CHAPTER II

X-RAY DIFFRACTION

II.1 Relationships of Reciprocal Lattice to Bragg's Law and Laue's Conditions.

II.1.1 Introduction of x-ray diffraction

Like visible light, x-rays which are also electromagnetic waves, when passing through a crystal cause diffraction if certain geometrical conditions are fulfilled.

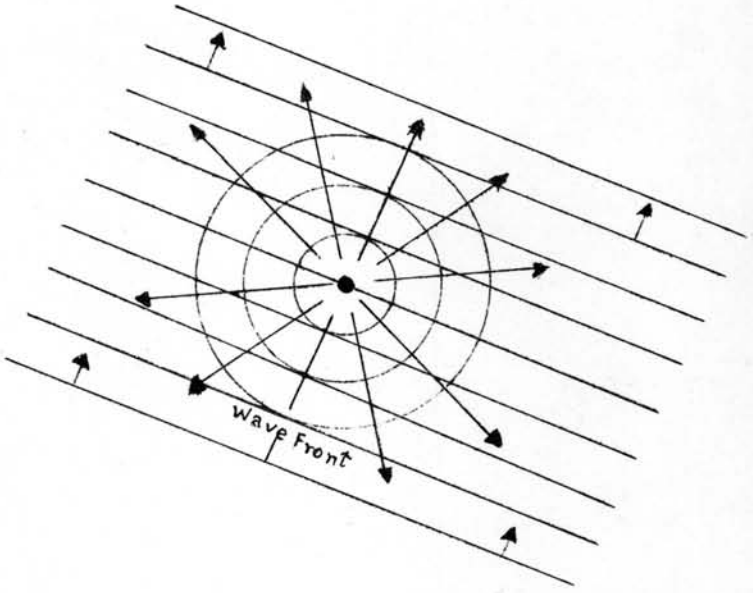


Fig.2.1 An electron acts as a source of secondary x-rays.

All atoms in the path of an x-ray beam scatter x-rays simultaneously but the atom is not a point source of x-rays.(15) An electron within the atom is set in vibratory motion under the influence of a beam of x-rays, and generates a new set of coherent electromagnetic waves having the same frequency and

wavelength as the incident beam. In this explanation we neglect the interaction between the incident beam and the seattered waves including no re-scattered waves by other lattice points. Then the electron has the effect of scattering the incident radiation and acts as a source of secondary x-rays. Each electron scatters x-rays and they combine to give the effect of a point source. Therefore, the atom as a whole scatters x-rays. This cooperative scattering is known as diffraction.[3,15]

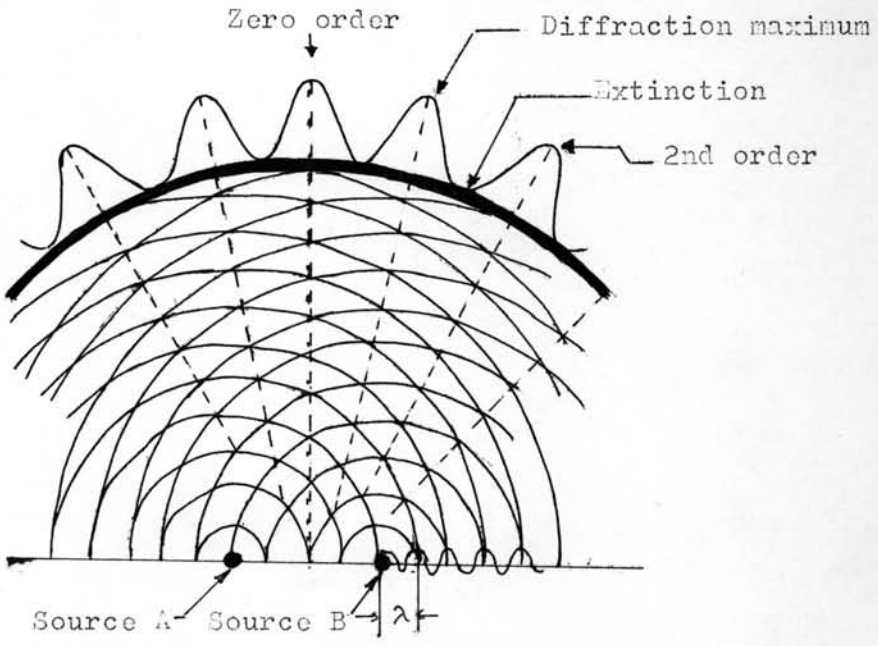


Fig.2.2 Cooperative scattering by two sources

II.1.2 The Laue conditions

In order to understand three dimensional Laue's conditions we must first understand simple diffraction by a row of identical, equally spaced atoms. Each atom in the row can be considered as the center of radiating, spherical wave shells, as a beam of x-rays passes it. These scattered waves interfere with one

another and when they are in phase they combine to give moximum diffraction. This happens when the path difference between rays scattered from adajacent atoms is zero or any whole number of wavelengths, i.e.

path difference = $h\lambda$ where h is some integer 0, $\pm$ 1, $\pm$ 2, ... which designetes the order of diffraction. See Fig.2.3.

Two rays of x-ray beam strike the row of periodicity a, at an angle of incidence μ and make the diffracted angle ν_i (i = 0,1,2,3,...). Then from Fig. 2.3.

