BSc (Physics): Core III - Theory

3B03PHY: Allied physics

Semester-3, Credit-3, Contact hours -54, Max. Ext. Marks- 40, Max. Int. marks-10

Module 1: Solid State Physics

Crystal structure:-Introduction- crystal lattice and translation vectors- unit cell-basis-symmetry operations–point groups and space groups(qualitative) - types of lattices - Bravais lattices–lattice directions and planes-Miller indices-inter planar spacing for orthogonal lattice(no derivation)-simple crystal structures-close packed structures-loose packed structures-structure of diamond –structure of sodium chloride

X-ray diffraction:– Bragg's law –X-ray diffraction methods-Laue's method- Powder crystal method- powder method(Book 1,Chapter1,2) **14hrs**; Marks: Minimum 12.

Module 2: Properties of matter

Elasticity:- Stress, strain, elastic constants, Poisson's ratio relation connecting various elastic constants- angle of twist and angle of shear – twisting couple on a cylindrical rod of wire – torsion pendulum- Bending of beams –expression for bending moments-cantilever- expression for depression –beam supported at its ends and loaded in the middle-expression for depression –stiffness of a beam

Hydrodynamics: Streamline and turbulent flows-tubes of flow and equation of continuity-energy possessed by a liquid- Bernoulli's theorem-practical applications-Torricelli's theorem

Viscosity:-critical velocity-flow of liquid through a capillary tube (Poiseulle's formula)-Stokes formulae.

Surface tension:-surface energy-expression for excess pressure on a curved surface - measurement of surface tension by capillary tube method (Book 2-Chapters 12,14,15,16)

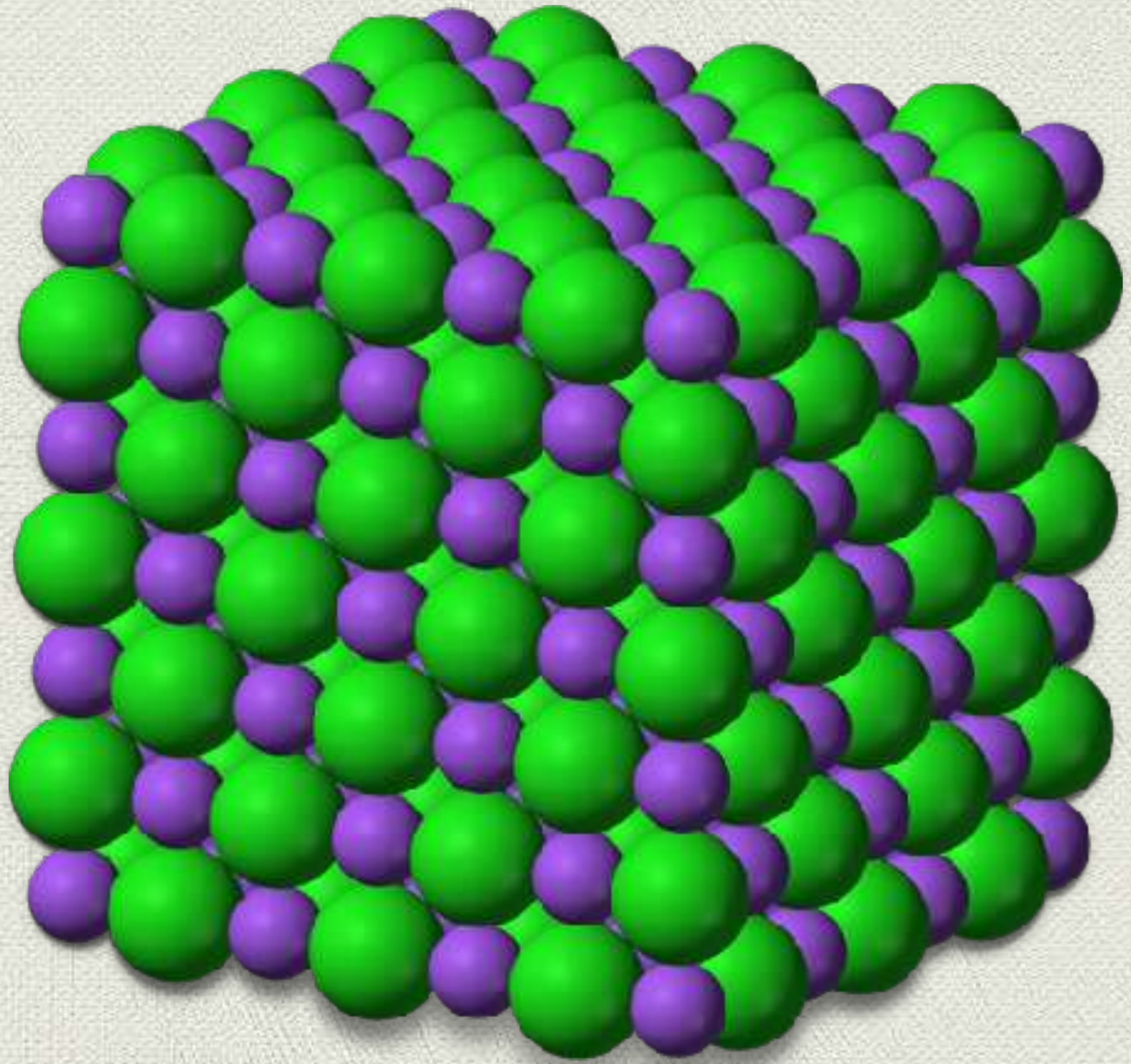
22hrs; Marks: Minimum 14

Module 3: Electricity

DC Network theorems:-Kirchoff's laws –voltage and current sources-source conversion-superposition theorem- Maximum power transfer theorem- reciprocity theorem- Thevenin's and Norton's theorems –equivalent circuits-star/delta ,delta/star transformations

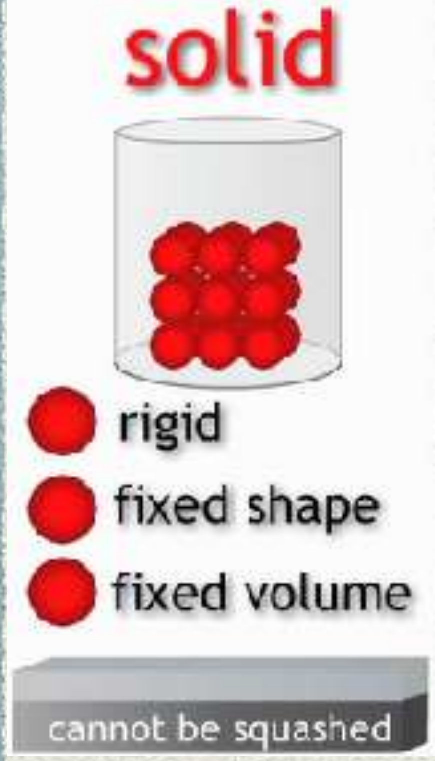
Transients and ac circuits:- Charging and discharging of capacitor- time constants-ac through R,L and C-choke coil-skin effect-ac through LR, CR and LCR series and parallel circuits-resonance-power in ac circuits-power factor(Book 3,Chapters 2,5,10,11,13.)

18hrs; Marks: Minimum 14

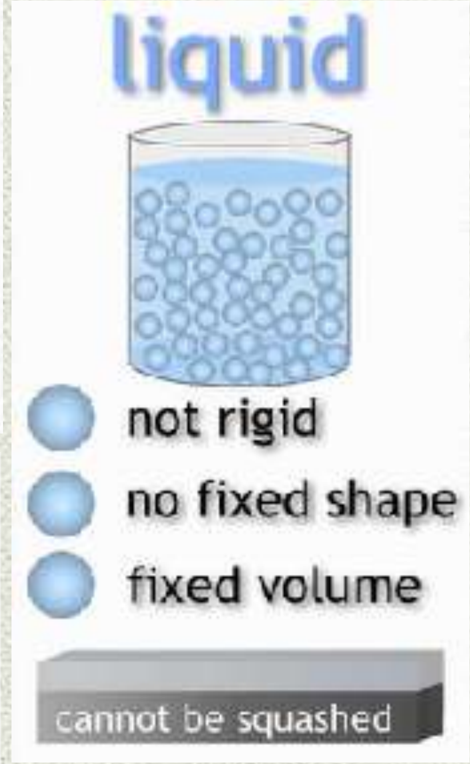


SOLID STATE PHYSICS

Solid, Liquid & Gas



Solid: atoms are packed together in a rigid structure with short- or long-range order (more later).
As the solid is heated up, the atoms oscillate around their equilibrium positions but retain a rigid structure.

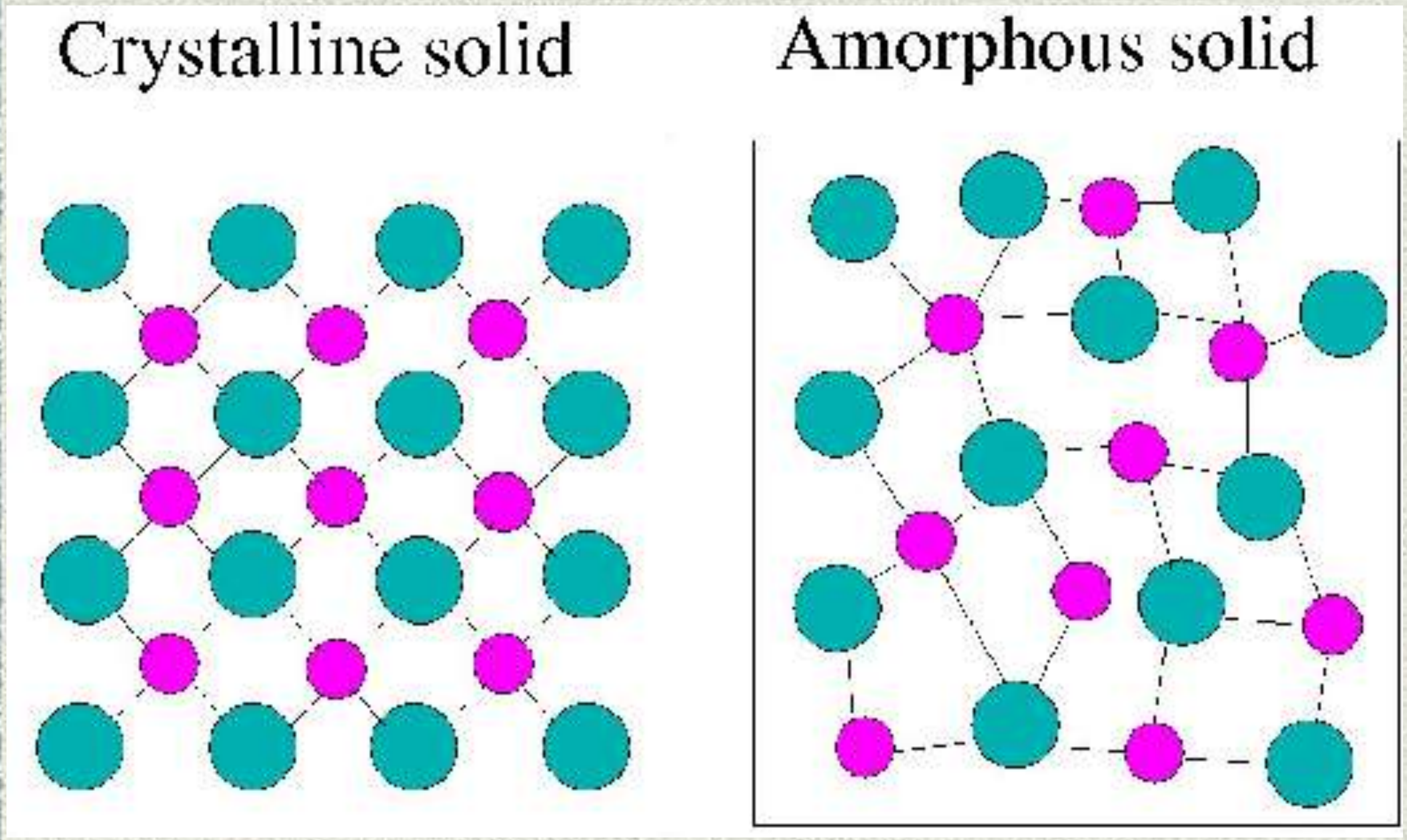


Liquid: atoms are closely packed but do not form a rigid structure. As the liquid is heated up the atoms move around but without clear relation to one another.

Gas: atoms are located far away from each other (a much lower density than for a liquid or gas) with little interaction with each other. As the gas is heated up the atoms become more energetic, increasing the probability of collision.

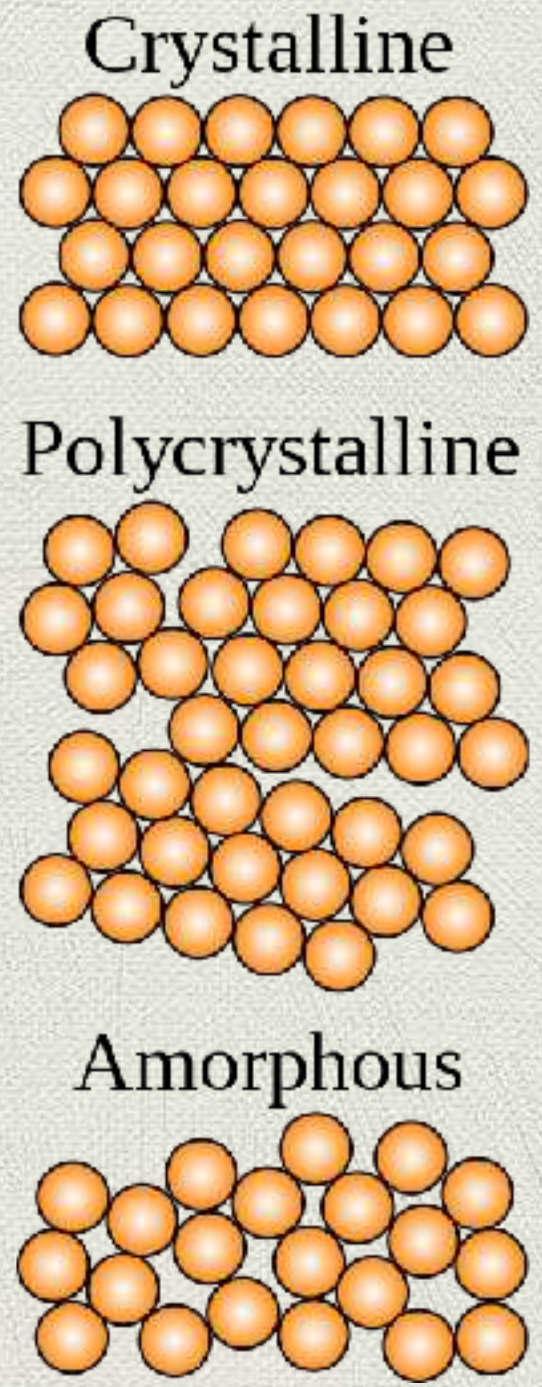
Crystalline & Amorphous

In *crystalline* solids the atoms form a periodic structure and there is *long range order* in the position of the atoms (e.g. metals, diamond, silicon etc.). More than 90% of solids form crystalline structures.



In *amorphous* solids there may be *short range order* between atoms but the atoms do not overall form a periodic structure. The atoms themselves are at equilibrium spacing (e.g. glasses)

Single crystalline & Poly crystalline



- Single crystal has an atomic structure that repeats periodically across its whole volume. Even at infinite length scales, each atom is related to every other equivalent atom in the structure by translational symmetry

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- Poly crystal is a material made up of an aggregate of *many small single crystals* (also called crystallites or grains).
- Polycrystalline material have a high degree of order over many atomic or molecular dimensions.
- These *ordered regions,* or single crystal regions, vary in size and orientation wrt one another.
- These regions are called as *grains (domain)* and are separated from one another by *grain boundaries. The atomic order can vary from one domain to the next.*
- The grains are usually *100 nm - 100 microns in diameter*. Poly crystals with grains that are <10 nm in diameter are called nano crystalline

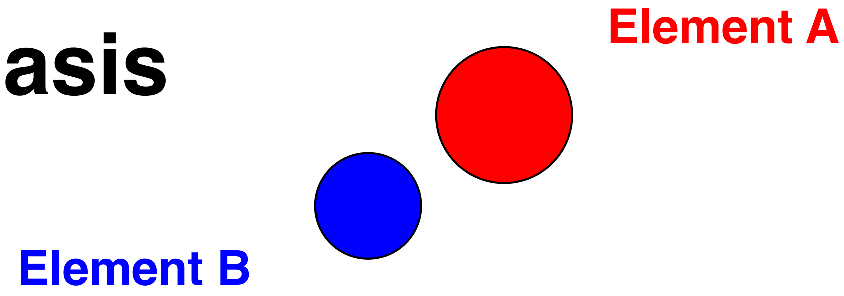
Crystal Lattice

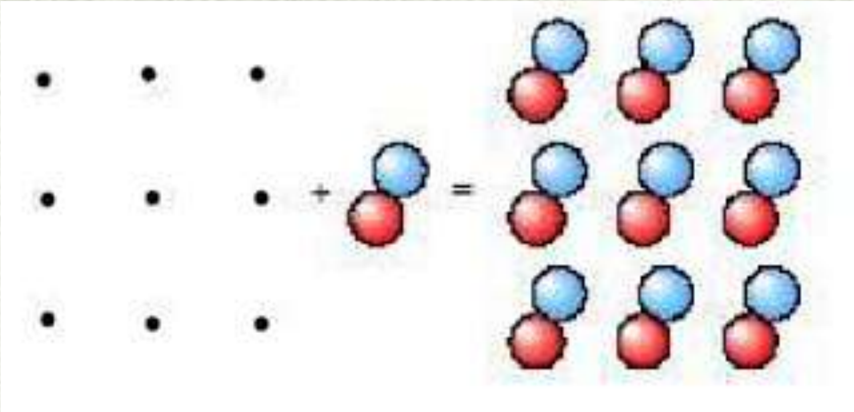
An ideal crystal is constructed from an infinite repetition of identical groups of atoms

- The group is known as the **basis** (this will contain one or more atoms)
- The set of points on which the basis sits is called the **lattice**
  (a mathematical construction)

Crystal structure = lattice + basis

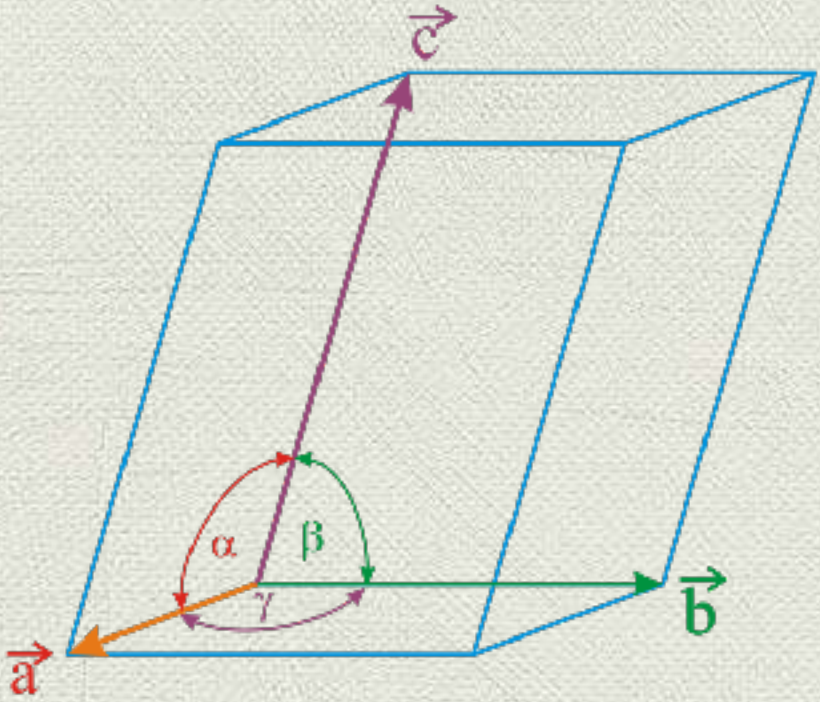
Basis

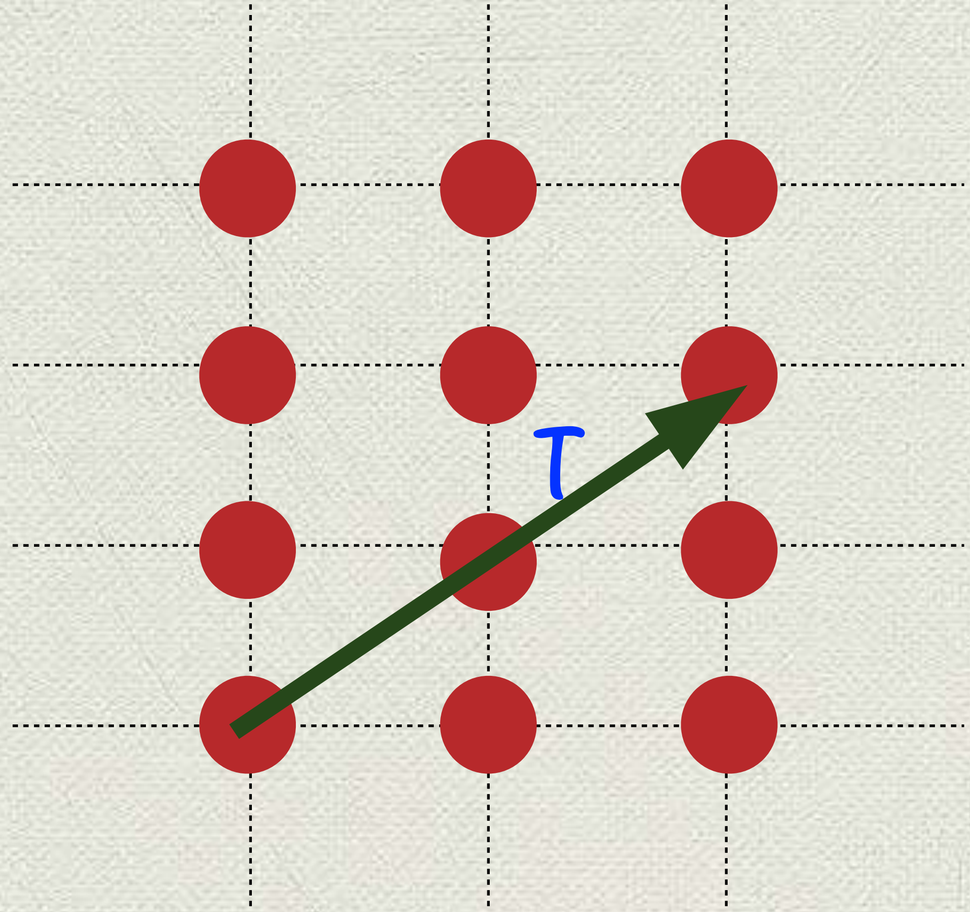




Translation vectors

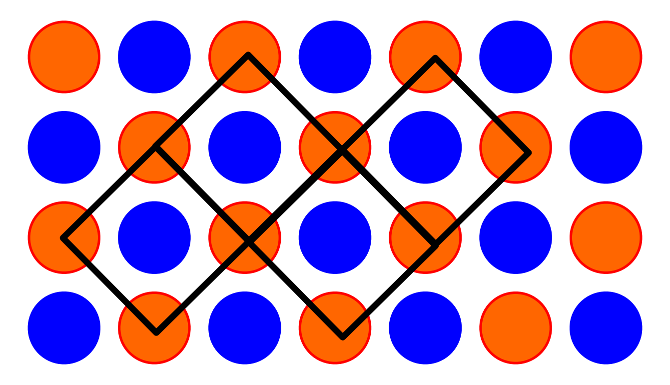
$$\mathbf{T} = n_1 \mathbf{a} + n_2 \mathbf{b} + n_3 \mathbf{c}$$

