Symmetry Groups. International Union of Crystallography, Kynoch Press.
†When planes are parallel to the paper, heights other than zero are indicated by writing the *z* coordinate next to the symbol (e.g., $\frac{1}{4}$ or $\frac{3}{8}$). The arrows indicate the direction of the glide component.

We will use Klein's (2002) CD-ROM tutorial material to demonstrate screw-axis and glide plane operations in class.

The following page is Table 5.10 from Klein, 2002, that lists the Space Group symbols for all the 230 space groups (and the associated crystal classes).

TABLE 5.10 The 230 Space Groups, and the Isogonal 32 Crystal Classes (Point Groups). The Space Group Symbols Are, in General, Unabbreviated*

Crystal Class	Space Group
1	$P1$
$\bar{1}$	$P\bar{1}$
2	$P2, P2_1, C2$
m	Pm, Pc, Cm, Cc
$2/m$	$P2/m, P2_1/m, C2/m, P2/c, P2_1/c, C2/c$
222	$P222, P222_1, P2_12_12, P2_12_12_1, C222_1, C222, F222, I222, I2_12_12_1$
$mm2$	$Pmm2, Pmc2_1, Pcc2, Pma2, Pca2_1, Pnc2, Pmn2_1, Pba2, Pna2_1, Pnn2, Cmm2, Cmc2_1, Ccc2, Amm2, Abm2, Ama2, Aba2, Fmmc, Fdd2, Imm2, Iba2, Ima2$
$2/m2/m2/m$	$P2/m2/m2/m, P2/n2/n2/n, P2/c2/c2/m, P2/b2/a2/n, P2_1/m2/m2/a, P2/n2_1/n2/a, P2/m2/n2_1/a, P2_1/c2/c2/a, P2_1/b2_1/a2/m, P2_1/c2_1/c2/n, P2/b2_1/c2_1/m, P2_1/n2_1/n2/m, P2_1/m2_1/m2/n, P2_1/b2/c2_1/n, P2_1/b2_1/c2_1/a, p2_1/n2_1/m2_1/a, C2/m2/c2/m, C2/m2/c2_1/a, C2/m2/m2/m, C2/c2/c2/m, C2/m2/m2/a, C2/c2/c2/a, F2/m2/m2/m, F2/d2/d2/d, I2/m2/m2/m, I2/b2/a2/m, I2/b2/c2/a, I2/m2/m2/a$
4	$P4, P4_1, P4_2, P4_3, I4, I4_1$
$\bar{4}$	$P\bar{4}, I\bar{4}$
$4/m$	$P4/m, P4_2/m, P4/n, P4_2/n, I4/m, I4_1/a$
422	$P422, P42_12, P4_122, P4_12_12, P4_222, P4_22_12, P4_322, P4_32_12, I422, I4_122$
$4mm$	$P4mm, P4bm, P4_2cm, P4_2nm, P4cc, P4nc, P4_2mc, P4_2bc, I4mm, I4cm, I4_1md, I4_1cd$
$\bar{4}2m$	$P\bar{4}2m, P\bar{4}2c, P\bar{4}2_1m, P\bar{4}2_1c, P\bar{4}m2, P\bar{4}c2, P\bar{4}b2, P\bar{4}n2, I\bar{4}m2, I\bar{4}c2, I\bar{4}2m, I\bar{4}2d$
$4/m2/m2/m$	$P4/m2/m2/m, P4/m2/c2/c, P4/n2/b2/m, P4/n2/n2/c, P4/m2_1/b2/m, P4/m2_1/n2/c, P4/n2_1/m2/m, P4/n2_1/c2/c, P4_1/m2/m2/c, P4_2/m2/c2/m, P4_2/n2/b2/c, P4_2/n2/n2/m, P4_2/m2_1/b2/c, P4_2/m2_1/n2/m, P4_1/n2_1/m2/c, P4_2/n2_1/c2/m, I4/m2/m2/m, I4/m2/c2/m, \mathrm{I}4_1/a2/m2/d, I4_1/a2/c2/d$
3	$P3, P3_1, P3_2, R3$
$\bar{3}$	$P\bar{3}, R\bar{3}$
32	$P312, P321, P3_112, P3_121, P3_212, P3_221, R32$
$3m$	$P3m1, P31m, P3c1, P31c, R3m, R3c$
$\bar{3}2/m$	$P\bar{3}1m, P\bar{3}1c, P\bar{3}m1, P\bar{3}c1, R\bar{3}m, R\bar{3}c$
6	$P6, P6_1, P6_5, P6_2, P6_4, P6_3$
$\bar{6}$	$P\bar{6}$
$6/m$	$P6/m, P6_3/m$
622	$P622, P6_122, P6_522, P6_222, P6_422, P6_322$
$6mm$	$P6mm, P6cc, P6_3cm, P6_3mc$
$\bar{6}m2$	$P\bar{6}m2, P\bar{6}c2, P\bar{6}2m, P\bar{6}2c$
$6/m2/m2/m$	$P6/m2/m2/m, P6/m2/c2/c, P6_3/m2/c2/m, P6_2/m2/m2/c$
23	$P23, F23, I23, P2_13, I2_13$
$2/m\bar{3}$	$P2/m\bar{3}, P2/n\bar{3}, F2/m\bar{3}, F2/d\bar{3}, I2/m\bar{3}, P2_1/a\bar{3}, I2_1/a\bar{3}$
432	$P432, P4_232, F432, F4_132, I432, P4_332, P4_132, I4_132$
$\bar{4}3m$	$P\bar{4}3m, F\bar{4}3m, I\bar{4}3m, P\bar{4}3n, F\bar{4}3c, I43d$
$4/m\bar{3}2/m$	$P4/m\bar{3}2/m, P4/n\bar{3}2/n, P4_2/m\bar{3}2/n, P4_2/n\bar{3}2/m, F4/m\bar{3}2/m, F4/m\bar{3}2/c, F4_1/d\bar{3}2/m, F4_1/d\bar{3}2/c, I4/m\bar{3}2/m, I4_1/a\bar{3}2/d$

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