$a(\cos\nu_0 - \cos\mu) = 0\lambda$ for zero order diffraction,

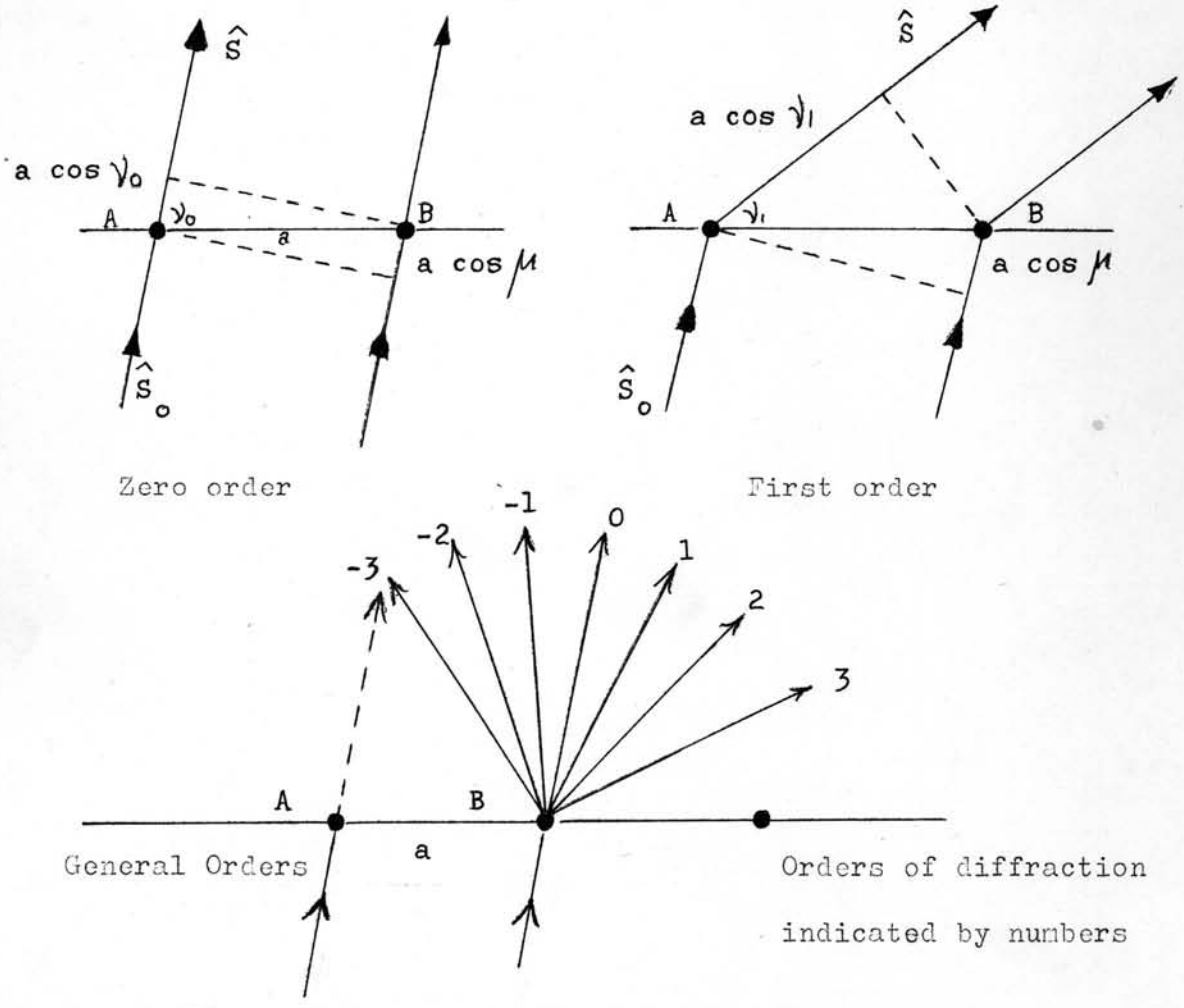


Fig.2.3 The conditions for diffraction by a row of atoms.

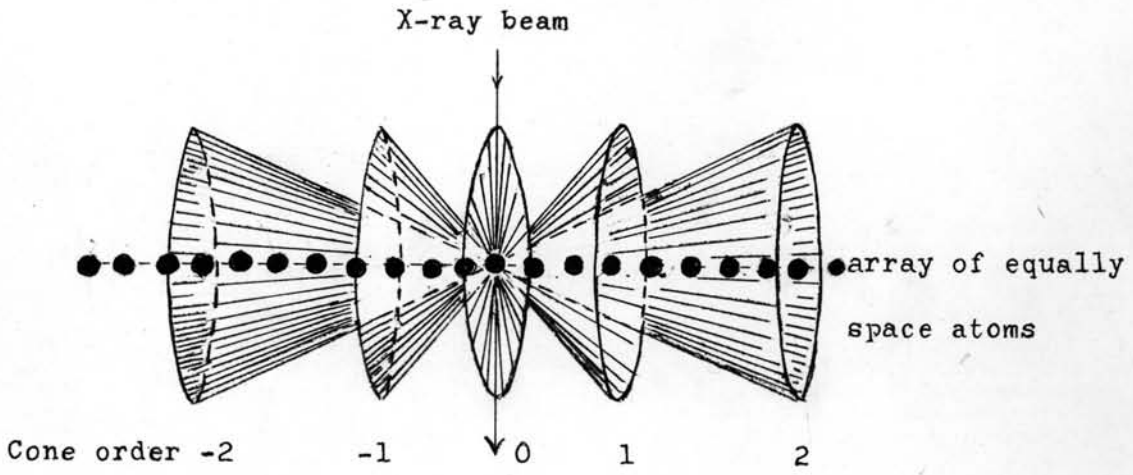


Fig. 2.4 Showing cones of diffracted beam formed by a row of identical regularly spaced atoms.

$a(\cos\gamma_1 - \cos\mu) = 1\lambda$ for 1st order diffraction where a is the distance between atom A and B. In general

$$a(\cos\gamma - \cos\mu) = h\lambda \text{ where h is an integer} \quad (1.a)$$

In vector notation we can write

$$\bar{a}\cdot(\hat{S} - \hat{S}_o) = h\lambda \quad (1.b)$$

where $\hat{S}_o$ is the unit vector for incident beam and $\hat{S}$ is the unit vector for diffracted beam. For a given incident direction $\hat{S}_o$, lattice spacing a, wavelength λ, and integer value h, there is only one possible scattering angle

$$\cos\gamma = \cos\mu - \frac{h\lambda}{a} \quad (2)$$

This defines a cone of rays which all atoms of a row are scattering in phase and coaxial with the row with half apex

angle equals to γ as illustrated in Fig. 2.4.

The expression of equation (1) is called Laue's equation for a row of atoms.

If there is a plane containing a lattic array of atoms with spacing a in one direction and b in the other, there will be two simultaneous diffractions to be fulfilled :

$$\begin{aligned} \bar{a} \cdot (\hat{S} - \hat{S}_o) &= h\lambda \\ \bar{b} \cdot (\hat{S} - \hat{S}_o) &= k\lambda \quad \text{where k is an integer.} \end{aligned} \tag{3}$$

Because each row has its own set of cones about its axis, the intersection of these two concentric cones of h and k order is a direction for diffraction. (Fig. 2.5)

The same argument applied for three dimensional lattic array of atoms with spacing c for the third dimension. Therefore Laue's conditions for diffraction to occur are as follow[1,2,3,15]

$$\begin{aligned} \bar{a} \cdot (\hat{S} - \hat{S}_o) &= h\lambda \ , \\ \bar{b} \cdot (\hat{S} - \hat{S}_o) &= k\lambda \ , \\ \bar{c} \cdot (\hat{S} - \hat{S}_o) &= \ell\lambda \ , \end{aligned} \tag{4}$$

where h, k, and ℓ are integers. The requirement that three equations are simultaneously satisfied acts as a limitation for diffraction to occur, that is, it can occur only if the diffracted angles. γ_a , γ_b , and γ_c define the same direction (Fig. 2.6). This fulfilling of Laue's equations, h th order cone of spacing a, k th order of spacing b, and ℓ th order of spacing c, is equivalent to a reffection of the incident beam by the atoms of the planes(h k ℓ).

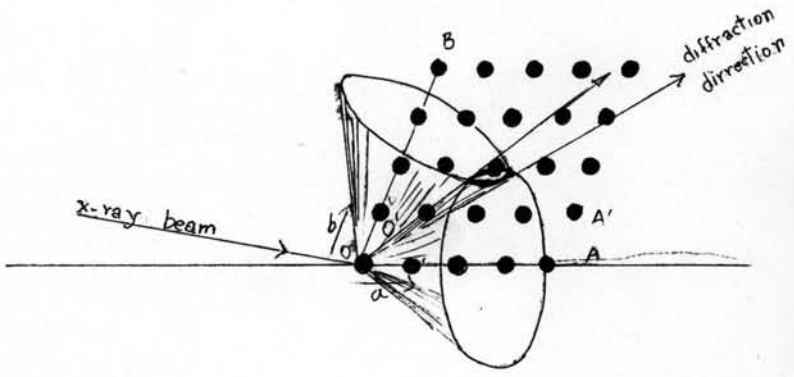


Fig.2.5 Intersection of two cones defining possible scattering direction.