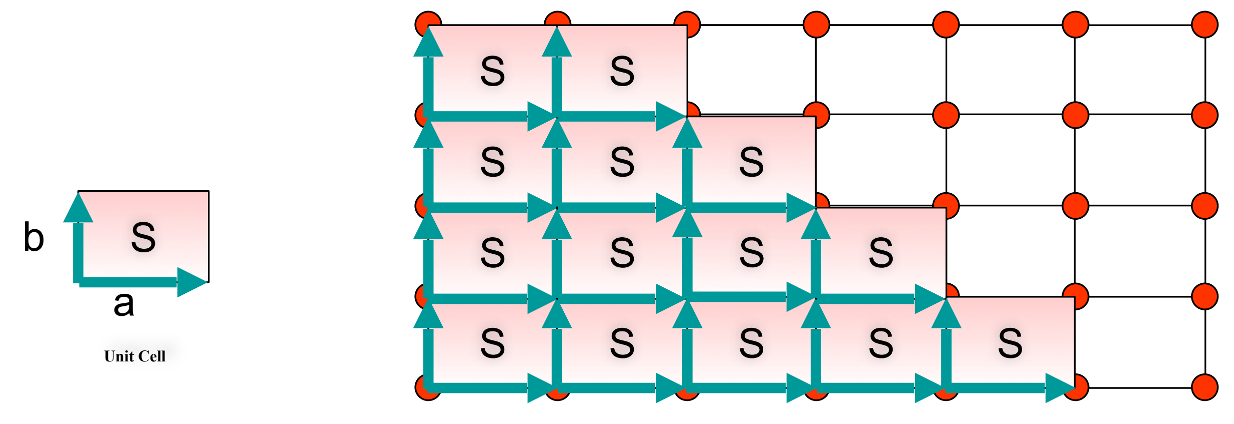




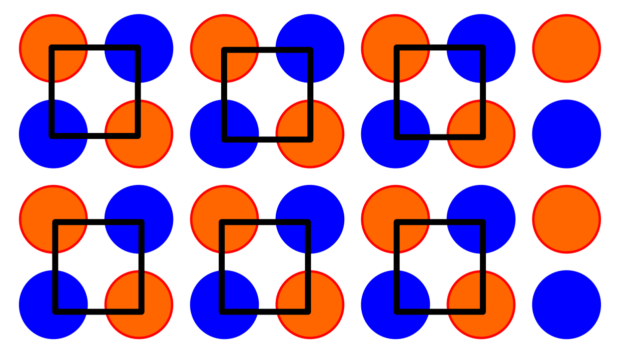
Unit Cell & Primitive Cell

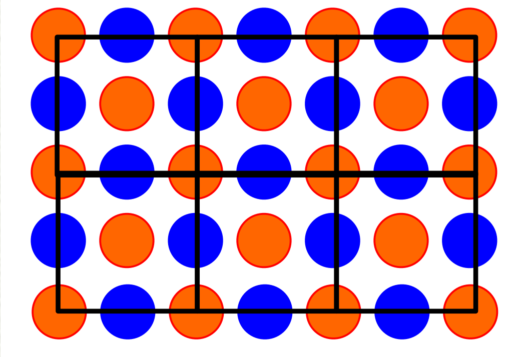
- The smallest component of the crystal (group of atoms, ions or molecules), which when stacked together with pure translational repetition reproduces the whole crystal.





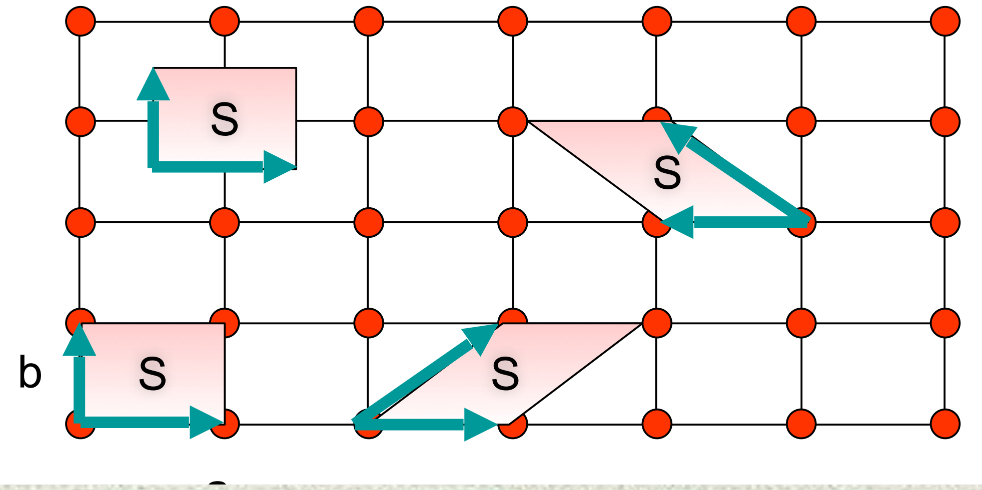
Crystal Structure

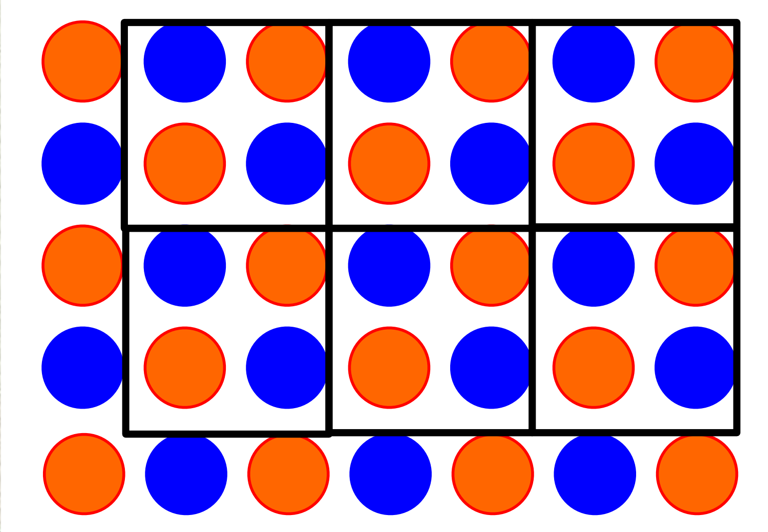




Crystal Structure

The choice of unit cell is not unique.



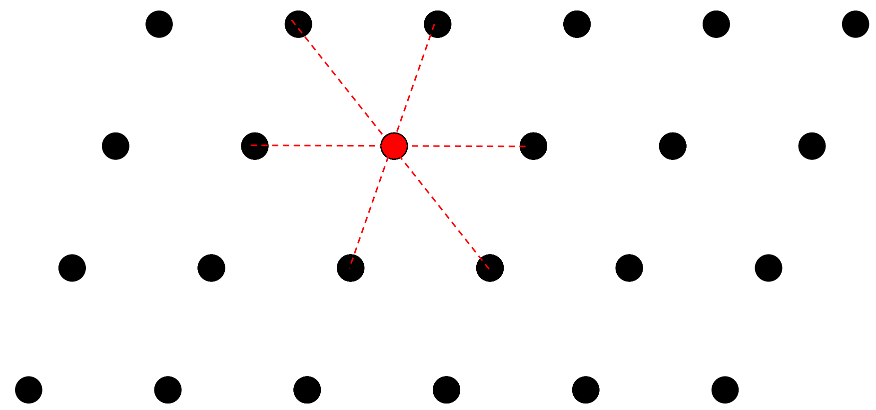


Weigner- Seitz Primitive Cell

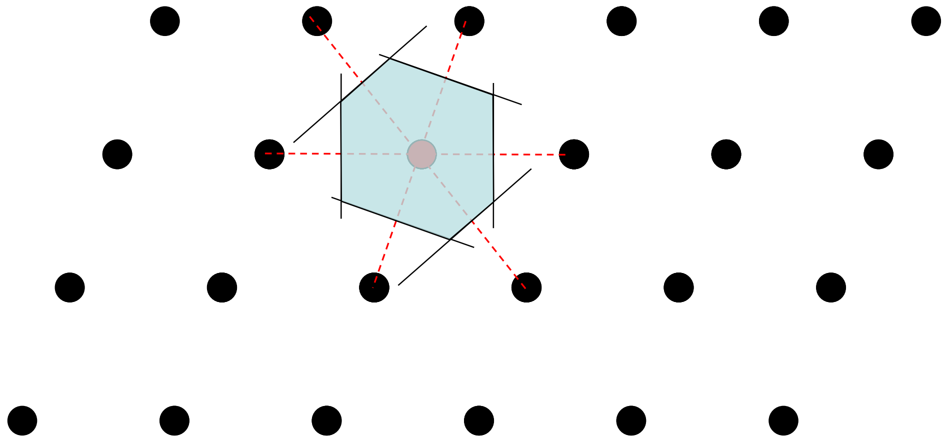
A **primitive** cell contains 1 lattice point!

A **primitive cell** can be defined in more than one way

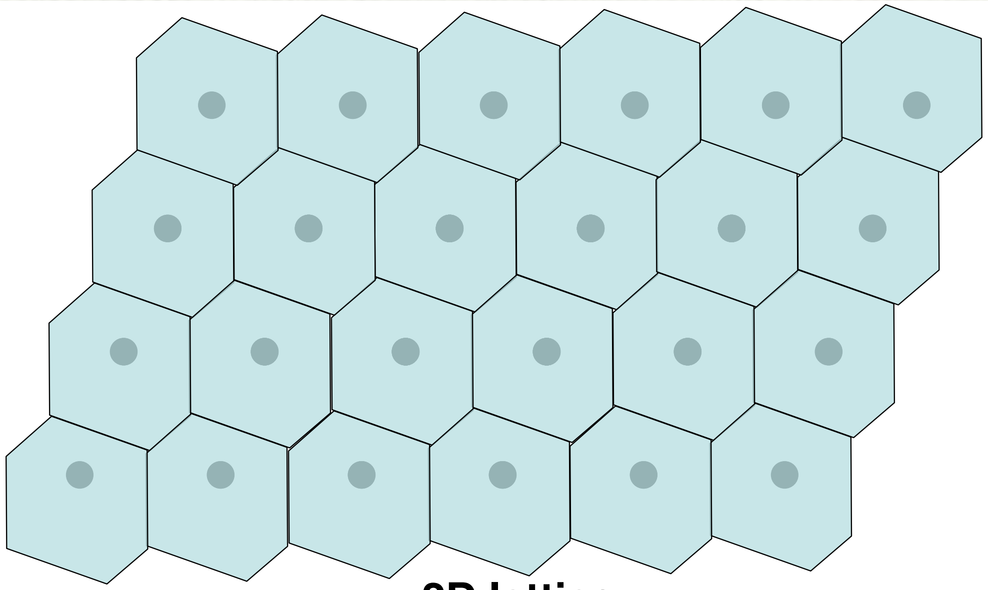
Define a primitive cell by bisecting lines connecting lattice points…



2D lattice



2D lattice



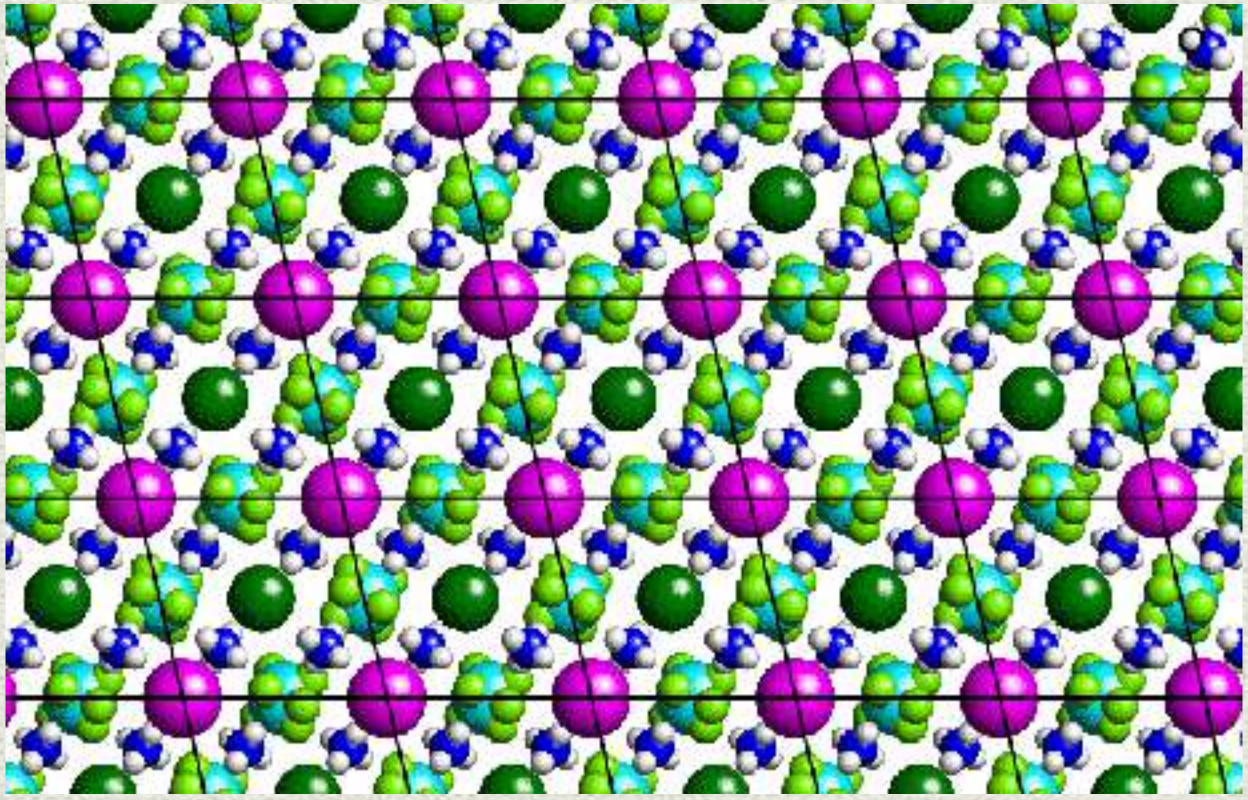
2D lattice

Symmetry Operations

A symmetry operation is that transforms the crystals to itself,
ie, a crystal remains invariant under a symmetry operation

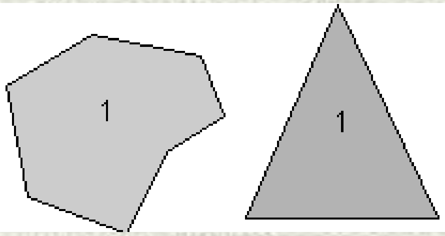
1. Translations 2. Rotations 3. Reflections 4. Inversions

Translations $r' = r + T$

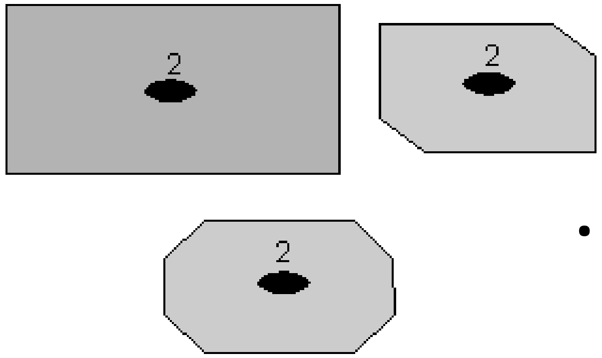


Rotations

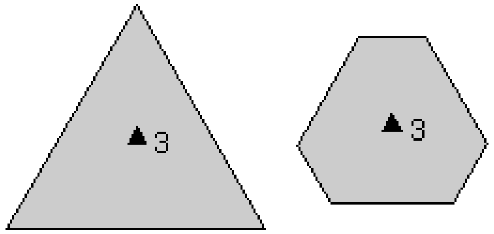
- ***1-Fold Rotation Axis*** - An object that requires rotation of a full 360^{o} in order to restore it to its original appearance has no rotational symmetry. Since it repeats itself 1 time every 360^{o} it is said to have a 1-fold axis of rotational symmetry.



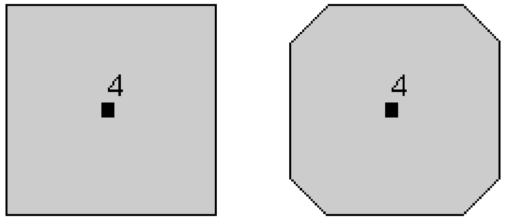
- ***2-fold Rotation Axis*** - If an object appears identical after a rotation of 180^{o}, that is twice in a 360^{o} rotation, then it is said to have a 2-fold rotation axis (360/180 = 2). Note that in these examples the axes we are referring to are imaginary lines that extend toward you perpendicular to the page or blackboard. A filled oval shape represents the point where the 2-fold rotation axis intersects the page.



- ***3-Fold Rotation Axis***- Objects that repeat themselves upon rotation of 120^{o} are said to have a 3-fold axis of rotational symmetry (360/120 =3), and they will repeat 3 times in a 360^{o} rotation. A filled triangle is used to symbolize the location of 3-fold rotation axis.

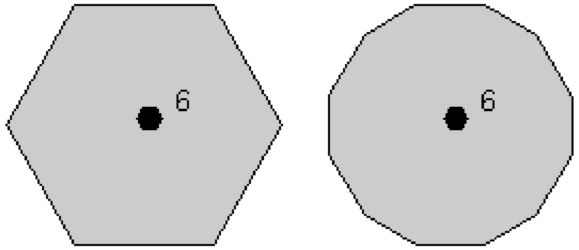


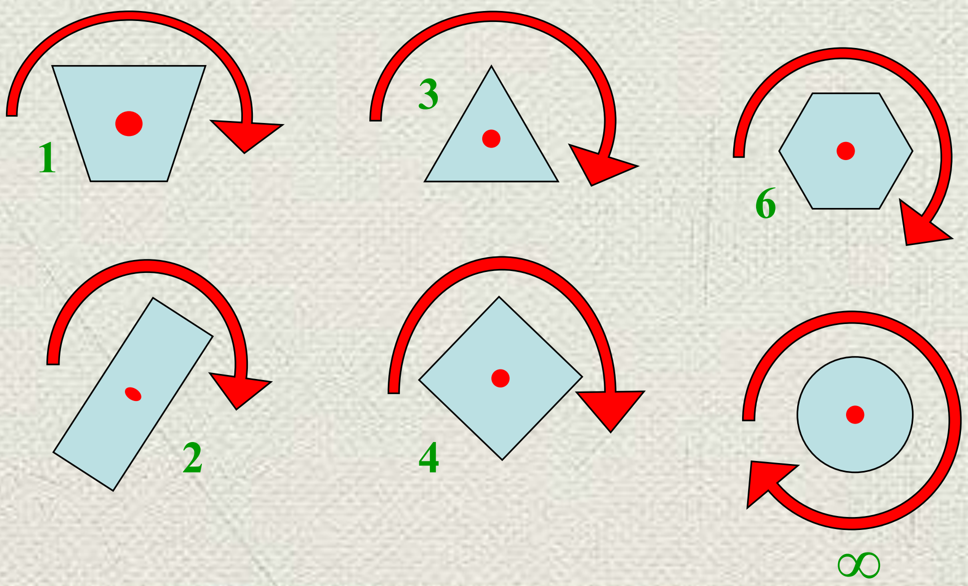
- ***4-Fold Rotation Axis*** - If an object repeats itself after 90^{o} of rotation, it will repeat 4 times in a 360^{o} rotation, as illustrated previously. A filled square is used to symbolize the location of 4-fold axis of rotational symmetry.