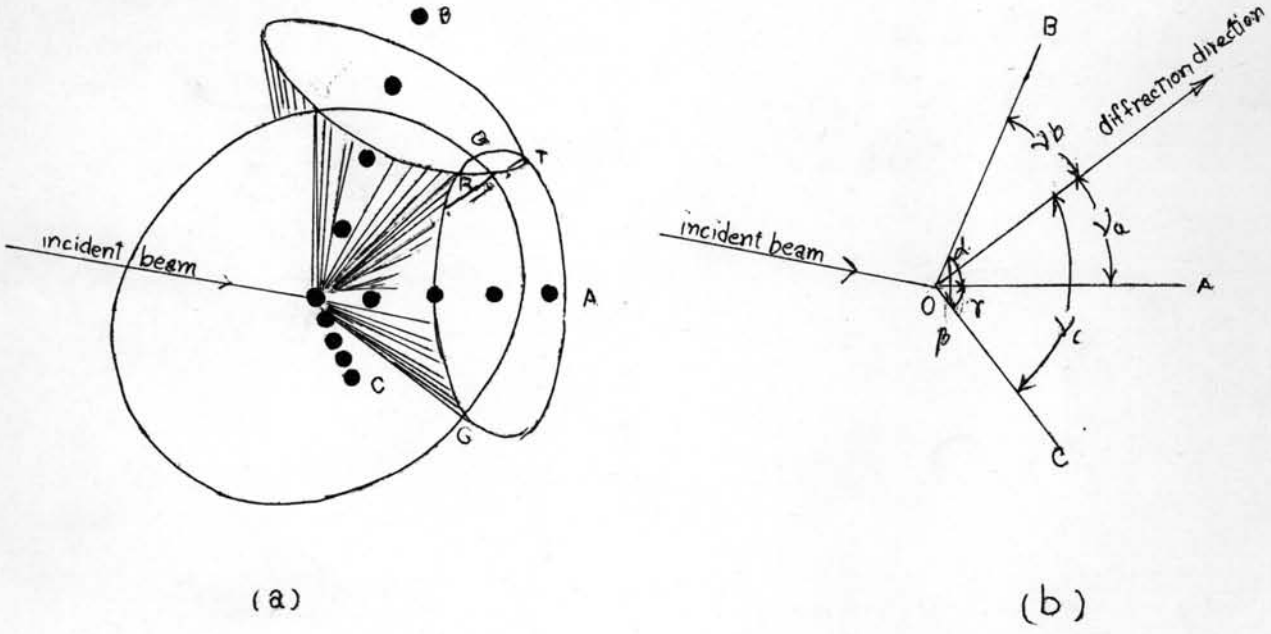


Fig.2.6 (a) Intersecting cones defining possible diffraction for three-dimensional lattice

(b) Defining possible diffraction direction (three cones intersect in one line.

II.1.3 The "reflection" of x-rays by crystal planes and Bragg's law.[2,3,8,14,15]

To understand the consequences of the principles explained above, consider the lattic in Fig. 2.7. When Laue's conditions are satisfied i.e. in the h th order cone around OA, in the k th order around OB, and in the th order around OC have the same line of intersection, this means that the rays scattered from point A and point O have a path difference of h wavelengths. Therefore the point A at a distance a/h from the origin O scatters a ray one wavelength ahead of those at the origin. Similarly at B and C rays are scattered with path differences of k and l wavelength from O and at B′ and C′ the path difference is one wavelength. Thus, points A′,B′, and C′ scattere rays differing in phase by the same number of wavelengths from those scattered at O, so they have no path difference from one another. These points lie on the crystal plane that has Miller indicies (h k l), therefore this plane acts as if it were reflecting the incident beam. There are families of these planes which are parallel to one another and each capable of scattering rays.

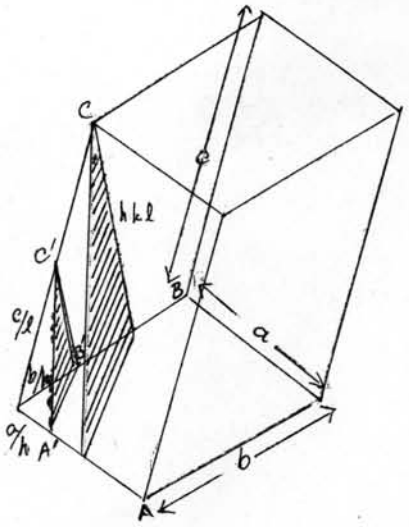
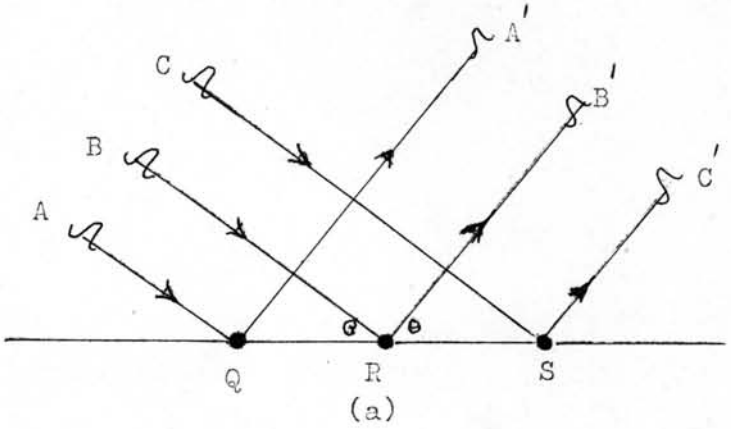
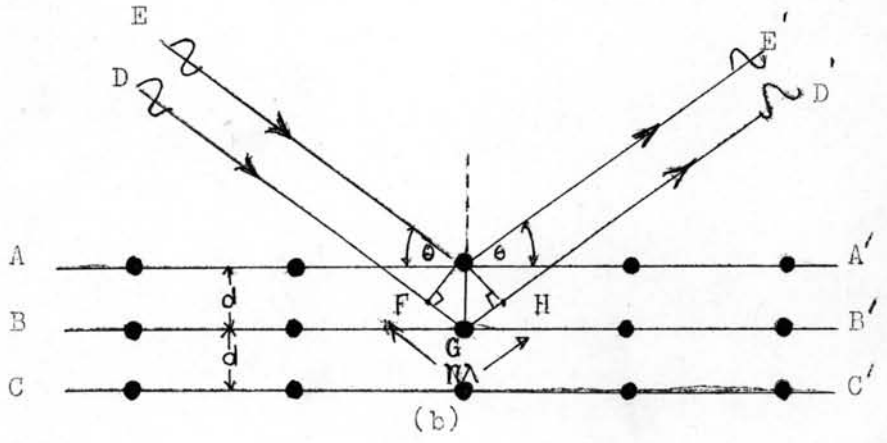


Fig. 2.7 A reflecting plane (h k ℓ)



(a)



(b)

Fig.2.8 (a) Reflection by a plane (h k ℓ)

(b) Reflection from stack of planes (h k ℓ)

Condsider a set of parallel planes of atoms in a crystal AA′, BB′, and CC′ with interplanar spacing d as shown in Fig. 2.8,(a) shows the condition for a plane (h k ℓ) and (b) illustrates the diffraction condition from the different planes to occur with the incident angle θ and reflected angle θ. The condition for constructive reflection is that

path difference = $n\lambda$ where n is an integer.

then $FG + GH = n\lambda$

and $FG = GH = d \sin\theta$.