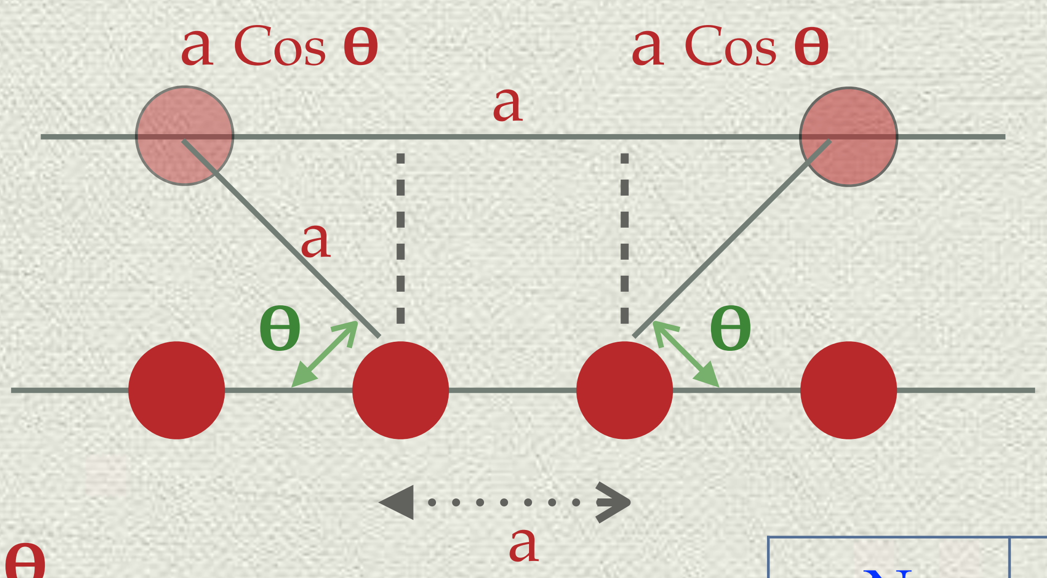
$$\theta = \frac{2\Pi}{n}$$

- ***6-Fold Rotation Axis*** - If rotation of 60^{o} about an axis causes the object to repeat itself, then it has 6-fold axis of rotational symmetry (360/60=6). A filled hexagon is used as the symbol for a 6-fold rotation axis.





“ 5 fold rotational symmetry is not Possible…”



$m*a = a + 2a \cos \theta$

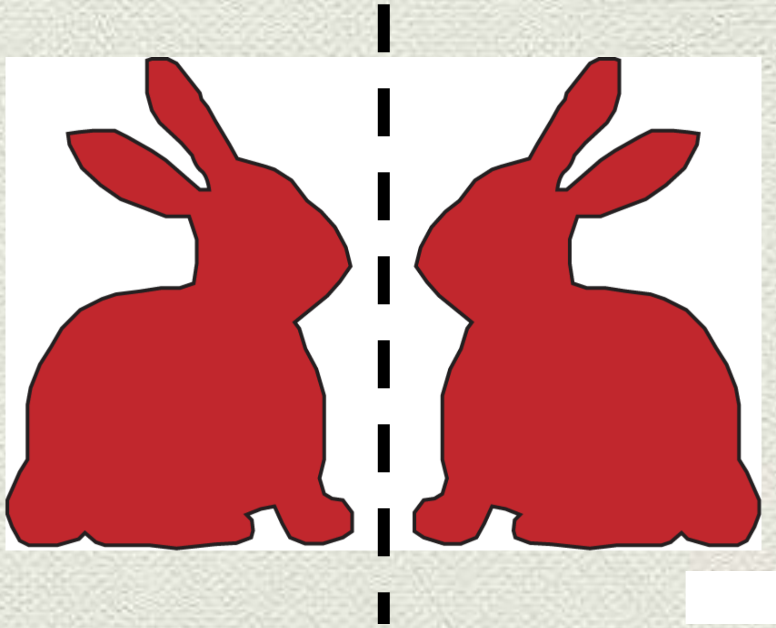
Where $m = 0, \pm 1, \pm 2, \pm 3, \ldots$

$N = 2 \cos \theta$

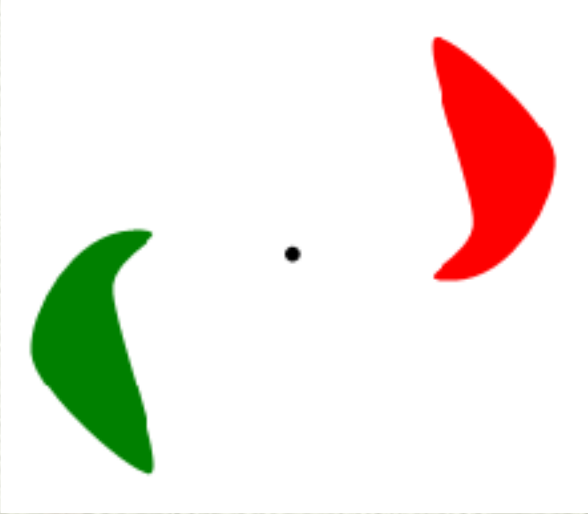
Where $N = 0, \pm 1, \pm 2, \pm 3, \ldots$

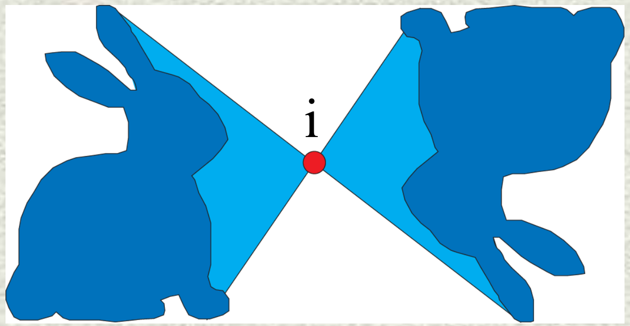
N	Cos θ	θ	n
-2	-1	180	2
-1	-1/2	120	3
0	0	90	4
+1	+1/2	60	6
+2	+1	360	1

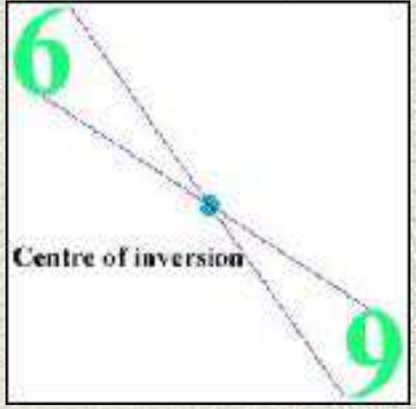
Reflections



Inversions

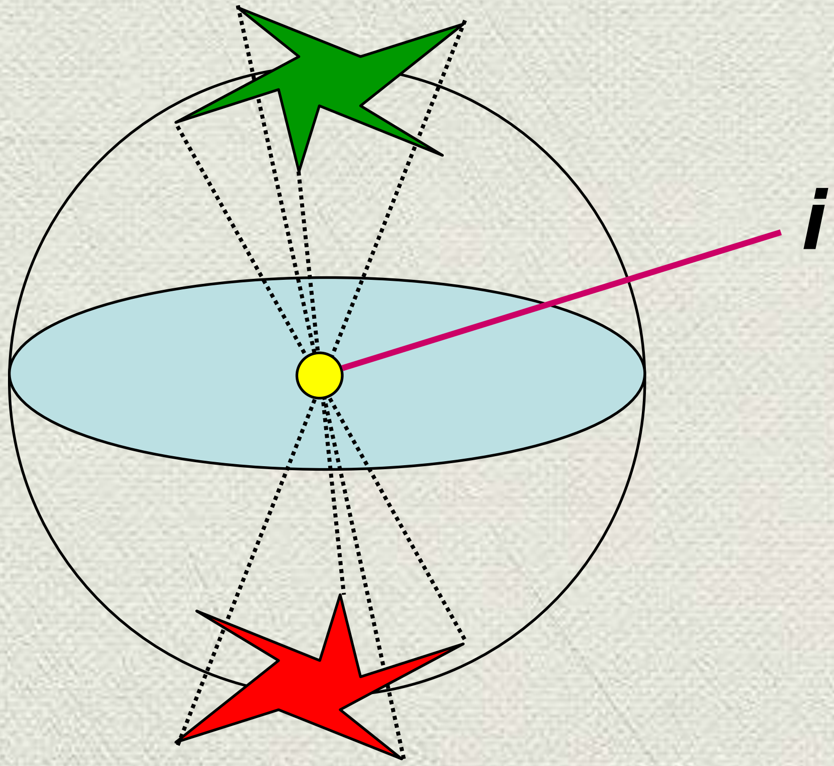






An *inversion (i)* produces an inverted object through an *inversion center*.

Draw lines from every point on the object through the inversion center and out an equal distance on the other side.



The combining of the single operations, rotation and inversion, generates a ***rotoinversion***

Bravais lattice

A crystal is made up of one or more atoms (the basis) which is repeated at each lattice point. The crystal then looks the same when viewed from any of the lattice points. In all, there are 14 possible Bravais lattices that fill three-dimensional space.

Point Groups

A crystallographic point group is a set of symmetry operations, like rotations or reflections, that leave a point fixed while moving each atom of the crystal to the position of an atom of the same kind.

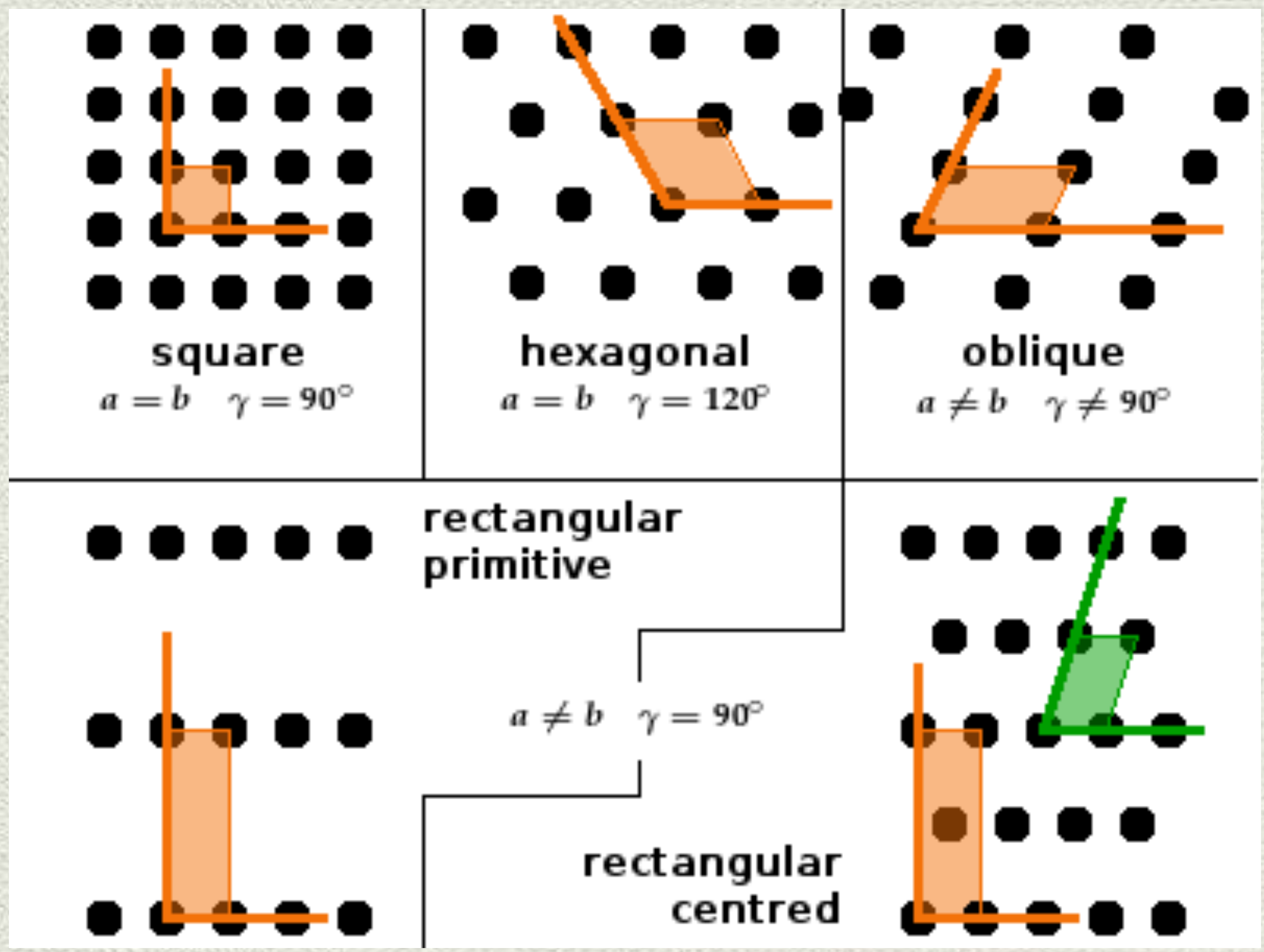
Space Groups

The space group of a crystal is a mathematical description of the symmetry inherent in the structure. The space groups in three dimensions are made from combinations of the 32 crystallographic point groups with the 14 Bravais lattices which belong to one of 7 crystal systems.

2D Lattice

4 Crystal Systems and 5 Bravais Lattices

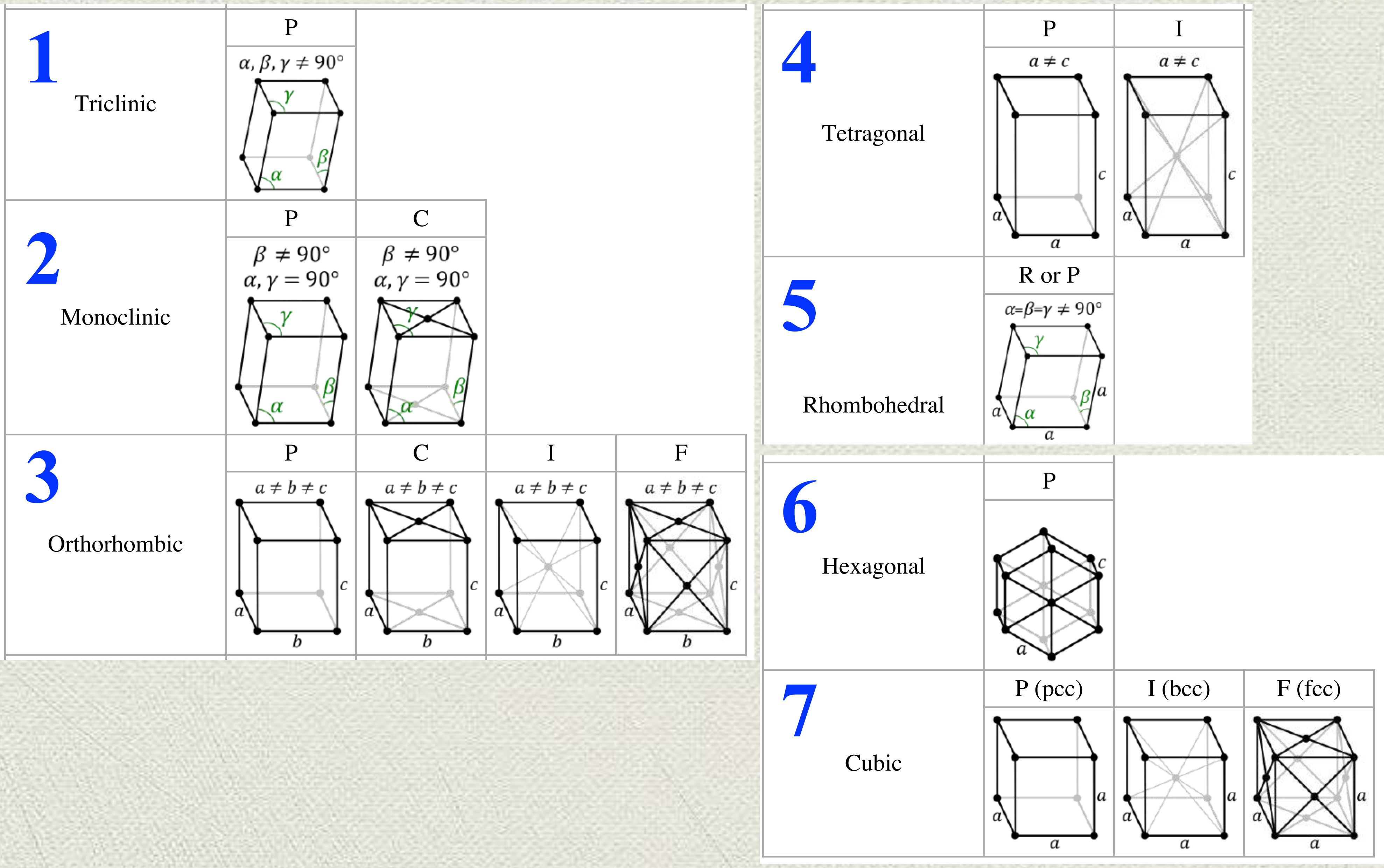
1. Oblique
2. Rectangular
3. Square
4. Hexagonal



3D Lattice

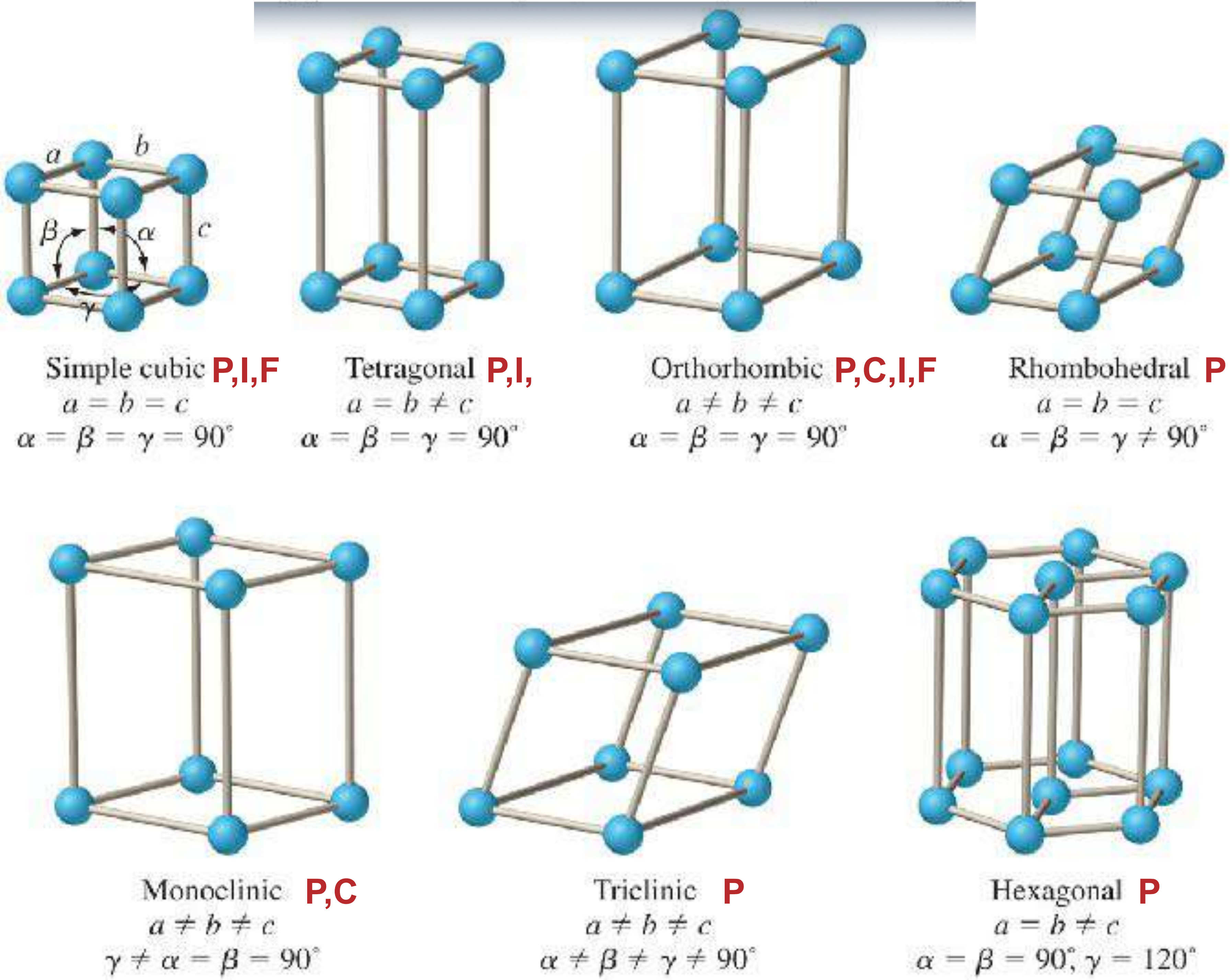
7 Crystal Systems and 14 Bravais Lattices

1. Triclinic
2. Monoclinic
3. Orthorhombic
4. Tetragonal
5. Rhombohedral
6. Hexagonal
7. Cubic



1	Triclinic	P $\alpha, \beta, \gamma \neq 90°$			
2	Monoclinic	P $\beta \neq 90°$ $\alpha, \gamma = 90°$	C $\beta \neq 90°$ $\alpha, \gamma = 90°$		
3	Orthorhombic	P $a \neq b \neq c$	C $a \neq b \neq c$	I $a \neq b \neq c$	F $a \neq b \neq c$
4	Tetragonal	P $a \neq c$	I $a \neq c$		
5	Rhombohedral	R or P $\alpha = \beta = \gamma \neq 90°$			
6	Hexagonal	P			
7	Cubic	P (pcc)	I (bcc)	F (fcc)	