Thus $2d \sin\theta = n\lambda$ (5)

which is Bragg's law for diffraction.

II.1.4 The Reciprocal lattice with Bragg's law and Laue's equations.

There is a relationship between the reciprocal lattice and Bragg's law. Since the diffraction is related to Laue's equations and Bragg's equation therefore they are all interalated. Consider Bragg's equation (5) which can be written as

$$\sin\theta = \frac{n\lambda}{2d}$$

By eliminating the term n we can write

$$\sin\theta_{h\,k\,\ell} = \frac{\lambda}{2\,d_{h\,k\,\ell}}$$

or

$$\sin\theta_{h\,k\,\ell} = \frac{\lambda / d_{hk\ell}}{2} \qquad (6)$$

Equation (6) can be expressed by a right angled triangle inscribed in a circle with a diameter of its hypotenuse side (Fig. 2.9)

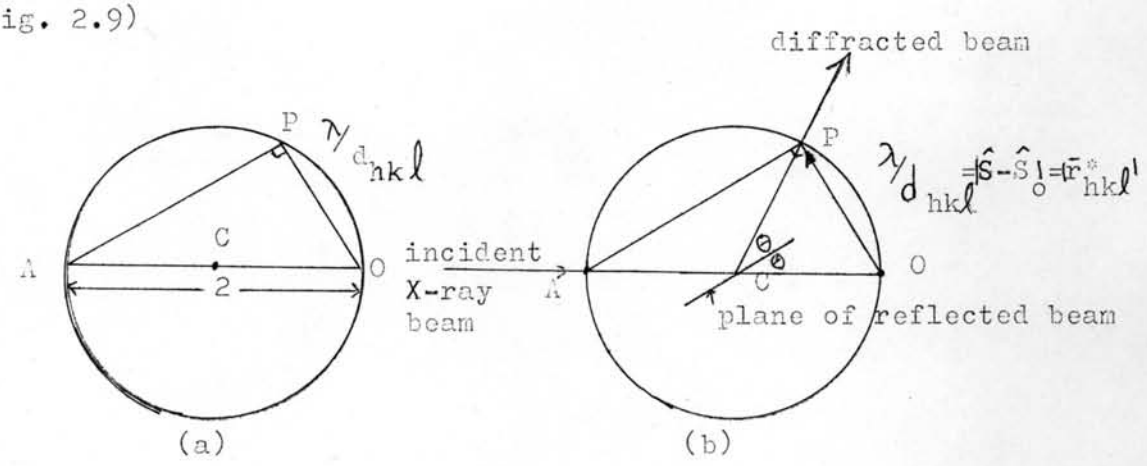


Fig. 2.9 Geometrical representation of Bragg's law.

In physical terms we can assume the incident beam enters and passes out in the direction AO. Then there is a crystal plane (h k ℓ) at the center of the circle which makes an angle θ with AO. Then CP must be the direction of the reflected beam. To relate this to the recipocal lattice concept, let us first define the basis vectors of a reciprocal lattice (11,12) $\bar{a}^*$, $\bar{b}^*$, and $\bar{c}^*$ in relation to the direct lattice constant as

$$\bar{a}^* \cdot \bar{a} = \bar{b}^* \cdot \bar{b} = \bar{c}^* \cdot \bar{c} = \lambda$$

and $$\bar{a}^* \cdot \bar{b} = \bar{a}^* \cdot \bar{c} = \bar{b}^* \cdot \bar{c} = \bar{b}^* \cdot \bar{a} = \bar{c}^* \cdot \bar{a} = \bar{c}^* \cdot \bar{b} = 0 \qquad (7)$$

Then a reciprocal lattice vector can be written as

$$\bar{r}^*_{hk\ell} = h\bar{a}^* + k\bar{b}^* + \ell\bar{c}^* \qquad (8)$$

where h,k and ℓ are all integers. Bragg's law can be

interpreted in terms of reciprocal lattice by defining[1,2,12]

$$\frac{\lambda}{d_{hk\ell}} = |r^*_{hk\ell}| \quad \ldots\ldots\ldots \quad (9)$$

Point O is the origin of the reciprocal lattice and point P is the end of the reciprocal lattice vector $\bar{r}^*_{hk\ell}$ (Fig.2.9 (b)). Since OP is normal to AP and AP is parallel to the crystal plane therefore OP must be normal to the crystal plane and $\overline{OP}$ can be the vector normal to the reflected plane. From equation (4) we get

$$\begin{aligned} \bar{a}.(\hat{S} - \hat{S}_o) &= \lambda h = \bar{a}.\bar{r}^*_{hk\ell} = \bar{a}.(h\bar{a}^* + k\bar{b}^* + \ell\bar{c}^*), \\ \bar{b}.(\hat{S} - \hat{S}_o) &= \lambda k = \bar{b}.\bar{r}^*_{hk\ell} = \bar{b}(h\bar{a}^* + k\bar{b}^* + \ell\bar{c}^*), \\ \bar{c}.(\hat{S} - \hat{S}_o) &= \lambda \ell = \bar{c}.\bar{r}^*_{hk\ell} = \bar{c}(h\bar{a}^* + k\bar{b}^* + \ell\bar{c}^*). \end{aligned} \quad (10)$$

Then $\hat{S} - \hat{S}_o = \bar{r}^*_{hk\ell}$.

This is illustrated in Fig. 2.10

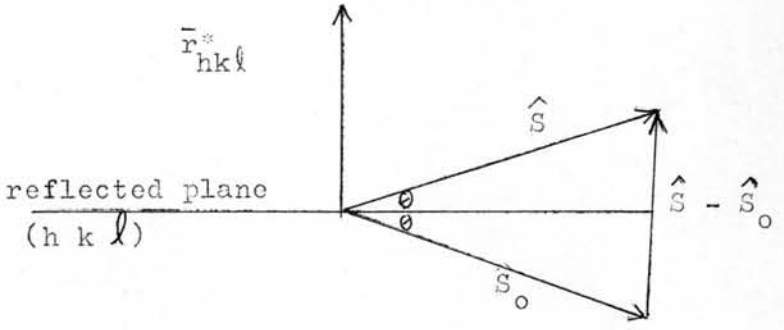


Fig.2.10 Bragg reflection and the reciprocal lattice.

Since the vector $\hat{S} - \hat{S}_o$ is at right angles to the reflected plane and parallel to the vector $\bar{r}^*_{hk\ell}$ then these two can be normal vectors of the reflected plane. From Fig. 2.10 we can easily seen that

$$|\hat{S} - \hat{S}_o| = 2 \sin \theta$$

and $$|\hat{S} - \hat{S}_o| = |\bar{r}^*_{hk\ell}| \quad \ldots\ldots (12)$$

and from equation (9) and (12) we have

$$\frac{2 \sin \theta}{\lambda} = \frac{1}{d_{hk\ell}} \quad \ldots\ldots (13)$$

which is Bragg's law. Then the reciprocal lattice, Bragg's law, and Laue's conditions are all related to one another.

Bragg's law is satisfied whenever a reciprocal lattice point lies anywhere on the circle or on the surface of a sphere in three dimensions. This sphere is called the "sphere of reflection" or "Ewald's sphere." Then the reciprocal lattice can be used in combination with the sphere of reflection to explain any x-ray diffraction experiment. Reflection occurs only when the orientation of the crystal is such that a reciprocal lattice point lies on the circumference of a circle. So a photographic record of the reflected x-ray beams is nothing more than a photographic record of the reciprocal lattice.

Since all three of them are related to one another, then they are two ways in which reflection can occur, viz : by varying λ or θ in Bragg's law one at a time.

	Radiation	θ	Method
Variable	White	Fixed	Laue; stationary single crystal
Fixed	Monochromatic	Variable	Powder; poly crystalline
			Rotation; Weissenberg;
			single crystal-nonstationary.

(a) Varying λ by using white radiation on a fixed single crystal. The Bragg angle θ is therefore fixed and each set picks out the λ that satisfied Bragg's law for the particular value of d and θ. Each diffracted beam thus has a different wavelength. This is called the Laue method :

(b) Varying θ ,

(1) Rotation method.[1,2,3,6,10,15,16] A single crystal is mounted with one of its axis normal to a monochromatic x-ray beam, and rotates about this axis. This allows a particular set of lattice planes to reflect the beams as the crystal reaches each of the several special preintations. The result is that the diffracted beams from cones that are coaxial about the rotation axis of the crystal. By using a cylindrical film coinciding with the crystal's axis of rotation the diffracted beams intersect the film in a set of circles which appear as straight lines when flattened out and are called layer lines. This method is called the rotation method and with it the direct lattice constant of the rotation axis can be determined. Consider Fig. 2.11, the angle γ is the semi- apex angle of the cone, depends on the spacing y of the reciprocal planes. For convenience in measurements complementary angle ν is used. For the first layer cone, ν_1 is fixed by

$$\sin \nu_1 = \frac{\xi}{1} = \lambda/c \quad \ldots\ldots\ldots (14)$$

where ζ is the cylindrical coordinate of a reciprocal lattice as shown in Fig. 2.11 (c), and c is the direct lattice constant along a rotation axis.

For the nth layer line

$$\sin \nu_n = \frac{\zeta}{i}_n = \frac{n\lambda}{c} \qquad \ldots\ldots\ldots (15)$$

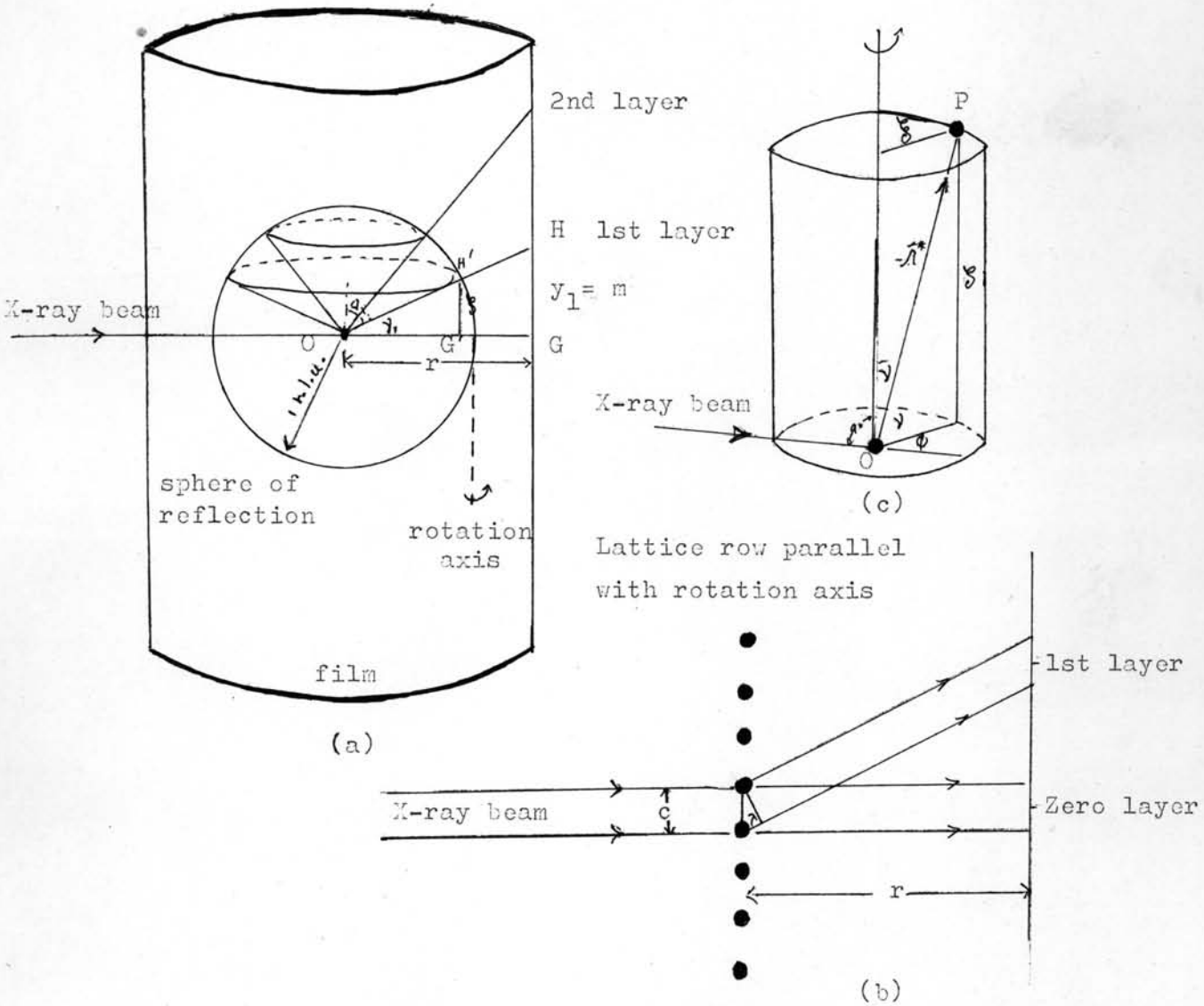


Fig.2.11 (a) The geometrical representation of rotation photograph.

(b) Showing the existence of layer lines in a rotation pattern.

(c) Cylindrical reciprocal lattice coordinate.