7 Crystal Systems



Simple cubic **P,I,F**
$a = b = c$
$\alpha = \beta = \gamma = 90^\circ$

Tetragonal **P,I,**
$a = b \neq c$
$\alpha = \beta = \gamma = 90^\circ$

Orthorhombic **P,C,I,F**
$a \neq b \neq c$
$\alpha = \beta = \gamma = 90^\circ$

Rhombohedral **P**
$a = b = c$
$\alpha = \beta = \gamma \neq 90^\circ$

Monoclinic **P,C**
$a \neq b \neq c$
$\gamma \neq \alpha = \beta = 90^\circ$

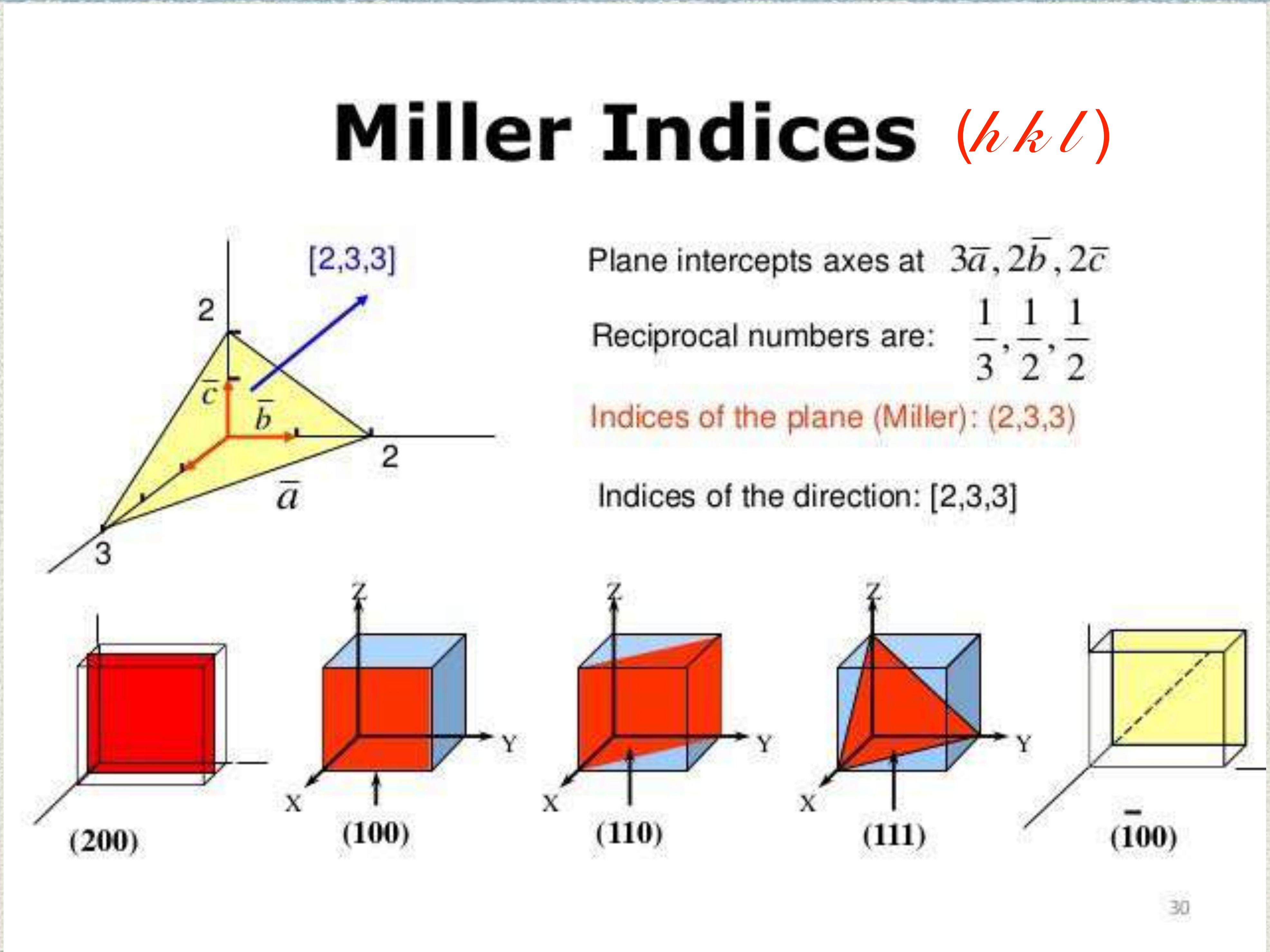
Triclinic **P**
$a \neq b \neq c$
$\alpha \neq \beta \neq \gamma \neq 90^\circ$

Hexagonal **P**
$a = b \neq c$
$\alpha = \beta = 90^\circ, \gamma = 120^\circ$

P - Primitive
I- Body centered
C- Base centered
F- Face centered

Lattice Directions and Planes

- ❑ Miller indices are used to specify directions and planes.
- ❑ These directions and planes could be in lattices or in crystals.



Miller Indices $(h\,k\,l\,)$

Plane intercepts axes at $3\overline{a}, 2\overline{b}, 2\overline{c}$

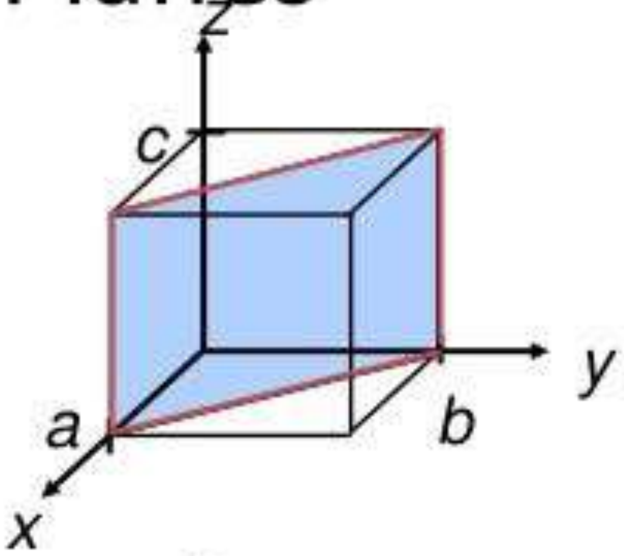
Reciprocal numbers are: $\frac{1}{3}, \frac{1}{2}, \frac{1}{2}$

Indices of the plane (Miller): (2,3,3)

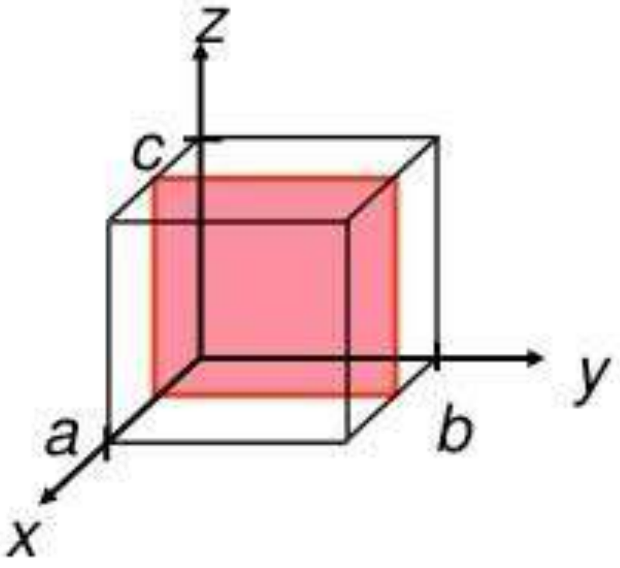
Indices of the direction: [2,3,3]

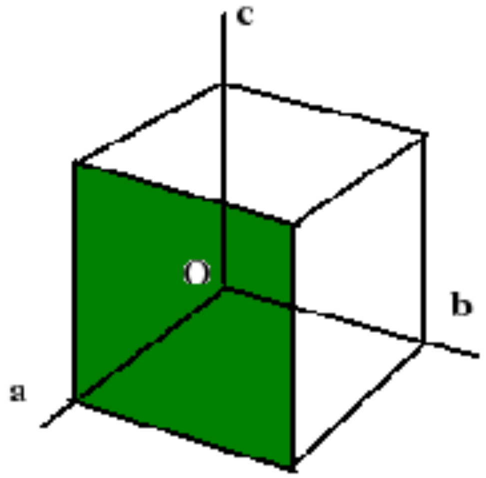
Crystallographic Planes

<u>example</u>		*a*	*b*	*c*
1.	Intercepts	1	1	∞
2.	Reciprocals	1/1	1/1	1/∞
		1	1	0
3.	Reduction	1	1	0
4.	Miller Indices	(110)		

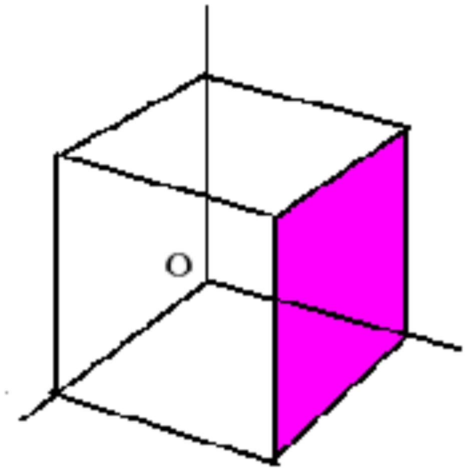


<u>example</u>		*a*	*b*	*c*
1.	Intercepts	1/2	∞	∞
2.	Reciprocals	1/½	1/∞	1/∞
		2	0	0
3.	Reduction	2	0	0
4.	Miller Indices	(100)		

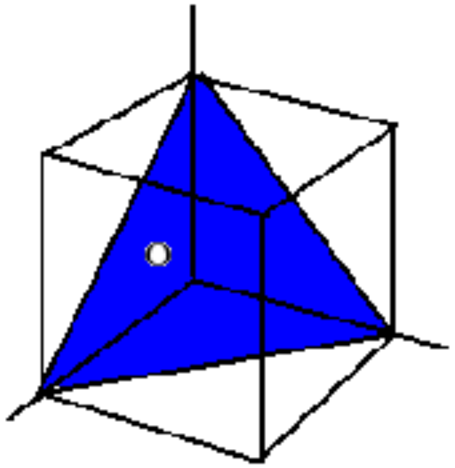




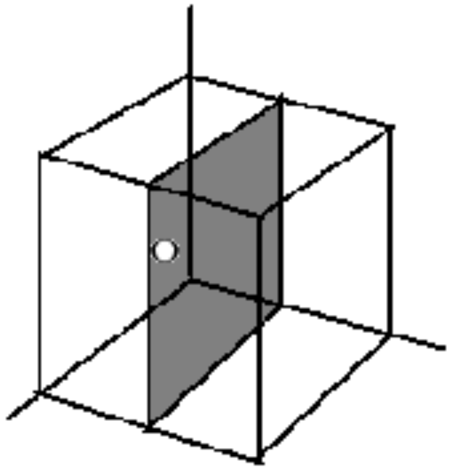
(1 0 0)



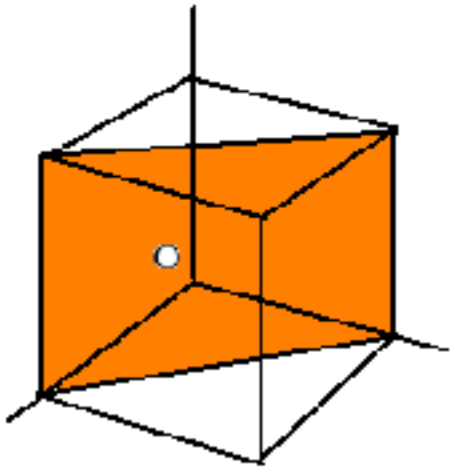
(0 1 0)



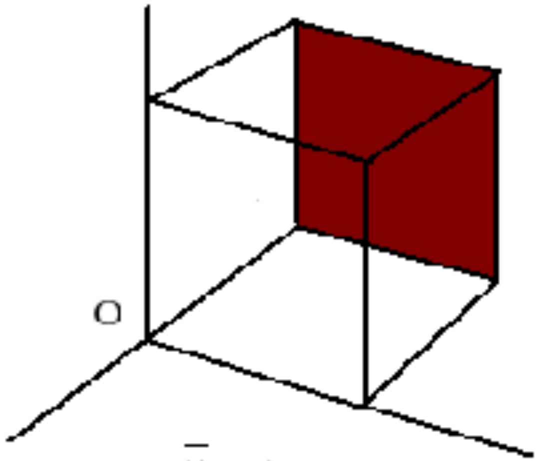
(1 1 1)



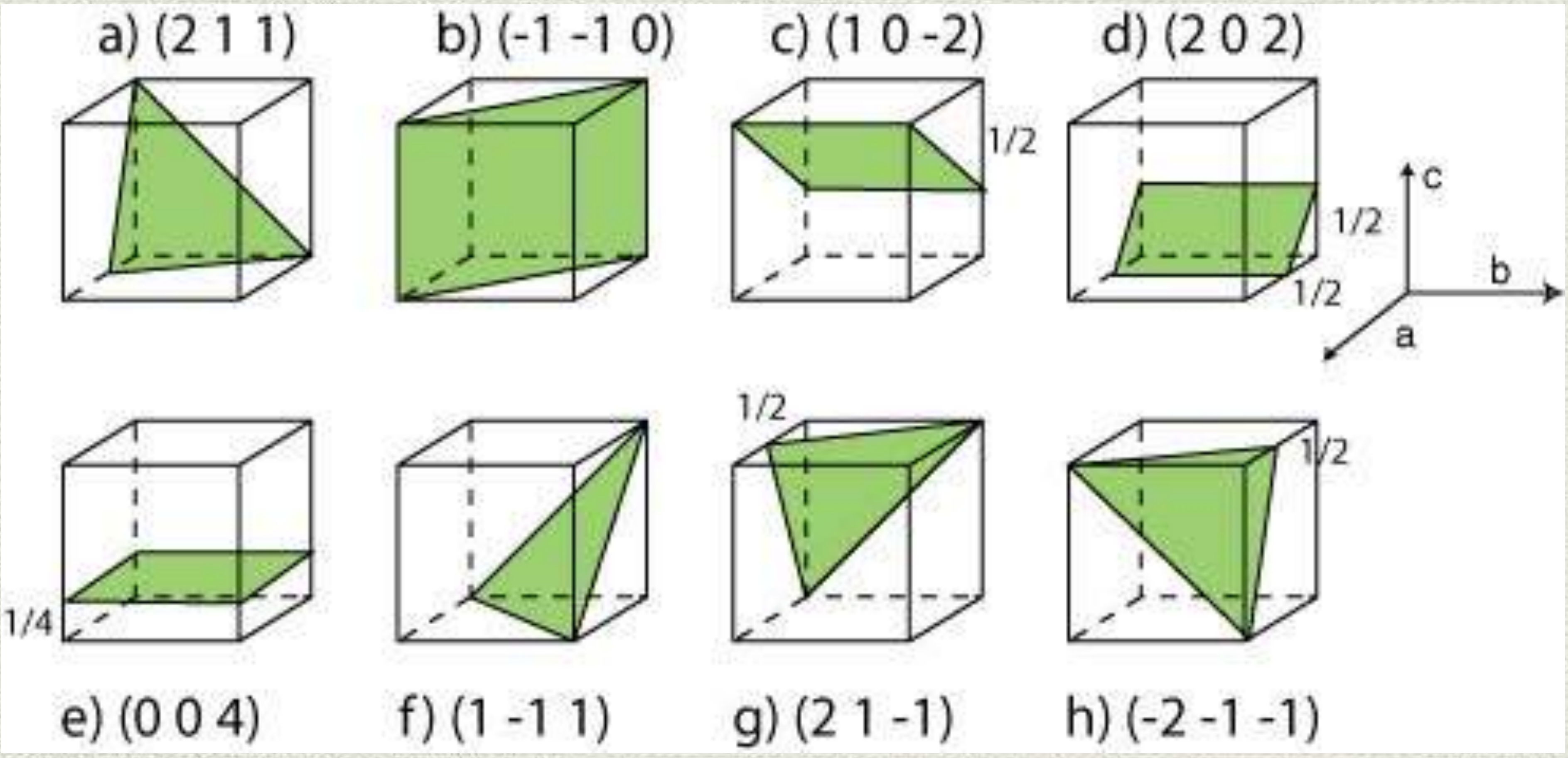
(0 2 0)



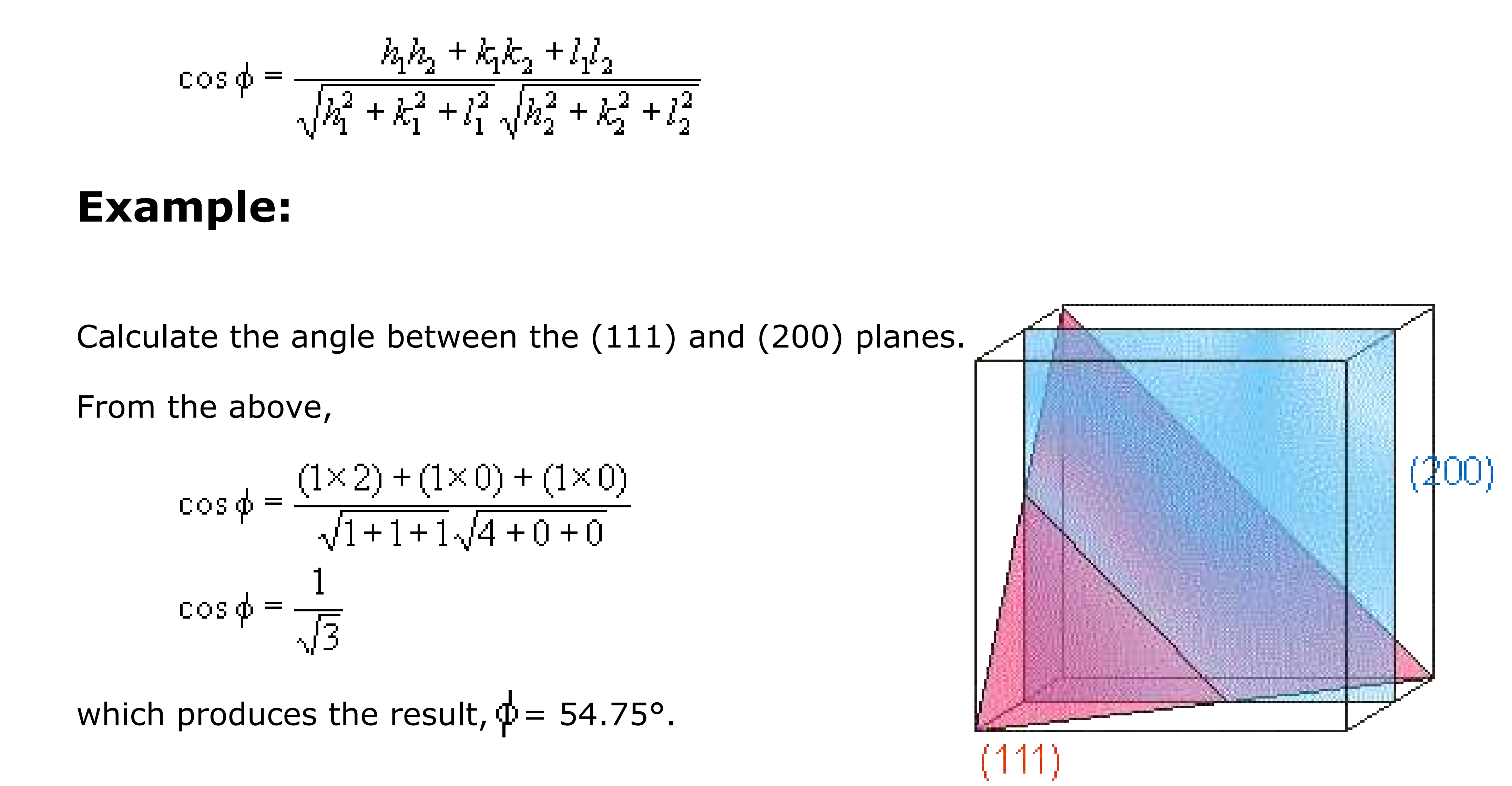
(1 1 0)



($\bar{1}$ 0 0)


a) (2 1 1)
b) (-1 -1 0)
c) (1 0 -2)
d) (2 0 2)
1/2
1/2
1/2
c
b
a
1/2
1/2
1/2
1/4
e) (0 0 4)
f) (1 -1 1)
g) (2 1 -1)
h) (-2 -1 -1)

Angle between Planes



$$\cos\phi = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2}\sqrt{h_2^2 + k_2^2 + l_2^2}}$$

Example:

Calculate the angle between the (111) and (200) planes.