Then from equation (14) and (15)

$$c = \frac{\lambda}{\sin \gamma_1} \qquad \ldots\ldots (16)$$

and

$$c = \frac{n \lambda}{\sin \gamma_n} \qquad \ldots\ldots (17)$$

To find γ_1 and γ_n, (see Fig.2.11(a)) : triangle OGH is similar to triangle OGH, therefore

$$\tan \gamma_1 = \frac{GH}{OG} ,$$

but GH = y_1 the distance between the zero and first layer lines and OG = r, the radius of the cylindrical camera.

Thus

$$\tan \gamma_1 = \frac{y_1}{r}$$

$$\gamma_1 = \tan^{-1} \frac{y_1}{r} \qquad \ldots\ldots (18)$$

From equation (16) and (18)

$$c = \frac{\lambda}{\sin (\tan^{-1} \frac{y_1}{r})} \qquad \ldots\ldots (19)$$

Similarly for the n th layer line

$$c = \frac{\lambda}{\sin (\tan^{-1} \frac{y_n}{r})} \qquad \ldots\ldots (20)$$

where y_n is measured from the average distance between the + n th and the - n th layer lines on the film.

(1,3,10,15,16)

(2) Weissenberg method. The development of the rotation method by applying the idea of a moving film is called the Weissenberg method. This method resolves each diffracted spot of a single cone onto different portions of the film by screening out unwanted cones, and the film is made to move in synchronism with the rotation of the crystal. So a particular set of reflections such as 0 k , 1 k , or 2 k is allowed to fall on the film in such a way that to each point on the photograph there corresponds a single value of k and . The method provides another two crystallographic constants, an angle between them, and indicies of spots whose space group can be determined. Indicies of more than one layer are needed to obtain all the necessary data inorder to specify the crystal's space groups.

For the zero layer the normal beam method in which the incident beam is normal to the rotation axis, is used. For other layers the equi-inclination method is used, in which the incident beam enters the reflecting circle along the generator of the reflected cone to avoid the blind region of certain reflections lying near the origin of that level. (see Fig. 2.12)

There are two instrumental settings for the upper level photograph.

(1) The inclination angle μ , the complement of the angle between the incident beam and the rotation axis, can be determined from Fig. 2.12(b)

$$\mu = \sin^{-1} \frac{\vartheta_n}{2} \qquad \ldots\ldots\ldots (21)$$

where ϑ_n can be obtained from the rotation photograph. From equation (15) and (18) we have

$$\vartheta_n = \sin \left[\tan^{-1} \frac{y_n}{r} \right] \qquad \ldots\ldots\ldots (22)$$

Conseguently

$$\mu = \sin^{-1} \left[\frac{\sin \tan^{-1} \frac{y_n}{r}}{2} \right] \ldots\ldots (23)$$

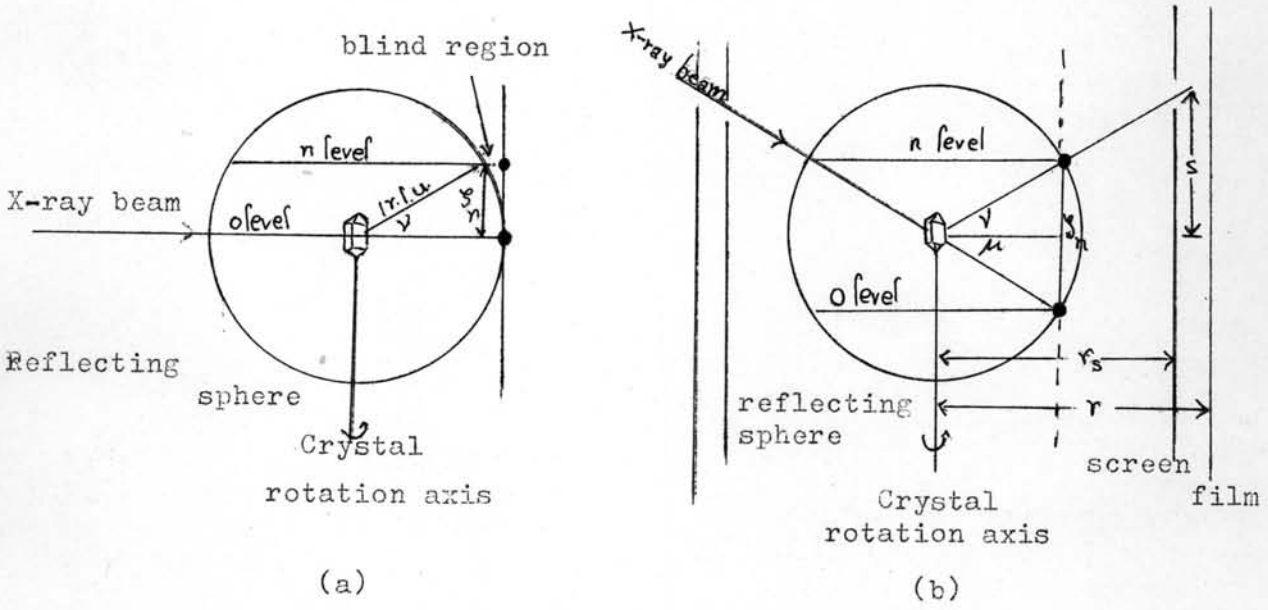


Fig.2.12 Geometrical arrangements for the Weissenberg method.
a) normal beam method, b) equi-inclination method.

(2) the layer line screen setting s which is the distance s mm. through which the layer line screen must be moved from its zero level position. From Fig.2.12 we see that the distance is related to the radius of the screen r_s and the inclination angle μ as follow

$$s = r_s \tan \mu \qquad \ldots\ldots\ldots\ldots (24)$$

But $\gamma = \mu$ where the angle γ is the complement of the semiangle of the diffracted cone.

Thus

$$s = r_s \tan \mu \qquad \ldots\ldots\ldots\ldots (25)$$

The reciprocal cylindrical coordinates δ (xi) and φ (see Fig.2.11 (c)) can be obtained directly from the spot on the film and the reciprocal lattice net can be constructed with chosen axes.

(3) Powder method. This method used powdered crystal or a fine grained polycrystal oriented at random to a monochromatic beam. The conditions for diffraction are just as in the rotation method. This method provides much useful information but in the present research its use is confined to obtaining a more refined measurement of the three cell dimensions.

We can obtain $\sin^2\theta_{hk}$ from the powder photograph and from Bragg's equation (5) and (6)

$$\sin^2 \theta_{hk\ell} = \frac{\lambda^2}{4d^2_{hk\ell}} \qquad \ldots\ldots\ldots\ldots (26)$$

where $d_{hk\ell}$ is the interplanar spacing for plane ($hk\ell$). For the orthorhombic system

$$d_{hk\ell} = \frac{1}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}} \qquad \ldots\ldots\ldots\ldots (27)$$

Knowing, a, b, and c from the rotation and Weissenberg photographs we can calculate $\sin^2 \theta_{hk\ell}$. By comparing the observed values of $\sin^2 \theta$ and $\sin^2 \theta_{hk\ell}$, we can obtain a value for new $d_{hk\ell}$ for each diffracted line consequently the new a, b, and c can be obtained.