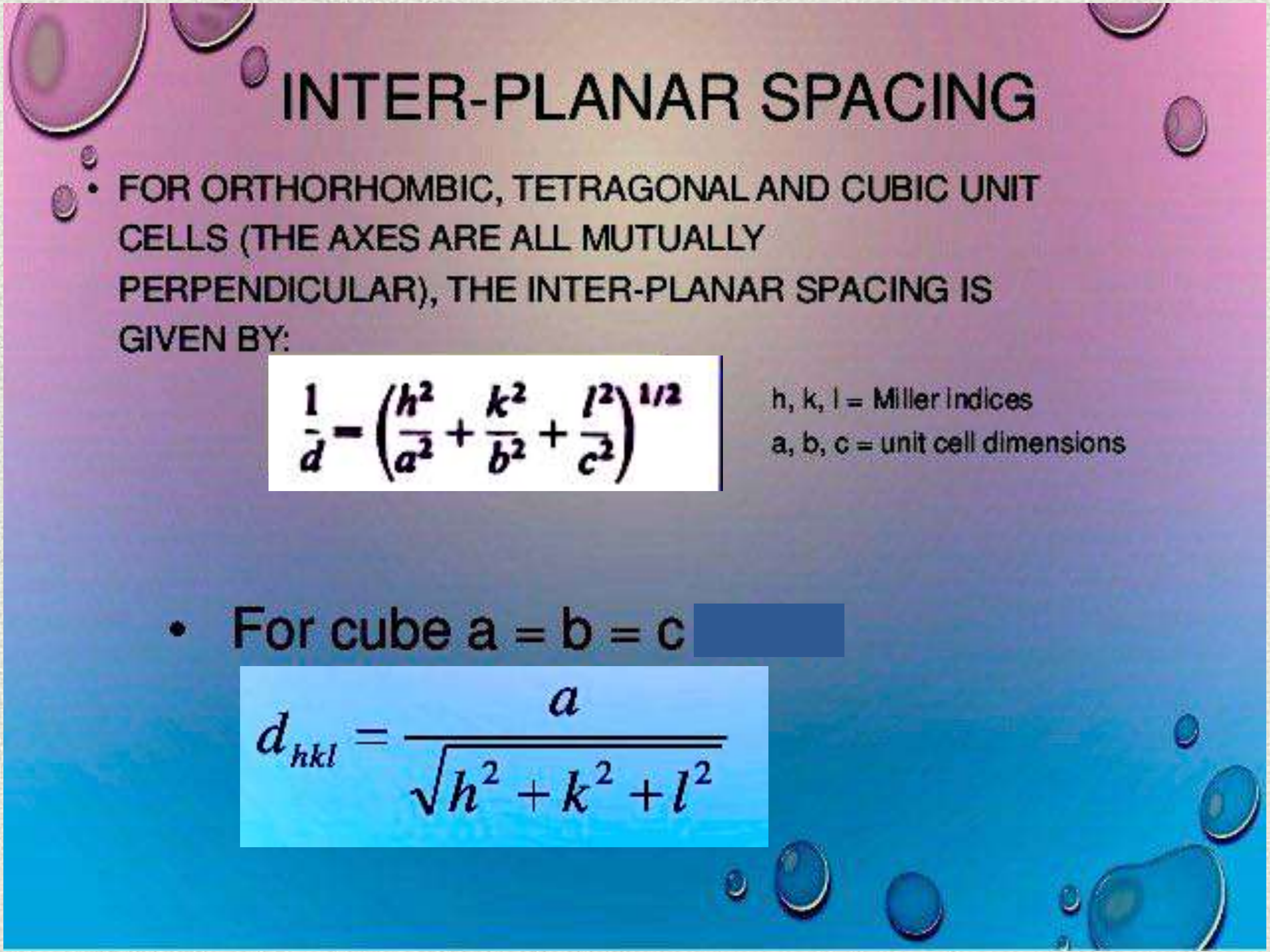
From the above,

$$\cos\phi = \frac{(1\times 2) + (1\times 0) + (1\times 0)}{\sqrt{1+1+1}\sqrt{4+0+0}}$$

$$\cos\phi = \frac{1}{\sqrt{3}}$$

which produces the result, ϕ = 54.75°.

Interplanar Spacing



INTER-PLANAR SPACING

- FOR ORTHORHOMBIC, TETRAGONAL AND CUBIC UNIT CELLS (THE AXES ARE ALL MUTUALLY PERPENDICULAR), THE INTER-PLANAR SPACING IS GIVEN BY:

$$\frac{1}{d} = \left(\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right)^{1/2}$$

h, k, l = Miller Indices

a, b, c = unit cell dimensions

- For cube a = b = c [redacted]

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Packing Fraction (f)

$$f = \frac{\text{Volume occupied by the atoms present in the unit cell}}{\text{Total Volume of the unit cell}}$$

Simple Crystal Structures

Close - Packed Structures

Hexagonal close-packed (hcp)

ABABAB….

12 atoms at corners

2 atoms at centres of basal plane

3 atoms completely inside the hexagon

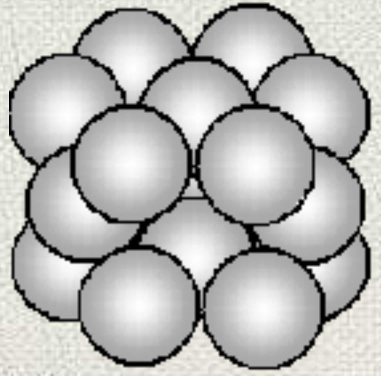
Effective number of atoms

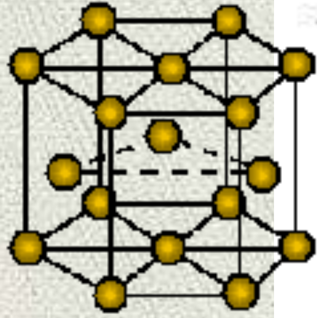
= 12(1/6)+2(1/2)+3=6

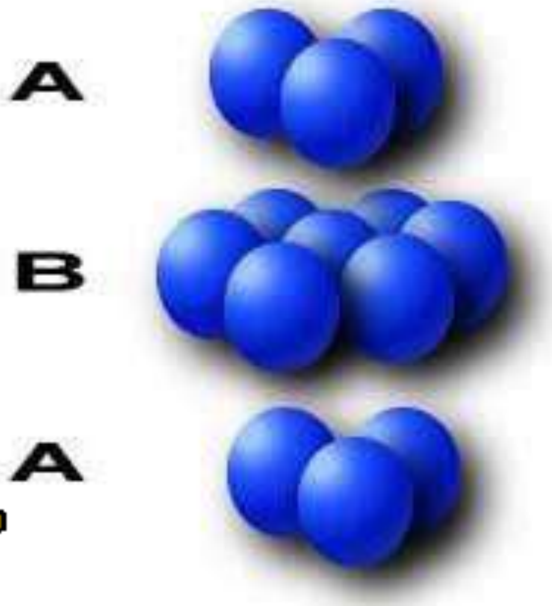
Coordination number =12

f = 0.74

Mg, Z, Cd, Ti







Hexagonal Close Packed Structure

Face centred cubic (fcc)

ABCABCABC….

8 atoms at corners

6 atoms at the face centres

Effective number of atoms

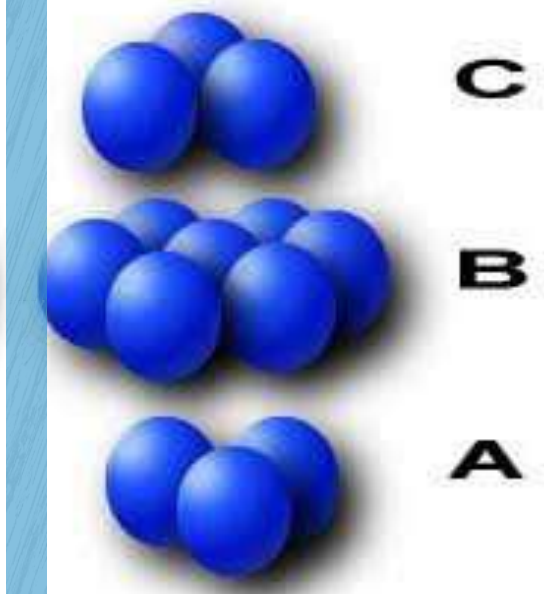
= 8(1/8)+6(1/2) = 4

Coordination number =12

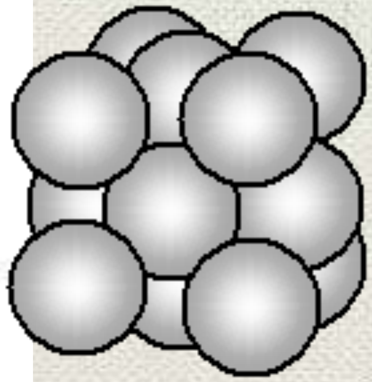
$4r = \sqrt{2}a$

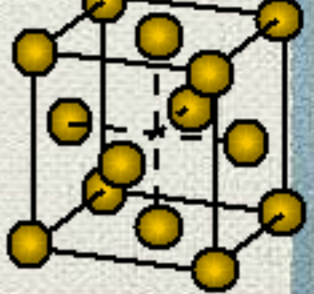
f = 0.74

Cu, Ag, Au, Al



Face Centered Cubic Structure





Loose- Packed Structures

Simple cubic

$a = 2r$

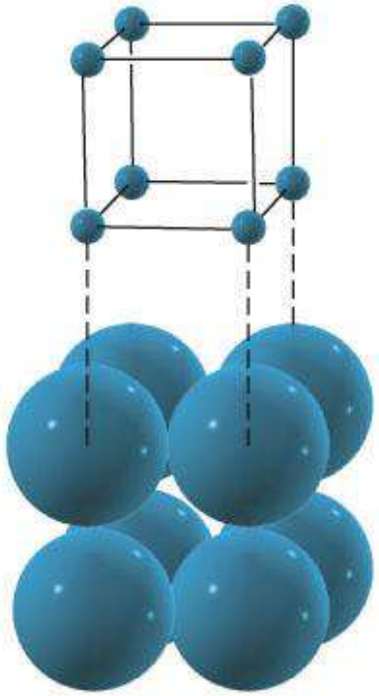
$f = 0.52$

8 atoms at corners

Effective number of atoms = 8(1/8)=1

Coordination number =6

Na, K ,Mo, W



Simple cubic (sc)

Body Centred

$4r = \sqrt{3}a$

$f = 0.68$

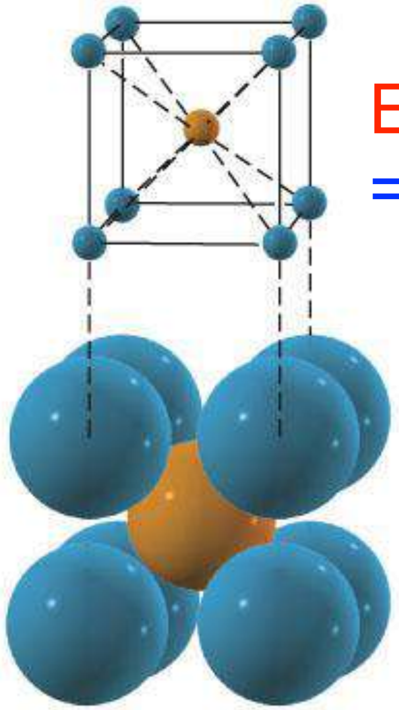
8 atoms at corners

1 atoms at body centre

Effective number of atoms = 8(1/8) +1=2

Coordination number =8

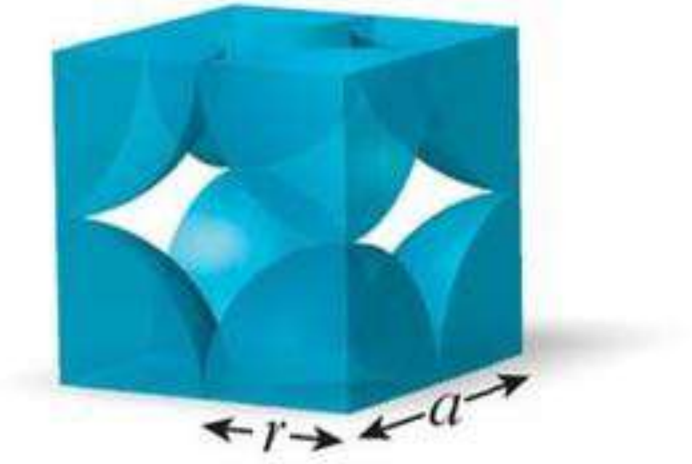
Polonium (Po)



Body-centred cubic (bcc)

Crystal Structure

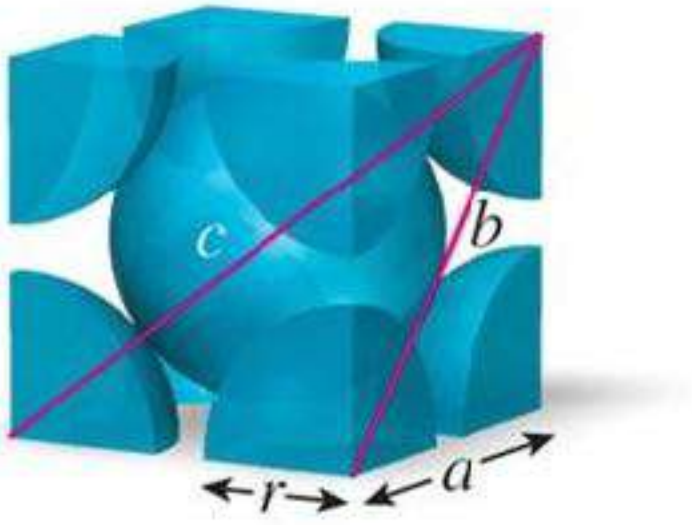
Edge length (a) and radius (r) are related:



scc

$$a = 2r$$

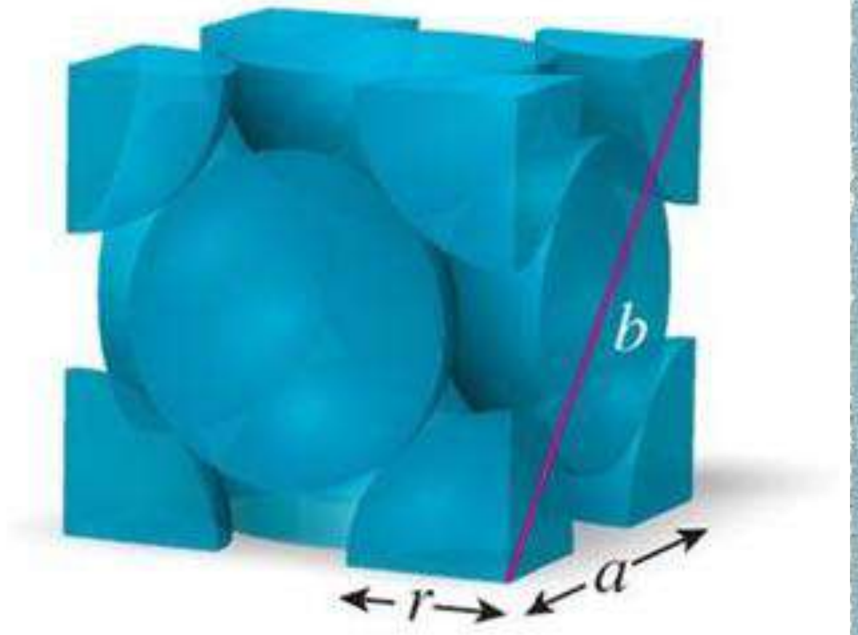
Simple cubic



bcc

$$\begin{aligned} b^2 &= a^2 + a^2 \\ c^2 &= a^2 + b^2 \\ &= 3a^2 \\ c &= \sqrt{3}a = 4r \\ a &= \frac{4r}{\sqrt{3}} \end{aligned}$$

Body-centered cubic



fcc

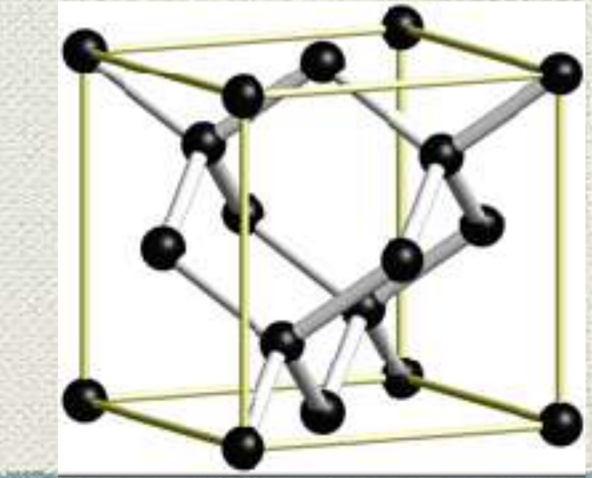
$$\begin{aligned} b &= 4r \\ b^2 &= a^2 + a^2 \\ 16r^2 &= 2a^2 \\ a &= \sqrt{8}r \end{aligned}$$

Face-centered cubic

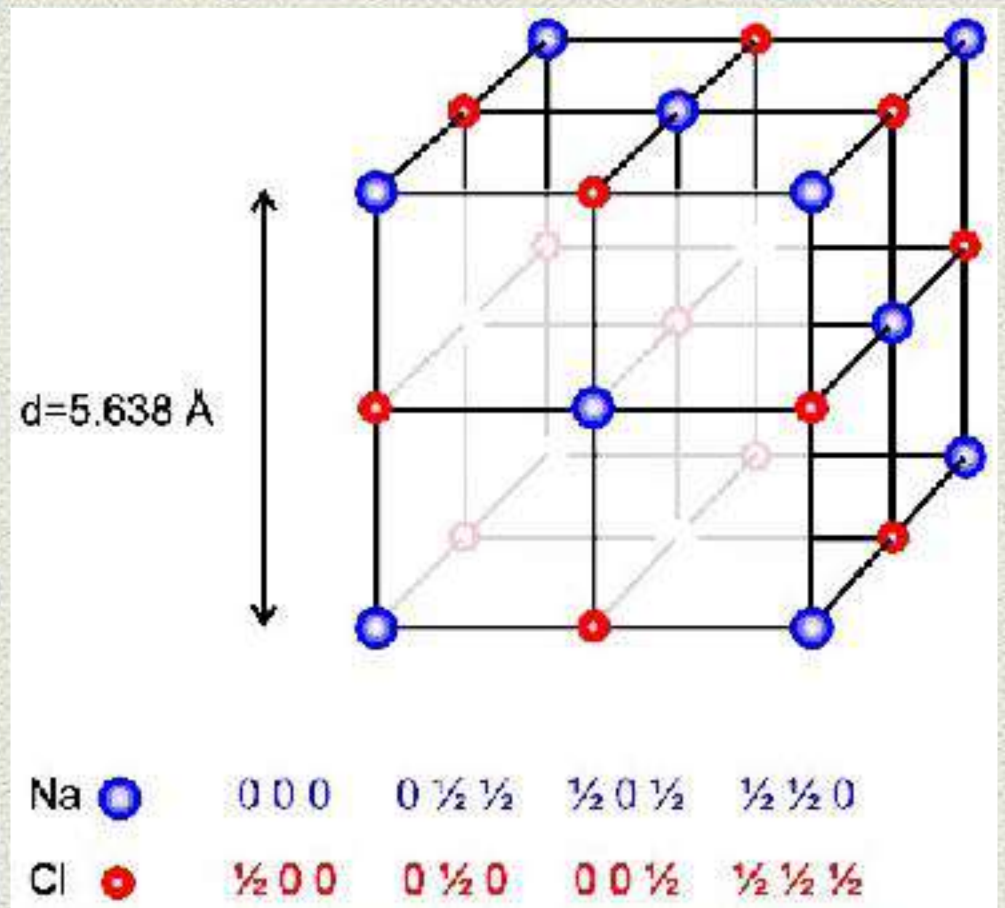
Structure of Diamond

Exhibits both cubic and hexagonal type structures. Diamond cubic structure is more common.

- It is formed by carbon atoms.
- Every carbon atom is surrounded by four other carbon atoms situated at the corners of regular tetrahedral by the covalent linkages.
- The diamond cubic structure is a combination of two interpenetrating FCC sub lattices displaced along the body diagonal of the cubic cell by 1/4th length of that diagonal.
- Thus the origins of two FCC sub lattices lie at (0, 0, 0) and (1/4, 1/4,1/4)
- No. of atoms contributed by the corner atoms to an unit cell is $8\times(1/8) = 1$.
- No. of atoms contributed by the face centred atoms to the unit cell is $6 \times (1/2) = 3$
- There are four more atoms inside the structure.
- No.of atoms present in a diamond cubic unit cell is $1 + 3 + 4 = 8$
- The co-ordination number is 4



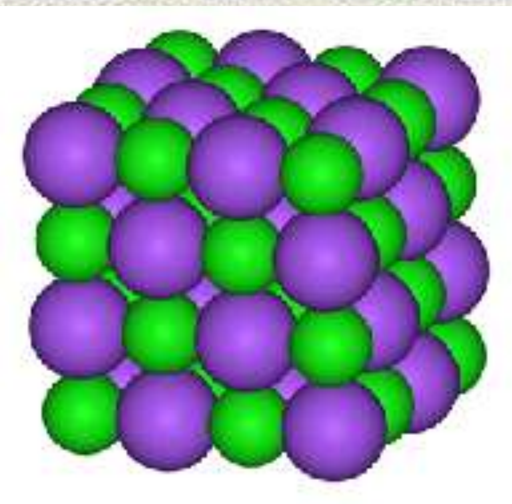
Structure of Sodium Chloride

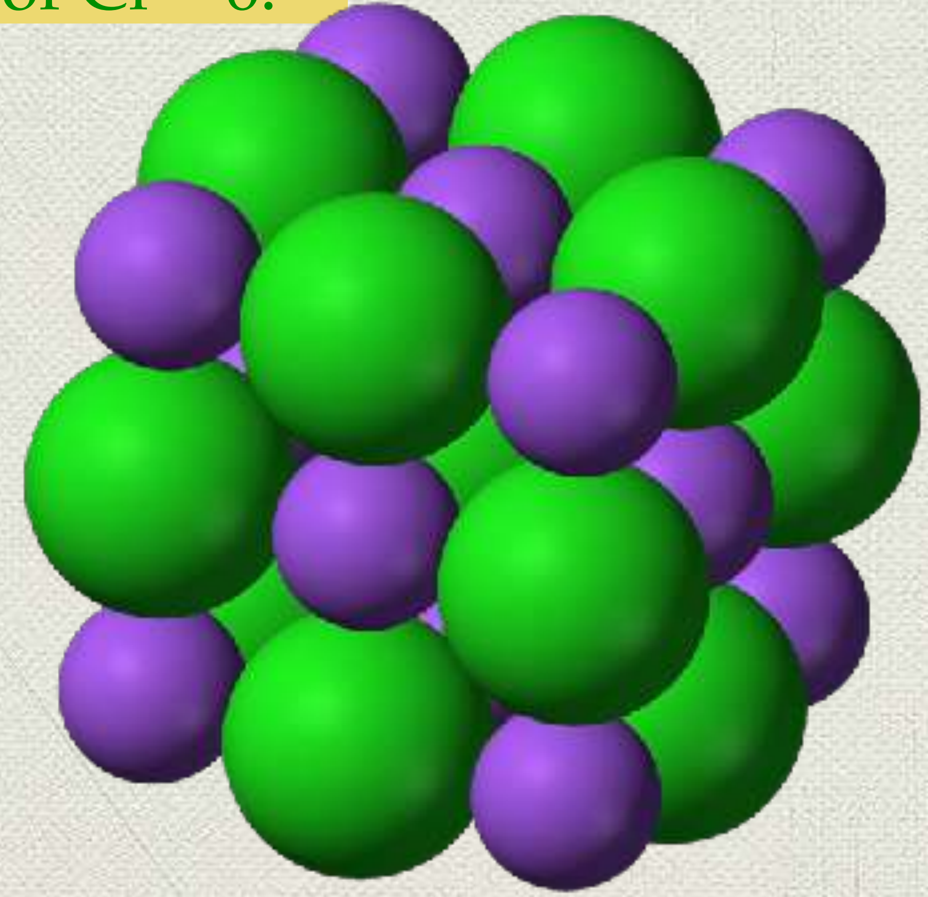


Na ●	0 0 0	0 ½ ½	½ 0 ½	½ ½ 0
Cl ●	½ 0 0	0 ½ 0	0 0 ½	½ ½ ½

Face centered cubic (fcc)

Coordination no of Na = 6;
Coordination no of Cl = 6.





For an fcc lattice there are 4 lattice points per cell,
Therefore the cell contents are
4 Na cations and 4 Cl anions.

X-ray crystallography

Study of atomic and molecular structure of a crystal by using X-ray diffraction technique

By measuring the angles and intensities of these diffracted beams, a crystallographer can produce a three-dimensional picture of the density of electrons within the crystal. From this electron density, the mean positions of the atoms in the crystal can be determined.

Why X ray ?

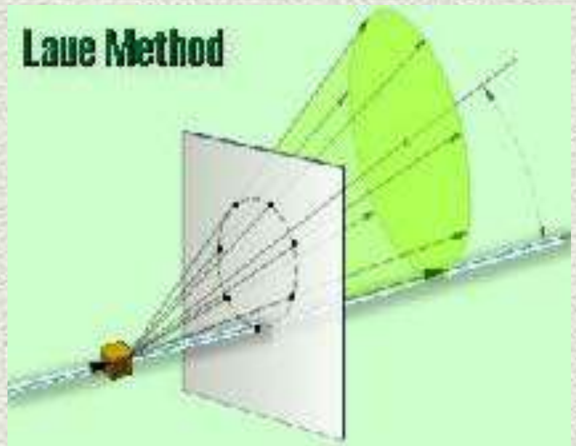
Wavelength is in the order of 0.1 nm

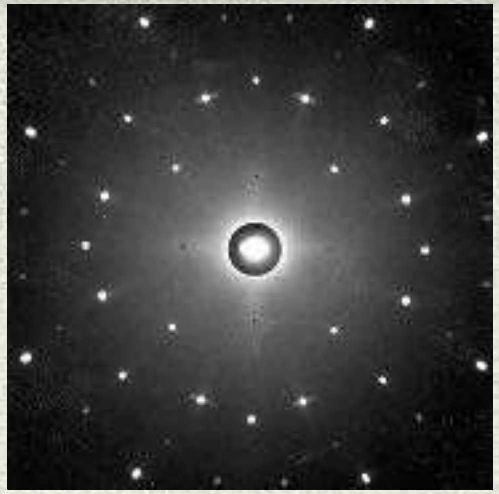
1912

Max Theodor Felix Laue

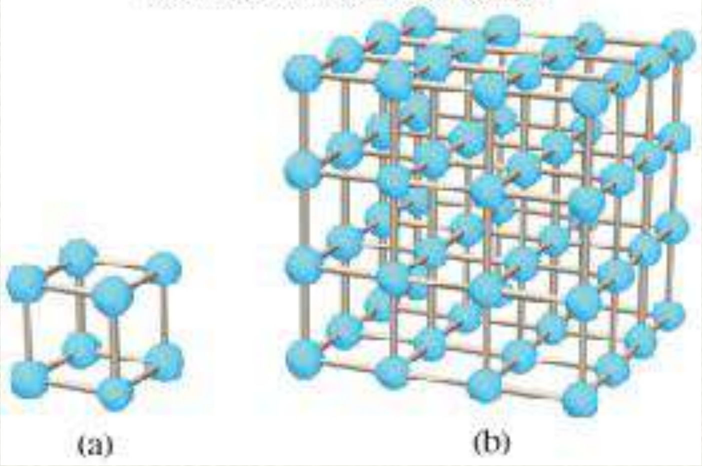
"Crystals act as a space grating"

Transmission Method

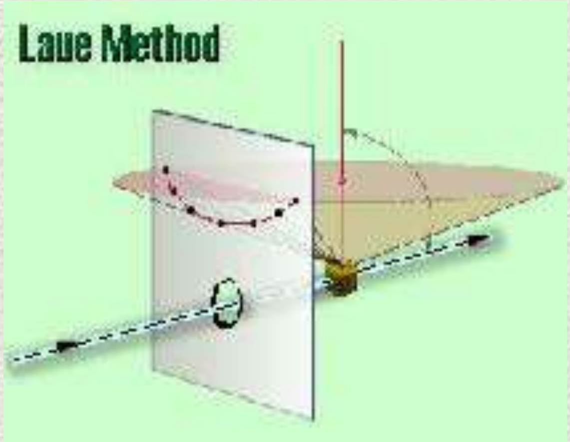




Laue pattern
Zinc blende



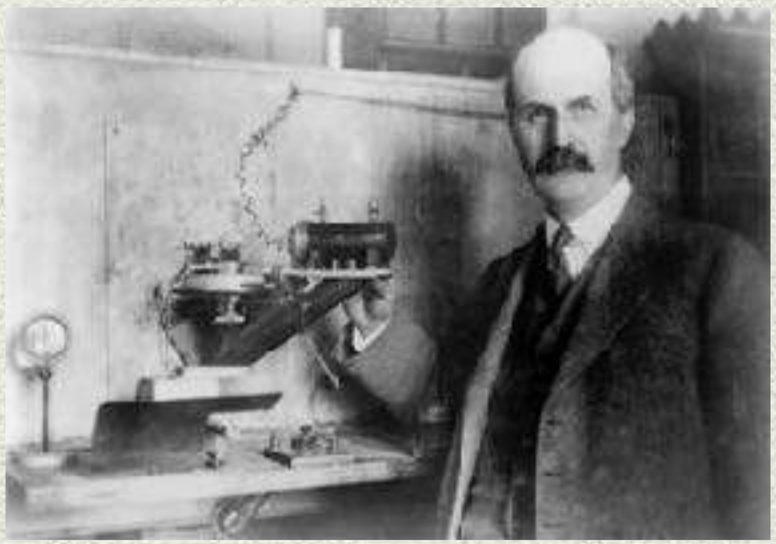
Back-reflection Method

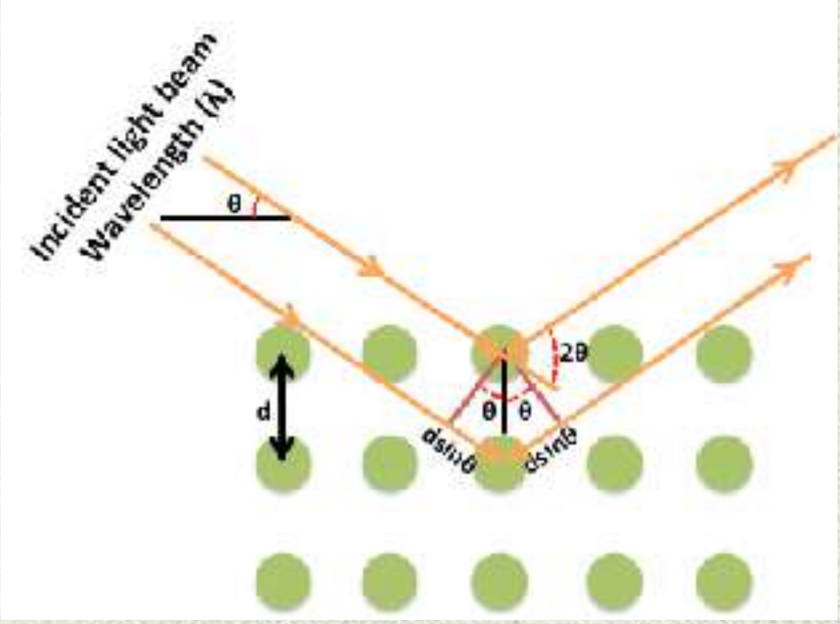


Proved that X-rays are electromagnetic radiation

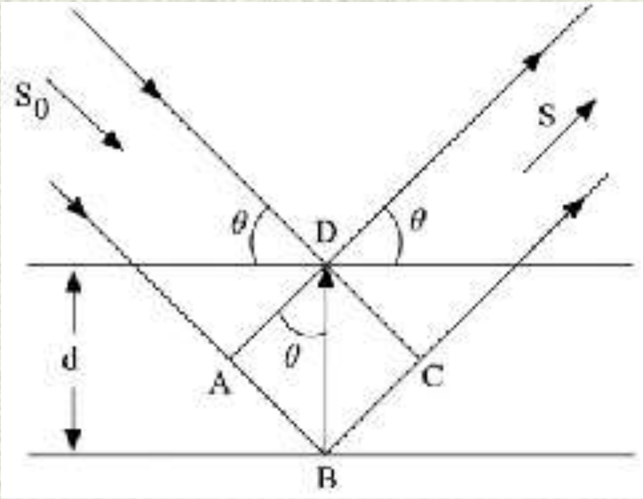
Bragg’s Law

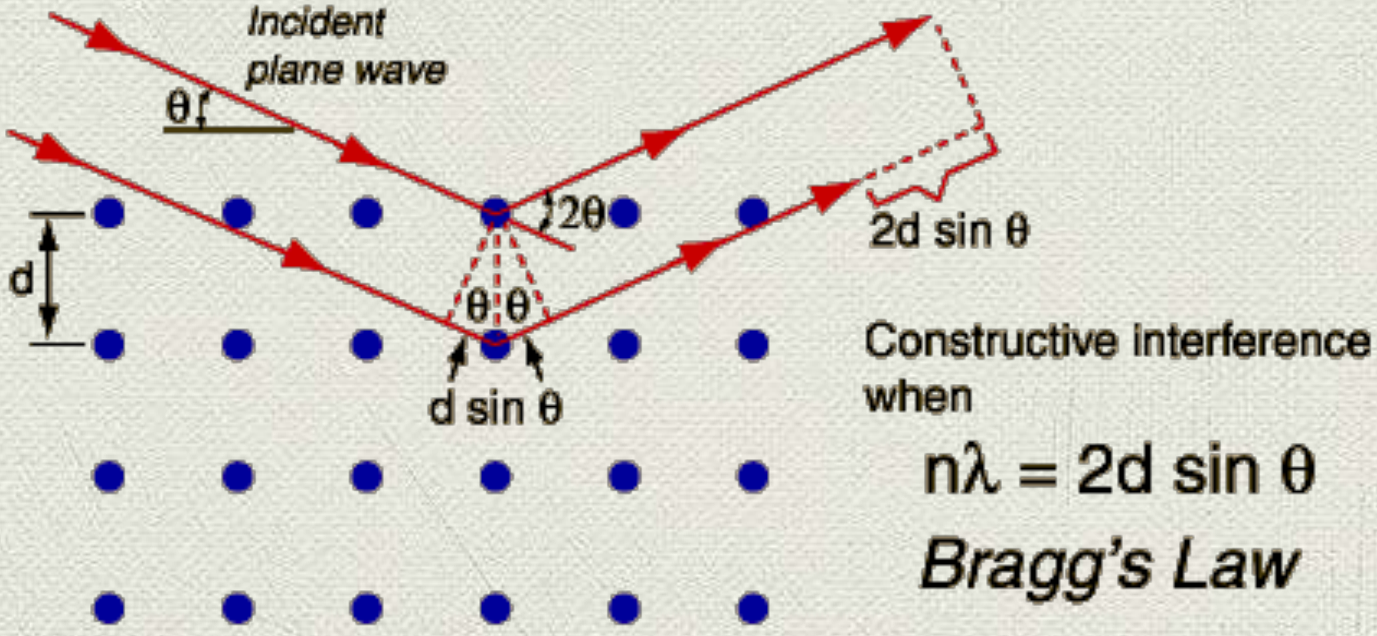
William Bragg





$$n\lambda = 2d \sin\theta$$



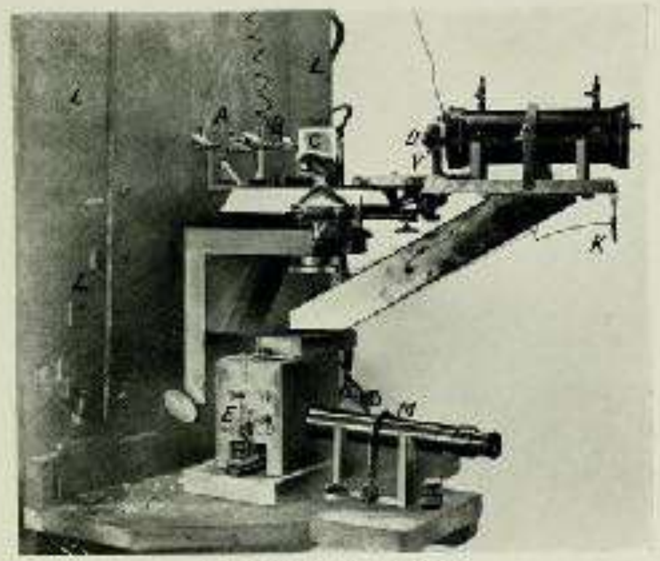


Constructive interference when

$$n\lambda = 2d \sin\theta$$

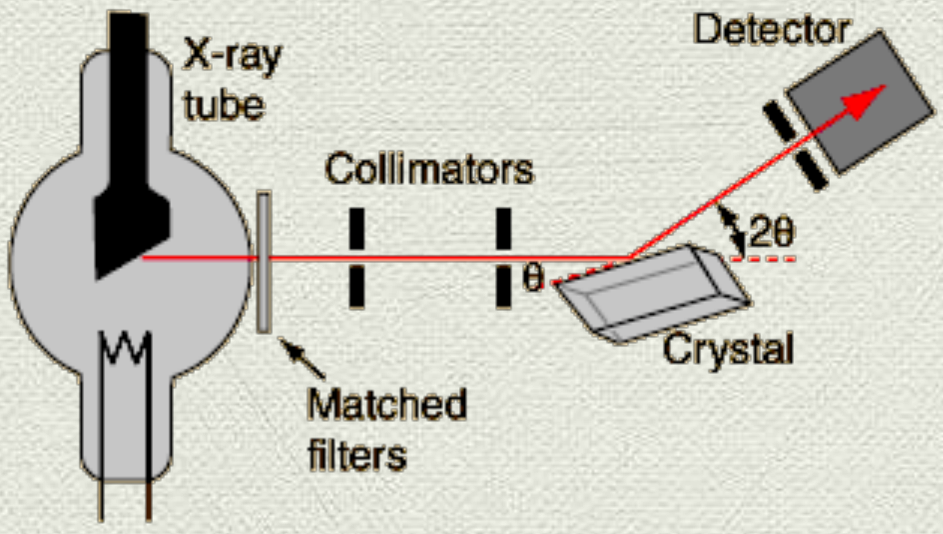
Bragg’s Law

Bragg’s X-ray Spectrometer



X-RAY SPECTROMETER.

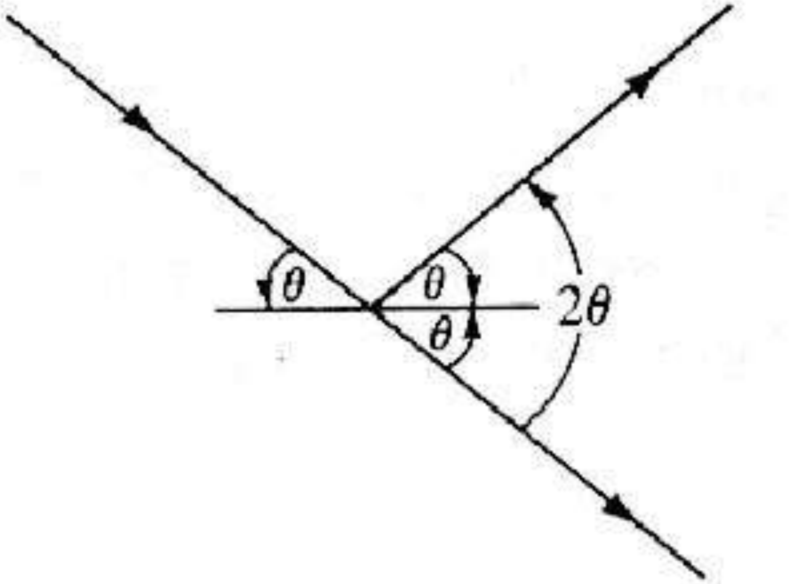
LLL. Lead box.
A, B, D. Slits.
C. Crystal.
I. Ionisation chamber.
V_1 Vernier of crystal table.
V_2 Vernier of ionisation chamber.
K. Earthing key.
E. Electroscope.
M. Microscope.



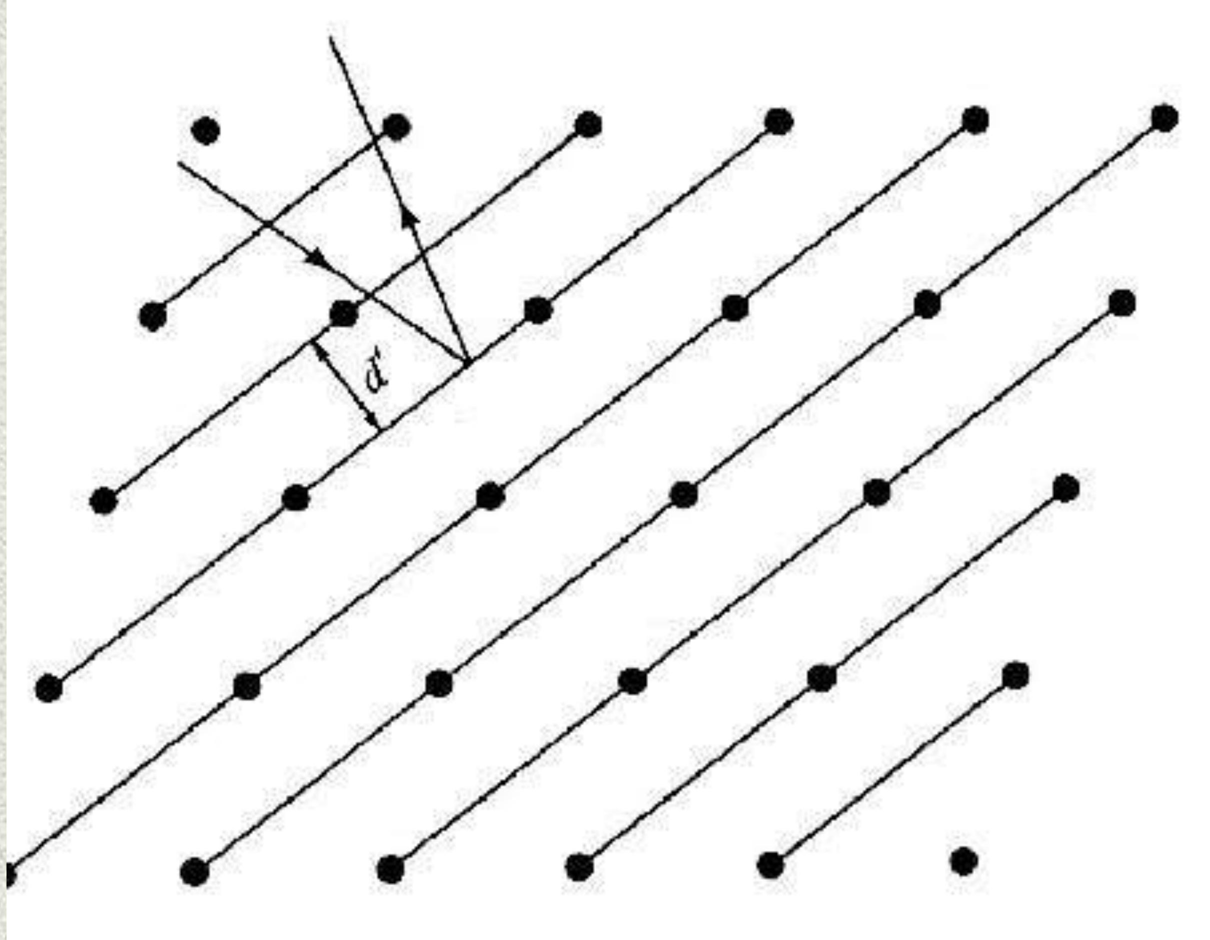
$$n=1, \qquad \lambda=2d\sin\theta_1$$
$$n=2, \qquad \lambda=2d\sin\theta_2$$
$$n=3, \qquad \lambda=2d\sin\theta_{3,\ etc}$$

$$\sin\theta_1 : \sin\theta_2 : \sin\theta_3 = 1 : 2 : 3$$

$$\frac{1}{\sin\theta_1} : \frac{1}{\sin\theta_2} : \frac{1}{\sin\theta_3} = d_{100} : d_{110} : d_{111}$$



Bragg angle θ is just the half of the total angle 2θ by which the incident beam is deflected.