II.2 Space Group

A crystal structure is a periodic space pattern which is an orderly periodic arrangement of atoms that constitues a crystal. There are 230 kinds of space group and each crystal belongs to one of them. A fundamental property of the patterns is a repetition, so in developing the classification of crystals, the elements of symmetry can be divided into three categories[3]:

1. translation
2. point group symmetry
3. space group symmetry

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[3] E.W. Nuffield, X-Ray Diffraction Method (New York : John Wiley Sons, Inc.,1966), p.p. 1 - 9.

II.2.1 Translation and plane lattice

From the crystal structure each repeat motif is replaced by a point called a lattice. The lattice can be considered as a collection of equipoints that portrays the translational periodicity of the structure. The translational periodicity can be represented by three primitive translation vectors, $\bar{a}$, $\bar{b}$, and $\bar{c}$. The axial lengths a, b, and c with three interaxial angles, α between $\bar{b}$ and $\bar{c}$, β between $\bar{a}$ and $\bar{c}$, and γ between $\bar{a}$ and $\bar{b}$, define a unit cell of the primitive type, i.e. it has points at the corners only. This translation lattice limits only five distinct plane lattices which are based on the magnitude of the translation and the angle between them as shown in Fig.2.13.

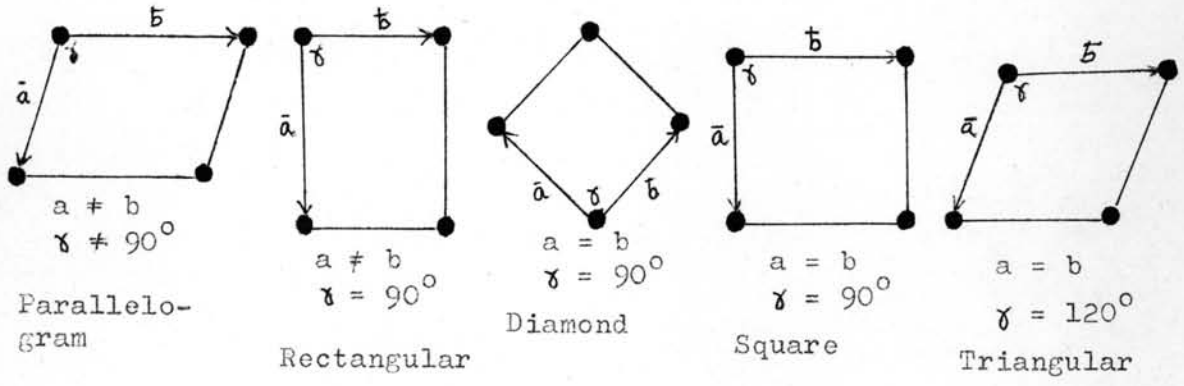


Fig. 2.13 Five plane lattices

II.2.2 Point groups and crystal systems

If a body can be divided into parts that are related to one another in certain ways then it is symmetrical, and the

operator that transforms one part to the other symmetrically related part is called a symmetry operation, leaving the body indistinguishable from its original state. The symmetry operations which are required for repetition are rotation, reflection, and inversion. This operation can be described by symmetry elements by which the equivalent points are brought into coincidence. They are divided into three main elements [13] ; symmetry axes, a symmetry plane, and a center of symmetry.

(1) Symmetry axes are produces by rotation through an angle $\frac{2\pi}{n}$, and are said to have n-fold axis of rotation. But this operation is limited to conform with that possible in a periodic extended lattice. This limits us to axes of one-, two-, three-, four-, and sixfold rotation symmetry axes.

(2) A symmetry plane operates by reflection across the plane which brings the equivalent point into coincidence with itself. This may be designated as mirror plane m.

(3) A center of symmetry operates by inversion across a center which matches the equivalent point on one side with those at other side. In vector expression $\bar{r}$ is converted to $-\bar{r}$ by inversion operator.

Two symmetries of rotation and inversion exhibit other symmetry axes called rotation-inversion axes. They are 1-,2-, 3-, 4-, and 6- fold rotation inversion axes, designated by

$\bar{1}$, $\bar{2}$, $\bar{3}$, $\bar{4}$, and $\bar{6}$. The $\bar{2}$ is equivalent to m, so it is actually 10 units of symmetry shown in table 2.1.

Table 2.1

Symmetry Elements (14,pp.15)

Symmetry	Symbol
No symmetry	1
Mirror plane of symmetry	m or ($\bar{2}$)
Twofold rotation	2
Threefold rotation	3
Threefold rotation inverter	$\bar{3}$
Fourfold rotation	4
Fourfold rotatory inverter	$\bar{4}$
Sixfold rotation	6
Sixfold rotatory inverter	$\bar{6}$
Inverter	$\bar{1}$

These features are the basis of the classification of the crystal into 32 crystal classes. These 10 units of symmetry element combine in 32 ways to represent all the kinds of symmetry found in a crystal. So there are 32 point groups. A point group may be defined as a group of symmetry operation which can operate on infinite three dimensional lattices so as to leave one point unmoved.

The 32 crystal classes may be divided into seven main crystal systems, each characterized by the possession of a certain minimum of symmetry elements, and referable to certain characteristic axis as shown in table 2.2.

Table 2.2

Crystal system and its minimum symmetry elements (11)

System	its minimum symmetry element
Triclinic	one fold symmetry only
Monoclinic	a single twofold axis
Orthorhombic	three mutually perpendicular twofold axes
Tetragonal	a single fourfold axis
Trigonal or Rhombohedral	a single threefold axis or sixfold axis
Hexagonal	a single sixfold axis
Cubic	four equivalent threefold axes.

LL.2.3 Space lattices and the 14 Bravais lattices

Space lattice can be thought of as a periodic stack of plane lattices with different ways of stacking and consistent with the symmetries of 32 point groups. They are only five unique space lattice types as shown in table 2.3.

Table 2.3

Space lattice types[1]

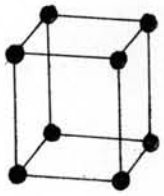
Name	Location of nonorigin points	Symbol
Primitive		P
Side-centered	Center of A face or (100) if A-centered	A
	Center of B face or (010) if B-centered	B
	Center of C face of (001) if C-centered	C
Face - centered	Centers of A,B, and C faces	F
Body - centered	Center of each cell	I
Rhombohedral	If primitive rhombohedron is referred to hexagonal cell	R

These five space lattices are distributed in the seven crystal systmes and constritute fourteen Bravais lattices as shown in table 2.4. The 14 Bravais lattices modify the primitive lattice but still conform to the symmetry of one of the seven crystal systems called nonprimitive lattices containing 2 or more lattice points per unit cell. So the 14 Bravais lattices consist of 7 primitives and 7 nonprimitives.