Incident x-ray: along direction $\hat{n}$

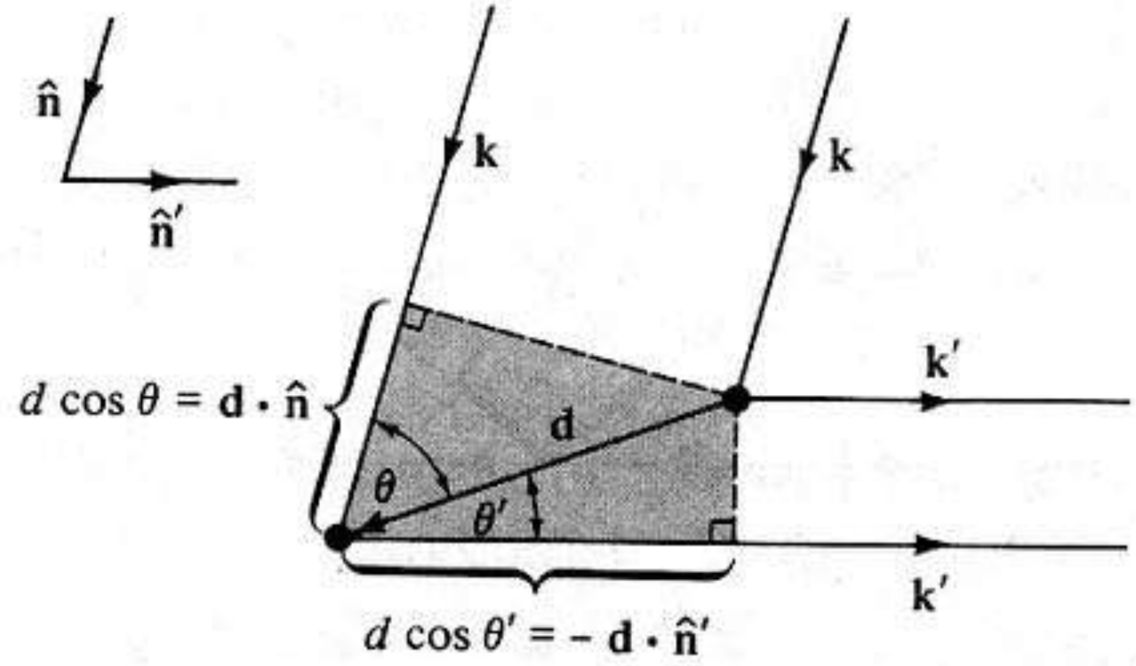
wavelength λ

wave vector $\vec{k} = \frac{2\pi}{\lambda}\hat{n}$

A scattered wave: direction $\hat{n}'$

wavelength λ

wave vector $\vec{k}' = \frac{2\pi}{\lambda}\hat{n}'$



$d\cos\theta = \mathbf{d}\cdot\hat{\mathbf{n}}$

$d\cos\theta' = -\mathbf{d}\cdot\hat{\mathbf{n}}'$

$$d\cos\theta + d\cos\theta' = \vec{d}\cdot(\hat{n}-\hat{n}')$$

Condition for constructive interference $\vec{d}\cdot(\hat{n}-\hat{n}') = m\lambda$ for integer m

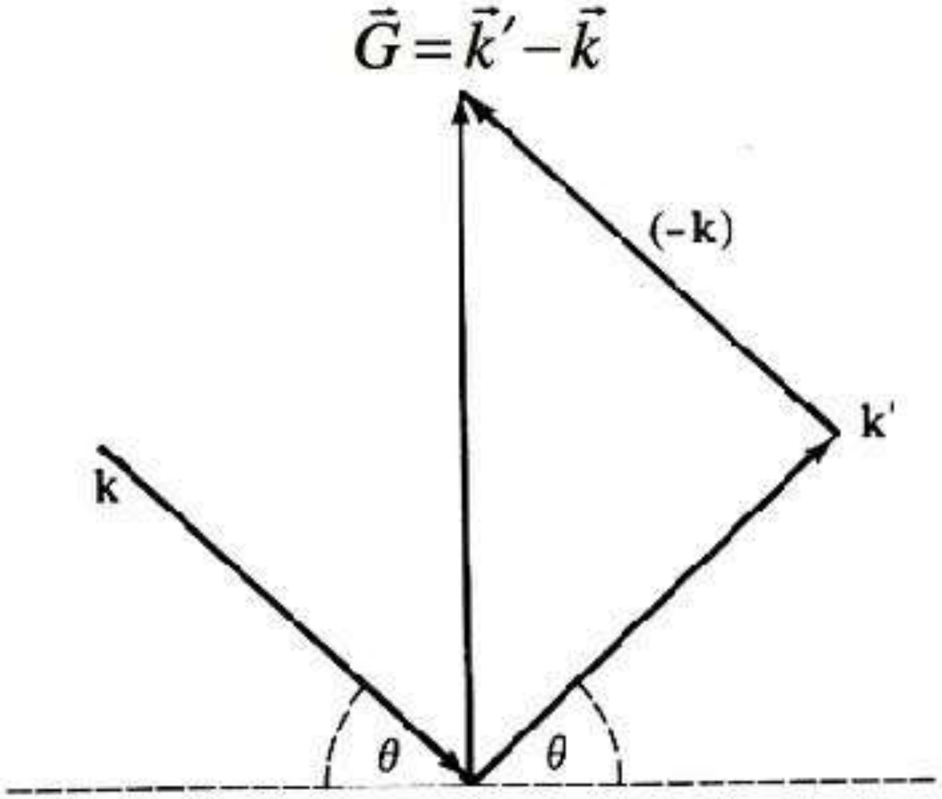
Multiply 2π $\vec{d}\cdot(\vec{k}-\vec{k}') = 2\pi m$

Equivalence of the Bragg and von Laue formulations

Suppose the incident and scattered wave vectors $\vec{k}$ and $\vec{k}'$, satisfy the Laue condition that $\vec{G}=\vec{k}'-\vec{k}$ be a reciprocal lattice vector

Elastic scattering: $\left|\vec{k}\right|=\left|\vec{k}'\right|$

It follows that $\vec{k}'$ and $\vec{k}$ make the same angle θ with the plane perpendicular to $\vec{G}$. Therefore the scattering can be viewed as a Bragg reflection with Bragg angle θ, from the family of direct lattice planes perpendicular to the reciprocal lattice vector $\vec{G}$.



The distance between successive planes in this family must satisfy:

$$\left|\vec{G}_0\right|=\frac{2\pi}{d}$$

where $\vec{G}_0$ is the shortest wave vector parallel to $\vec{G}$

$\vec{G}$ must be an integral multiple of $\vec{G}_0$, since reciprocal lattice is a Bravais lattice

$$\vec{G}=n\vec{G}_0$$

$$\left|\vec{G}\right|=n\left|\vec{G}_0\right|=\frac{2\pi n}{d}$$

From the figure, $\left|\vec{G}\right|=2k\sin\theta$

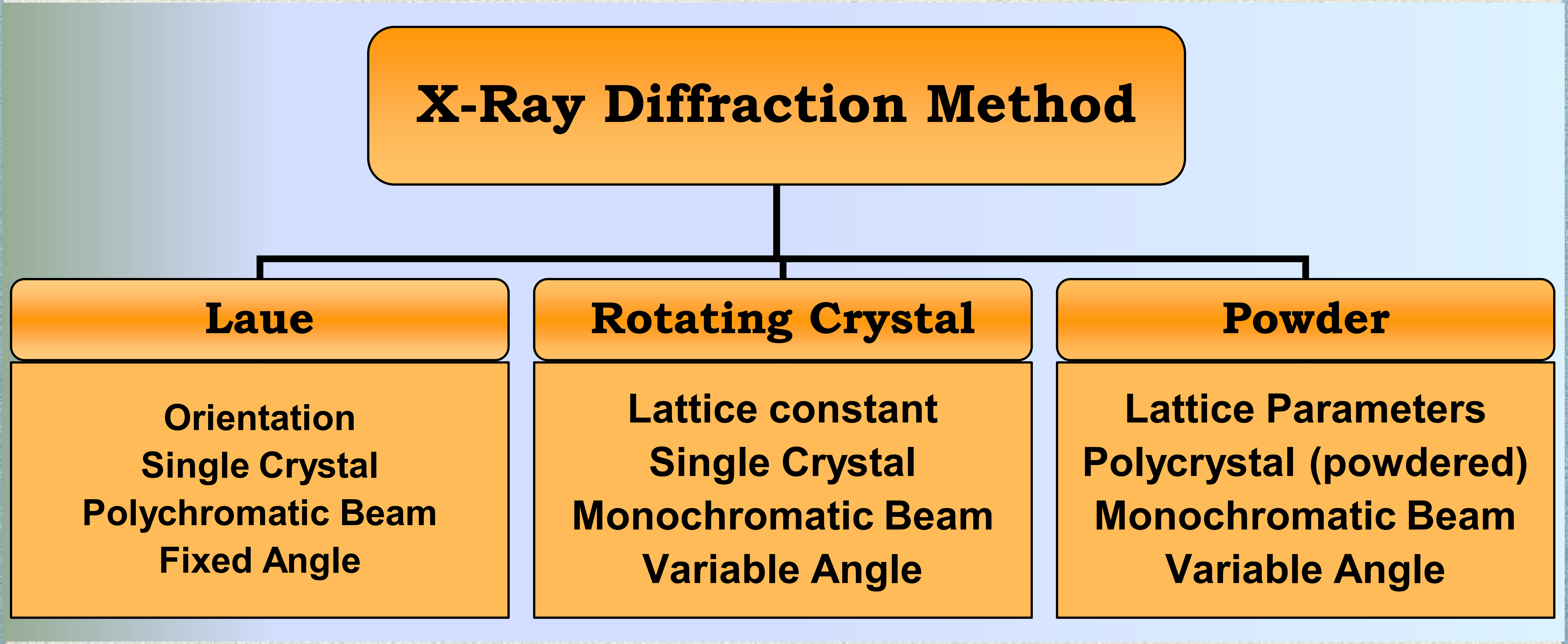
$$\therefore \quad k\sin\theta=\frac{\pi n}{d}$$

Note that $k=\dfrac{2\pi}{\lambda}$

$$n\lambda=2d\sin\theta$$

Bragg condition

X -ray Diffraction Methods



X-Ray Diffraction Method

Laue

Orientation
Single Crystal
Polychromatic Beam
Fixed Angle

Rotating Crystal

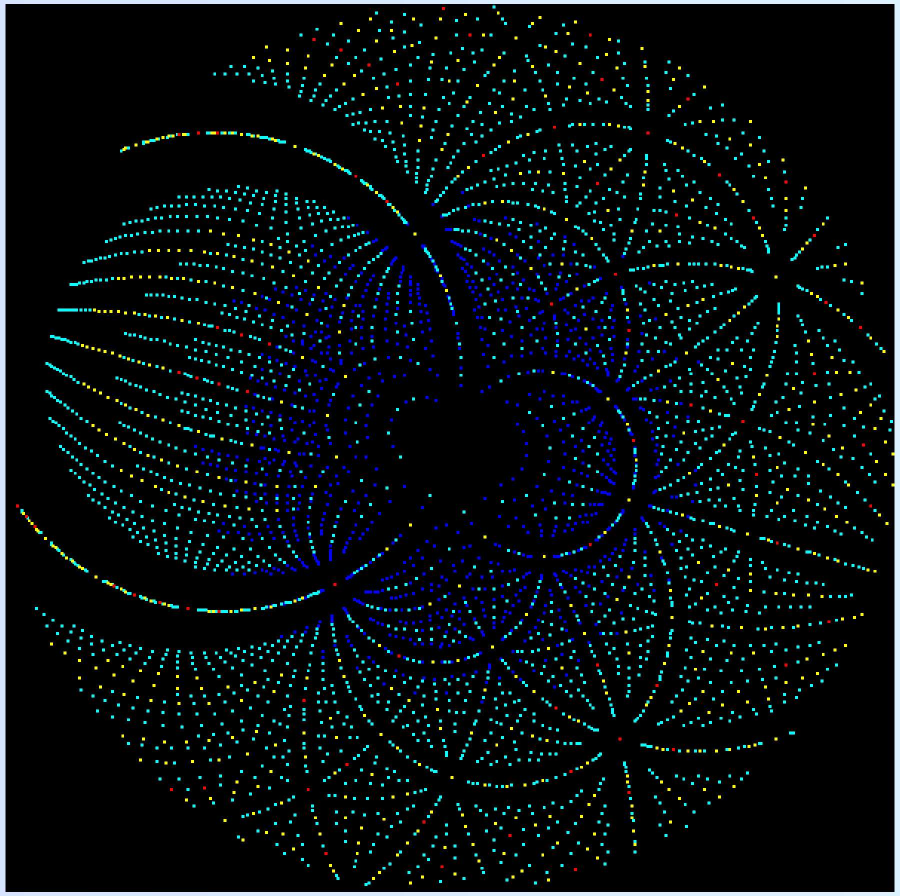
Lattice constant
Single Crystal
Monochromatic Beam
Variable Angle

Powder

Lattice Parameters
Polycrystal (powdered)
Monochromatic Beam
Variable Angle

Laue method

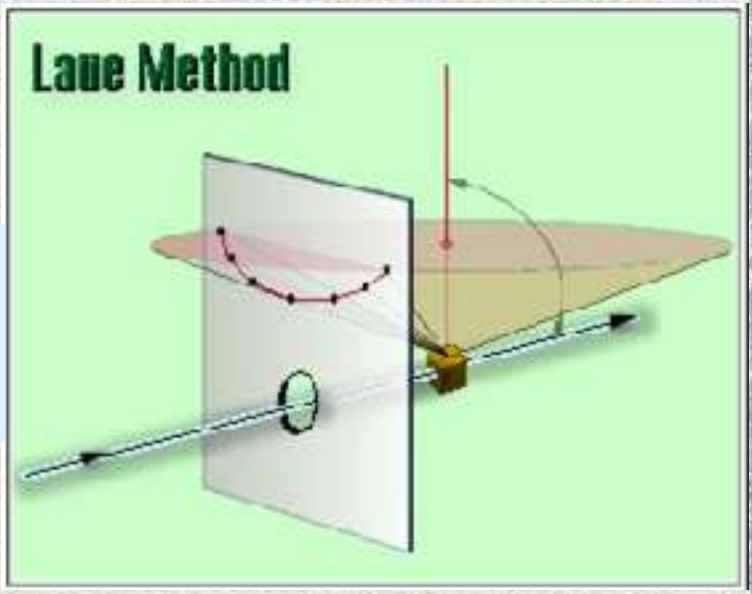
- The Laue method is mainly used to determine the orientation of large single crystals while radiation is reflected from, or transmitted through a fixed crystal.



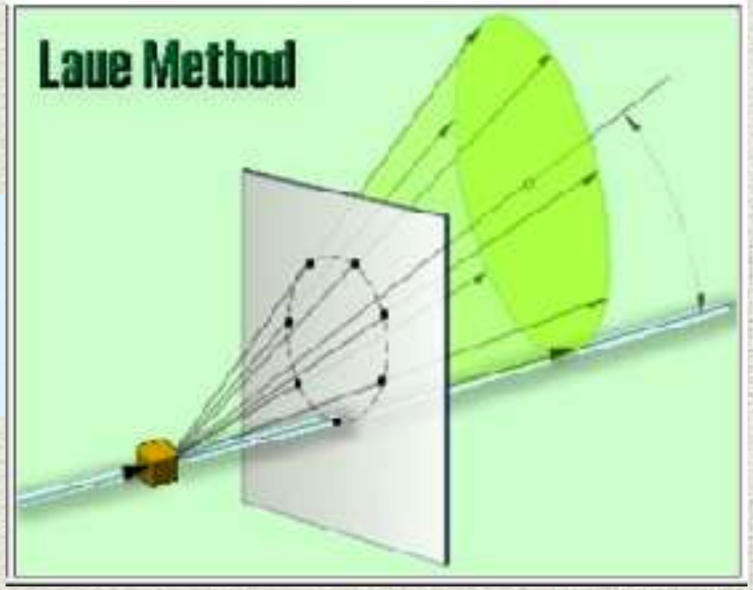
- The diffracted beams form arrays of spots, that lie on curves on the film.

- The Bragg angle is fixed for every set of planes in the crystal. Each set of planes picks out and diffracts the particular wavelength from the white radiation that satisfies the Bragg law for the values of *d* and θ involved.

- In the back-reflection method, the film is placed **between** the x-ray source and the crystal. The beams which are diffracted in a backward direction are recorded.



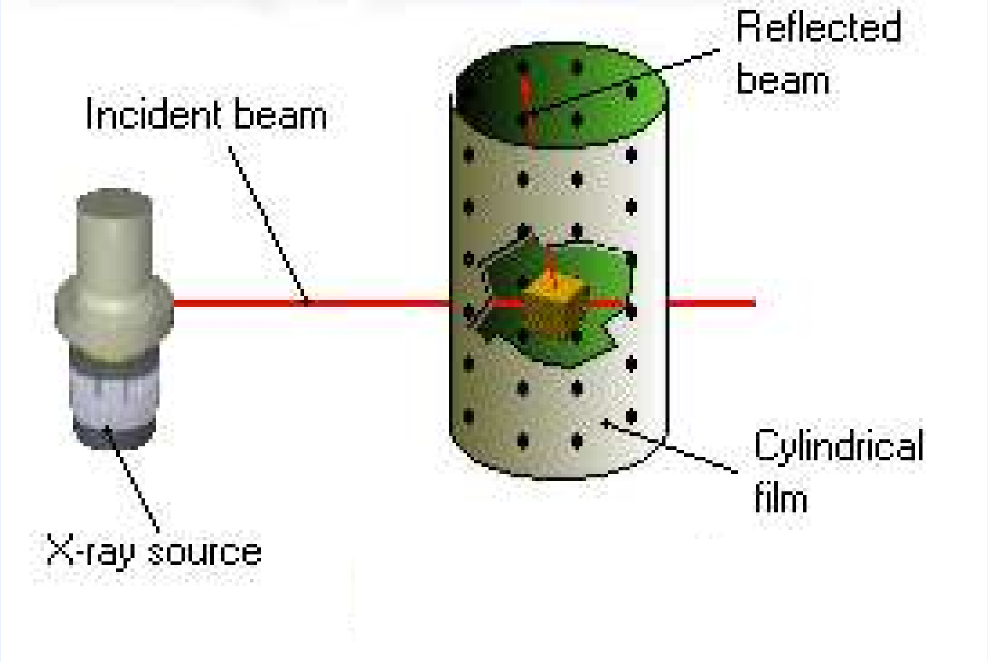
- In the transmission Laue method, the film is placed **behind** the crystal to record beams which are transmitted through the crystal.



- Therefore, the Laue method is mainly used to determine the crystal orientation.
- Although the Laue method can also be used to determine the crystal structure, several wavelengths can reflect in different orders from the same set of planes, with the different order reflections superimposed on the same spot in the film. This makes crystal structure determination by spot intensity diffucult.
- Rotating crystal method overcomes this problem. How?

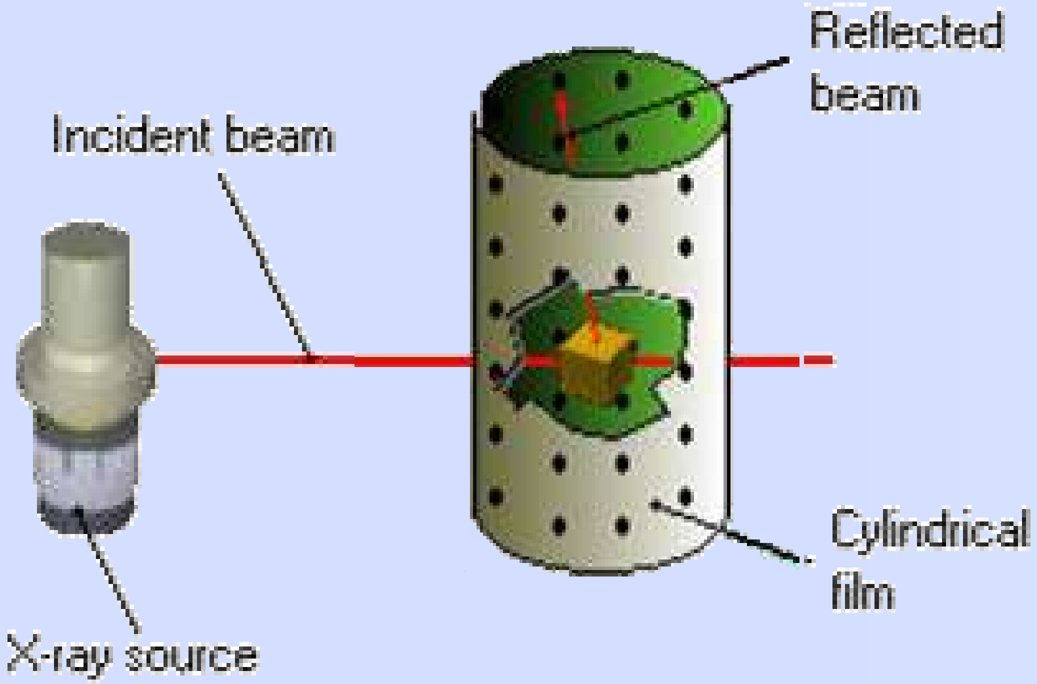
Rotating Crystal method

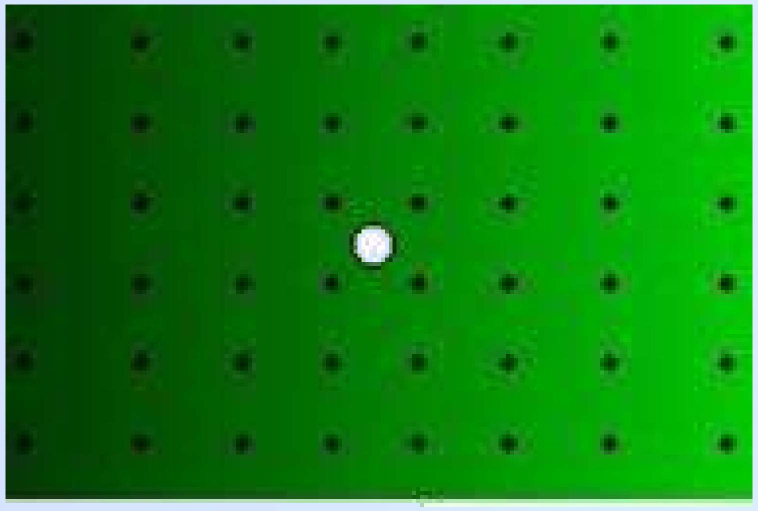
- In the rotating crystal method, a single crystal is mounted with an axis normal to a monochromatic x-ray beam. A cylindrical film is placed around it and the crystal is rotated about the chosen axis.



- As the crystal rotates, sets of lattice planes will at some point make the correct Bragg angle for the monochromatic incident beam, and at that point a diffracted beam will be formed.

The reflected beams are located on the surface of imaginary cones. By recording the diffraction patterns (both angles and intensities) for various crystal orientations, one can determine the shape and size of unit cell as well as arrangement of atoms inside the cell.





Film

Powder Diffraction Method

If a powdered specimen is used, instead of a single crystal, then there is ***no need to rotate*** the specimen, because there will always be some crystals at an orientation for which diffraction is permitted. Here a monochromatic X-ray beam is incident on a powdered or polycrystalline sample.

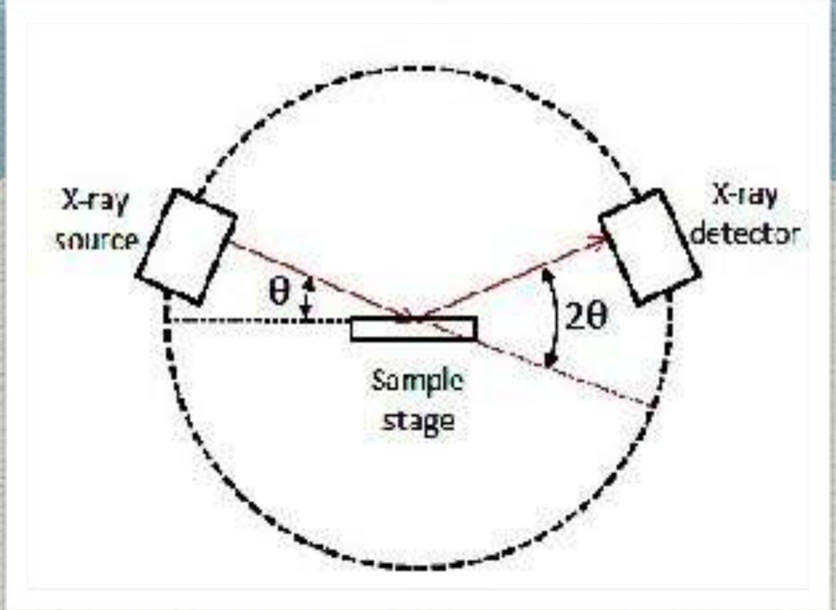
This method is useful for samples that are difficult to obtain in single crystal form.

The powder method is used to determine the value of the lattice parameters accurately. Lattice parameters are the magnitudes of the unit vectors **a**, **b** and **c** which define the unit cell for the crystal.

For every set of crystal planes, by chance, ***one or more crystals*** will be in the ***correct orientation*** to give the correct Bragg angle to satisfy Bragg's equation. Every crystal plane is thus capable of diffraction. Each diffraction line is made up of a large number of small spots, each from a separate crystal. Each spot is so small as to give the appearance of a continuous line.

Powder Diffraction

X-ray tube
Sample holder
X-ray detector.

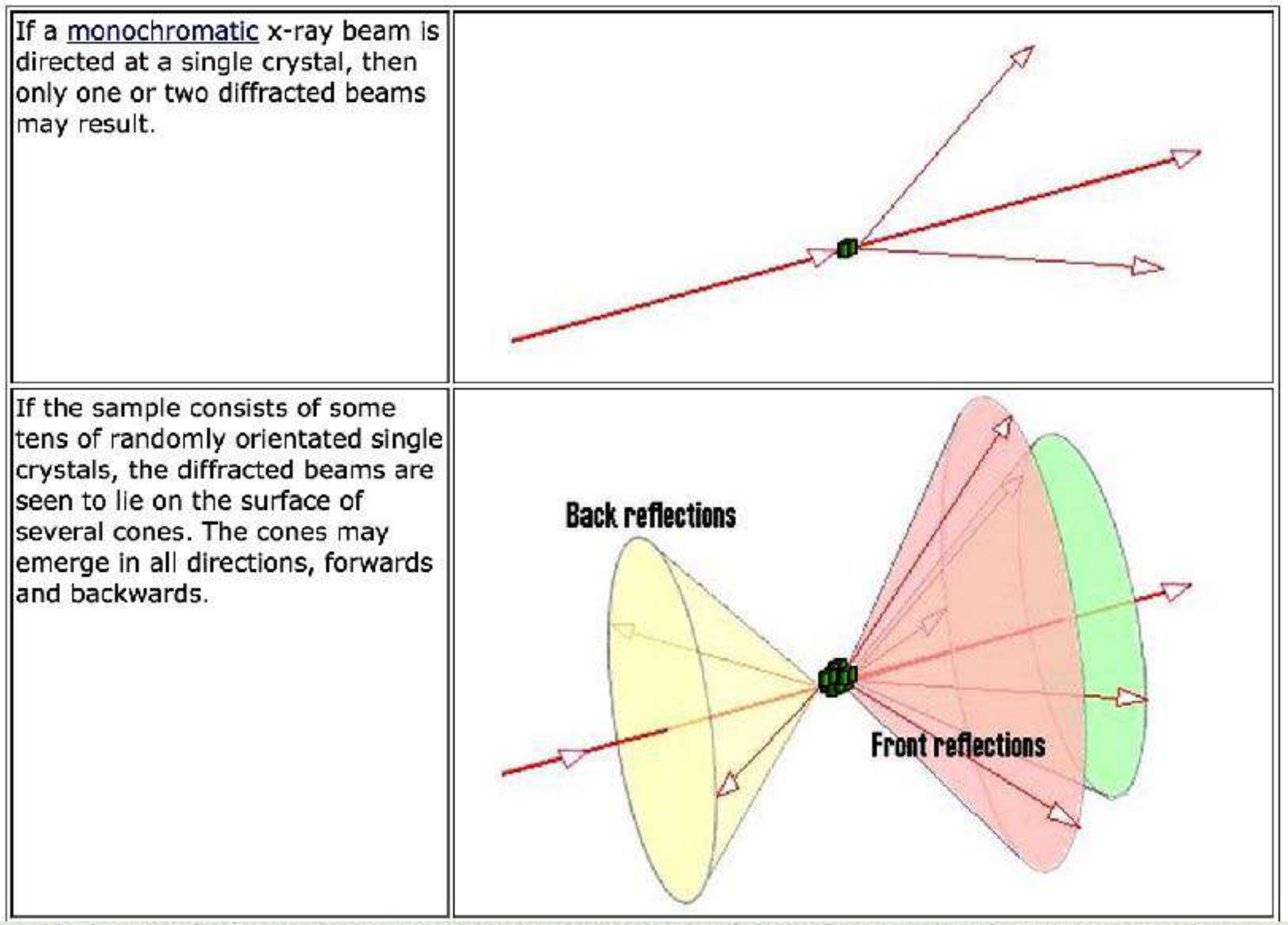


Rapid analytical technique primarily used for phase identification of a crystalline material and can provide information on unit cell dimensions.

By scanning the sample through a range of 2θangles, all possible diffraction directions of the lattice should be attained due to the random orientation of the powdered material. Conversion of the diffraction peaks to d-spacings allows identification of the mineral because each mineral has a set of unique d-spacings.

X-rays are collimated and directed onto the sample. As the sample and detector are rotated, the intensity of the reflected X-rays is recorded. When the geometry of the incident X-rays impinging the sample satisfies the Bragg Equation, constructive interference occurs and a peak in intensity occurs. A detector records and processes this X-ray signal

The powder method is used to determine the value of the lattice parameters accurately.

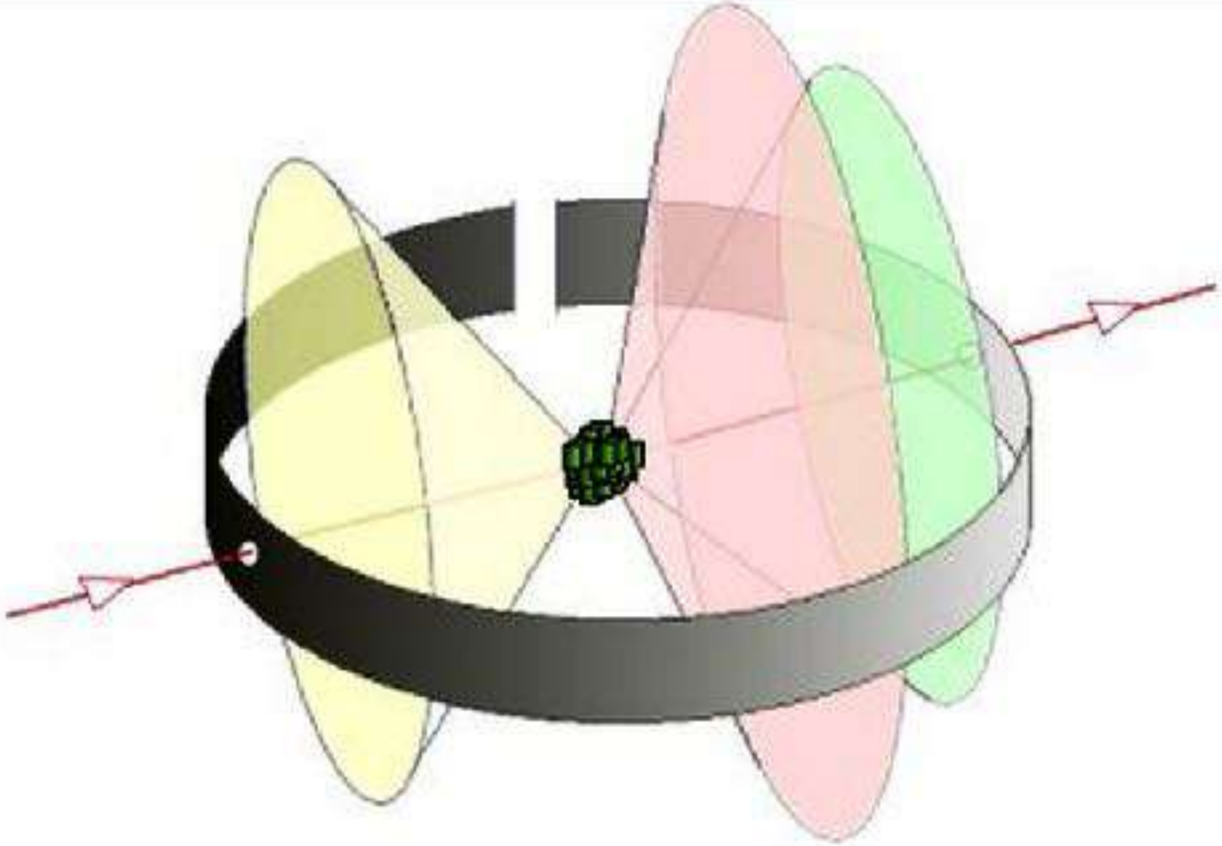


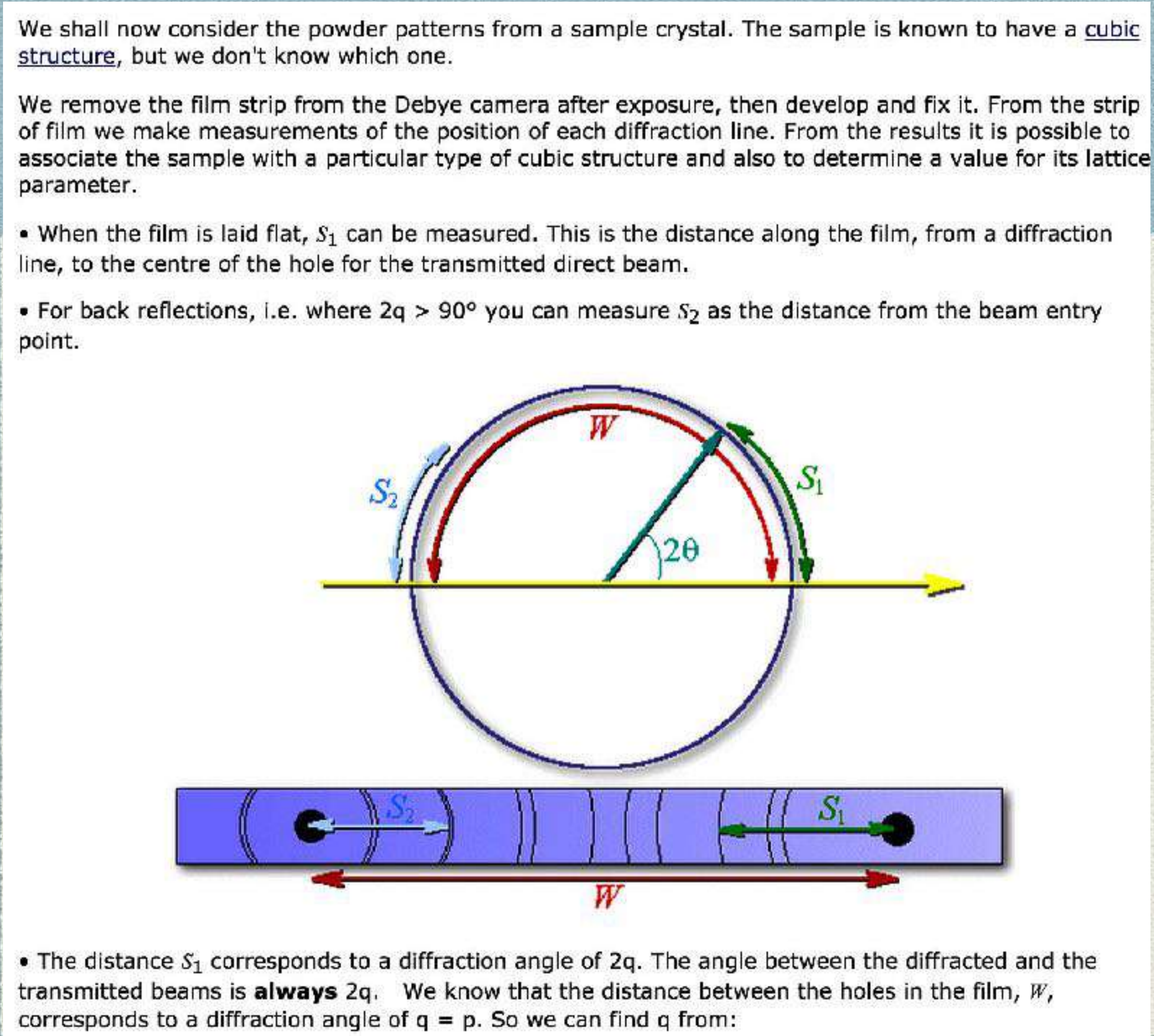
If a monochromatic x-ray beam is directed at a single crystal, then only one or two diffracted beams may result.

If the sample consists of some tens of randomly orientated single crystals, the diffracted beams are seen to lie on the surface of several cones. The cones may emerge in all directions, forwards and backwards.

A sample of some hundreds of crystals (i.e. a powdered sample) show that the diffracted beams form continuous cones.

A circle of film is used to record the diffraction pattern as shown. Each cone intersects the film giving diffraction lines. The lines are seen as arcs on the film.



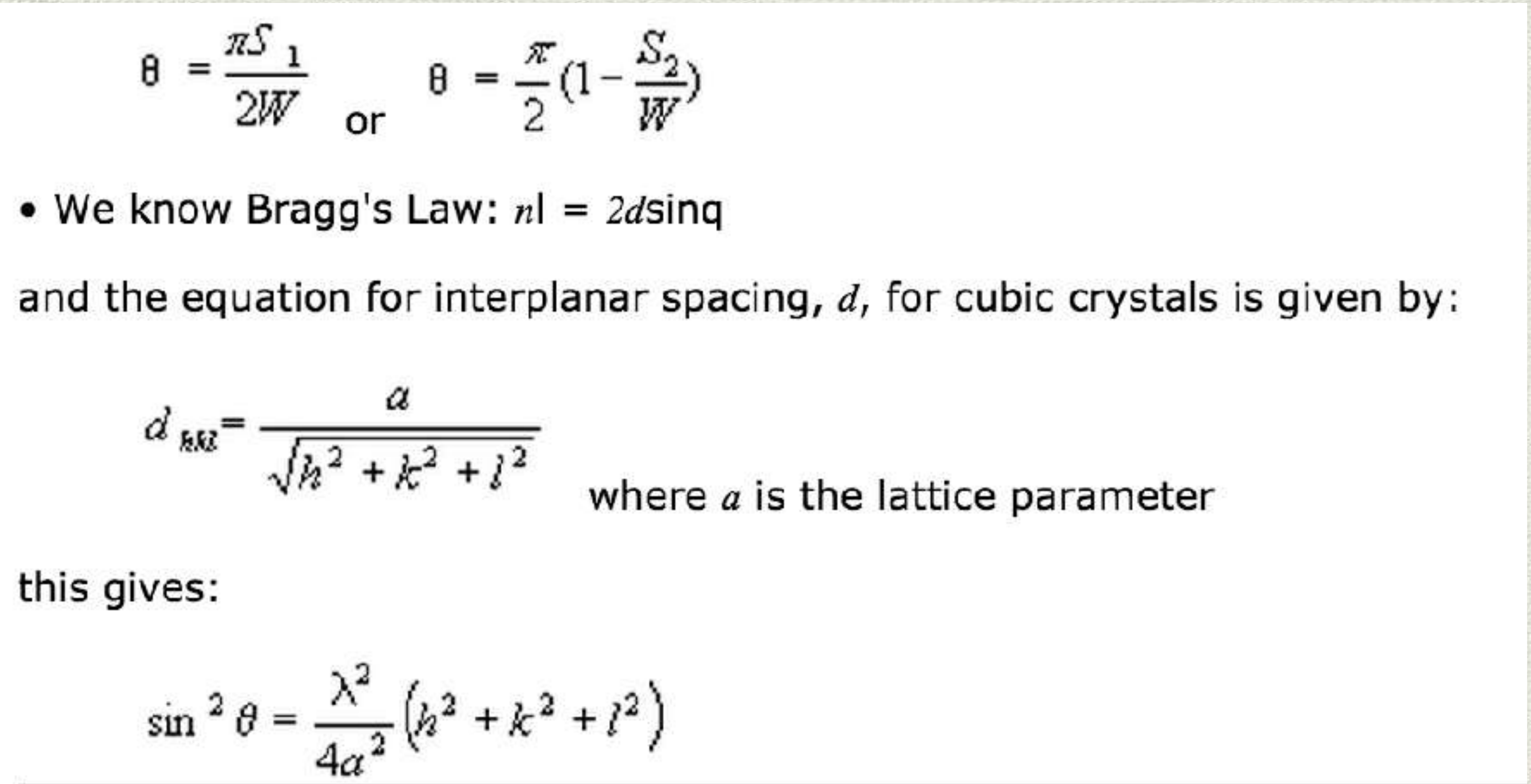


We shall now consider the powder patterns from a sample crystal. The sample is known to have a cubic structure, but we don't know which one.

We remove the film strip from the Debye camera after exposure, then develop and fix it. From the strip of film we make measurements of the position of each diffraction line. From the results it is possible to associate the sample with a particular type of cubic structure and also to determine a value for its lattice parameter.

- When the film is laid flat, S_1 can be measured. This is the distance along the film, from a diffraction line, to the centre of the hole for the transmitted direct beam.
- For back reflections, i.e. where 2q > 90° you can measure S_2 as the distance from the beam entry point.

- The distance S_1 corresponds to a diffraction angle of 2q. The angle between the diffracted and the transmitted beams is **always** 2q. We know that the distance between the holes in the film, W, corresponds to a diffraction angle of q = p. So we can find q from:



$$\theta = \frac{\pi S_1}{2W} \quad \text{or} \quad \theta = \frac{\pi}{2}\left(1 - \frac{S_2}{W}\right)$$

- We know Bragg's Law: *n*l = *2d*sinq

and the equation for interplanar spacing, *d*, for cubic crystals is given by:

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

where *a* is the lattice parameter

this gives:

$$\sin^2\theta = \frac{\lambda^2}{4a^2}\left(h^2 + k^2 + l^2\right)$$