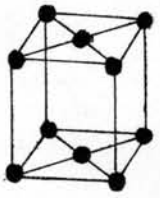
Table 2.4

The Fourteen Bravais Lattices

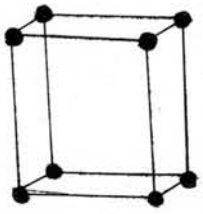
Triclinic



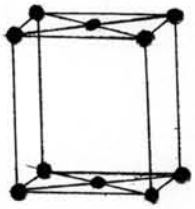
Monoclinic P



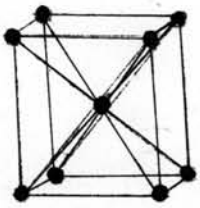
Monoclinic C



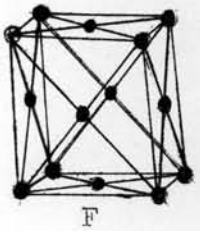
P



C

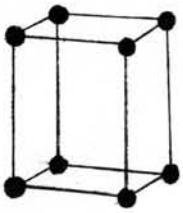


I

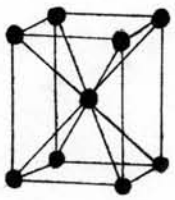


F

Orthorhombic

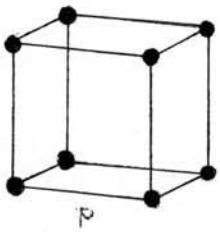


P

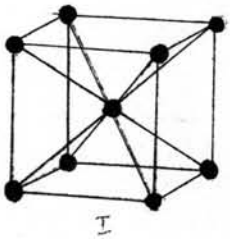


I

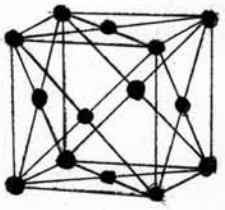
Tetragonal



P

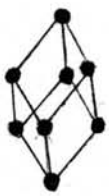


I

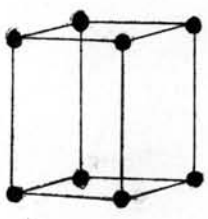


F

Cubic



Trigonal R



Trigonal and Hexagonal P

II.2.4 Space groups[3,14,15]

A space group is an array of symmetry elements that is consistent with an infinite extended regular repeated pattern. The 32 point groups combine with the 14 Bravais lattices resulting in 230 unique space groups. Also three-dimensional translation and symmetry operators introduce two new kinds of symmetry operations, screw axis and glide planes. When these are combined with the symmetry elements, they lead to the same 230 space groups.

The screw axis[13] is the combination of the rotation axis and a translation parallel to this axis, restricted by the translation periodicity of the crystal to repetition at angular intervals of 180, 120, 90 and 60 degrees. Screw axis are designated by an integer n and a subscript m, where n = 2,3,4, and 6 and m = 1,2,...,n -1. Thus 2_1 is a twofold rotation with a translation ½ of a unit translation parallel to this axis called the 2-fold screw axis.

Glide planes[3] represent reflection across a plane combine with a single fraction of translation ½ or ¼ of unit translation parallel to the plane. There are axial glide (a,b, or c), diagonal glide (n), and a diamond glide (d). The plane is describe as an axial glide plane (a, b, or c) if the glide is parallel to the edge of the unit cell with translation a/2, b/2, or c/2, n glide if $\frac{(a + b)}{2}$, $\frac{(a + c)}{2}$, or $\frac{(b + c)}{2}$, d glide if $\frac{(a + b)}{4}$, $\frac{(a + c)}{4}$, or $\frac{(b + c)}{4}$, for this d glide occurs only

in I and F unit cells.

Inturn these two new operators may combine with plane lattices to yield a nonprimitive cell. Combining 2-fold rotation axis with screw axis yields a body-centered lattice (I).

X-rays are extremply sensitive to the screw axis and glide planes because these operators cause a halving of certain classes of interplanar spacings which causes systematic extinctions in the x-ray diffraction patterns. From these extinctions the space groups can be specified first, then the point group since x-rays are subtly sensitive to symmetry. The diffraction pattern appears centrosymmetic which cause only 11 Laue symmetry elements to appear.

The sequence for determining the space group from the x-ray diffraction patterns is as follows. First consider the general type of indicies hkℓ , if no extinction the lattice is primitive (P) and if any of these are symmetrically absent the lattice is nonprimitive. (See the conditions in table 2.5). Then reflections with one zero index are considered; systematic absences amongst these give information about glide planes. Finally, reflections with two zero indicies are considered, systematic absences give information about screw axis.

Table 2.5

Symmetry interpretations of extinctions (3,pp.83)

Class of reflection	Condition for non extinction n = an integer	Interpretation of extinction	Symbol of symmetr elem.
hkℓ	h+k+ℓ = 2n	Body-centered lattice	I
	h+k = 2n	C-centered lattice	C
	h+ℓ = en	B-centered lattice	B
	k+ℓ = 2n	A-centered lattice	A
	h+k " 2n h+ℓ = 2n k+ℓ = 2n	Face-centered lattice	F
	h,k,ℓ all even or all odd		
	-h+k+ℓ = 3n	Rhombohedral lattice indexed on hexagonal system	R
	h+k+ℓ = 3n	Hexagonal lattice in dexed on rhombohedral system	H
	hkℓ no conditions		P
0kℓ	k = 2n	(100) glide plane, component b/2	b(P,B,C)
	ℓ = 2n	(100) glide plane, component c/2	c(P,C,I)
	k+ℓ = 2n	(100) glide plane, component (b/2+c/2)	n(P)
	k+ℓ = 4n	(100) glide plane, component (b/4+c/4)	d(F)

Class of reflection	Condition for non extinction n = an integer	Interpretation of extinction	Symbol of symmetry elem.
h0ℓ	h = 2n	(010) glide plane, component a/2	a(P,A,I)
	ℓ = 2n	(010) glide plane, component c/2	c(P,A,C)
	h+ℓ = 2n	(010) glide plane, component (a/2+c/2)	n(P)
	h+ℓ = 4n	(010) glide plane, component (a/4+c/4)	d(F),(B)
hk0	h = 2n	(001) glide plane, component a/2	a(P,B,I)
	k = 2n	(001) glide plane, component b/2	b(P,A,B)
	h+k = 2n	(001) glide plane, component (a/2+b/2)	n(P)
	h+k = 4n	(001) glide plane, component (a/4+b/4)	c(F)
h00	h = 2n	[100] screw axis, component a/2	2_1, 4_2
0k0	k = 2n	[010] screw axis, component b/2	2_1, 4_2
00ℓ	ℓ = 2n	[001] screw axis, component c/2	2_1,4_2,6_3

Table 2.6

(15,pp.373)

Space group determination of orthorhombic point group 222

Possible reflection	Space group
I hkℓ all orders (P)	
1) 0kℓ all orders	
1.1) h0ℓ all orders	
1.1.1) hk0 all orders	
1.1.1.1) h00 all orders	
1.1.1.1.1) 0kℓ all orders	
a) 00ℓ all orders	P_{222}
b) 00ℓ with ℓ = 2n	P_{222_1}
1.1.1.1.1.1) 0k0 with k = 2n	
a) 00ℓ all orders	P_{22_12}
b) 00ℓ with ℓ = 2n	$P_{22_12_1}$
1.1.1.2) h00 with h = 2n	
2.1) 0k0 all orders	
a) 00ℓ all orders	P_{2_122}
b) 00ℓ with ℓ = 2n	$P_{2_122_1}$
2.2) 0k0 with k = 2n	
a) 00ℓ all orders	$P_{2_12_12}$
b) 00ℓ with ℓ = 2n	$P_{2_12_12_1}$