X-ray Diffraction and crystal structure:

It was suggested by Von Laue in 1913, that it might be possible to diffract X-rays by means of crystals. The reason for this suggestion was that the wavelength of X-rays was of about the same order (10^{-3} cm) as the interatomic distances in the crystal.

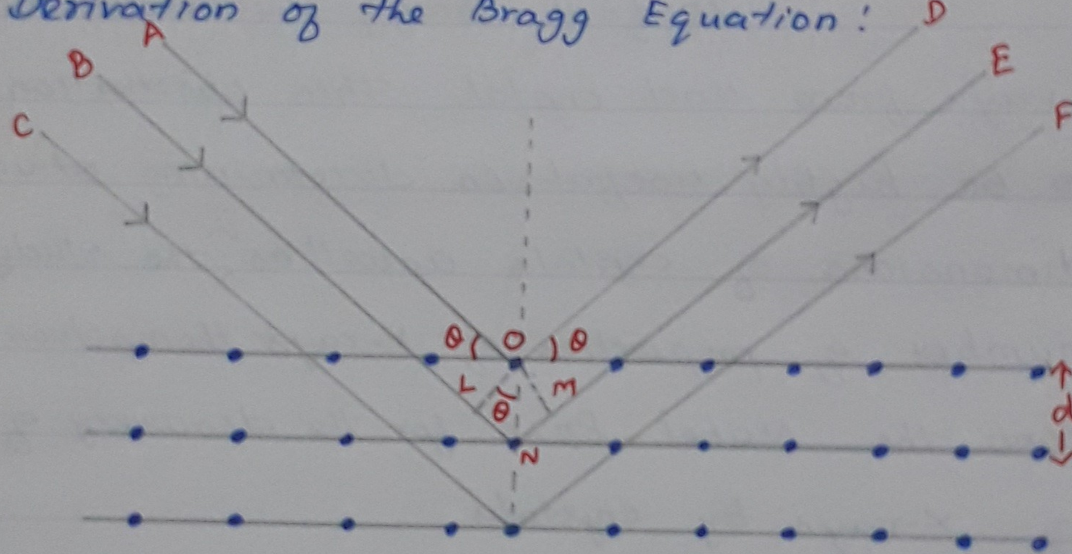
In fact Bragg succeeded in diffracting X-rays from NaCl crystal. This observation has proved to be highly useful in determining structures and dimensions of crystals as well as in the study of a number of properties of X-rays themselves. Laue won the Nobel Prize for the discovery of diffraction of X-rays by crystals.

The Bragg Equation:

W.H. Bragg pointed out that scattering of X-rays by crystals could be considered as reflection from successive planes of atoms in the crystals. However, unlike reflection of ordinary light, the reflection of X-rays can take place only at certain angles which are determined by the wavelength of the X-rays and the distance between the planes in the crystal.

The fundamental equation which gives a simple relation between the wavelength of the X-rays, the interplanar distance in the crystals and the angle of reflection is known as the Bragg equation.

Derivation of the Bragg Equation:



X-ray reflections from a crystal.

Consider the above diagram. The horizontal lines in the diagram represent parallel planes in the crystal structure separated from one another by the distance 'd'. Suppose a beam of X-rays falls on the crystal at glancing angle θ. Some of these X-rays will be reflected from the upper plane at the same angle θ, while some others will be absorbed and got reflected from the successive layers as shown.

Let the planes ABC and DEF be drawn perpendicular to the incident and reflected beams respectively. The waves reflected by different ~~layers~~ planes will coincide with one another in the plane DEF, only if the path length of the waves reflected from the successive planes is equal to the integral number of wavelengths.

Drawing OL and OM perpendicular to the incident and reflected beams, it will be seen that the difference in the path lengths (say δ) of the waves reflected from the first two planes is given by,

$$\delta = LN + NM$$

This should be equal to the whole number of multiple of wavelength λ i.e

$$LN + NM = n\lambda.$$

Since, the triangles OLN & OMN are congruent, hence $LN = NM$.

$\therefore \quad 2LN = n\lambda$.

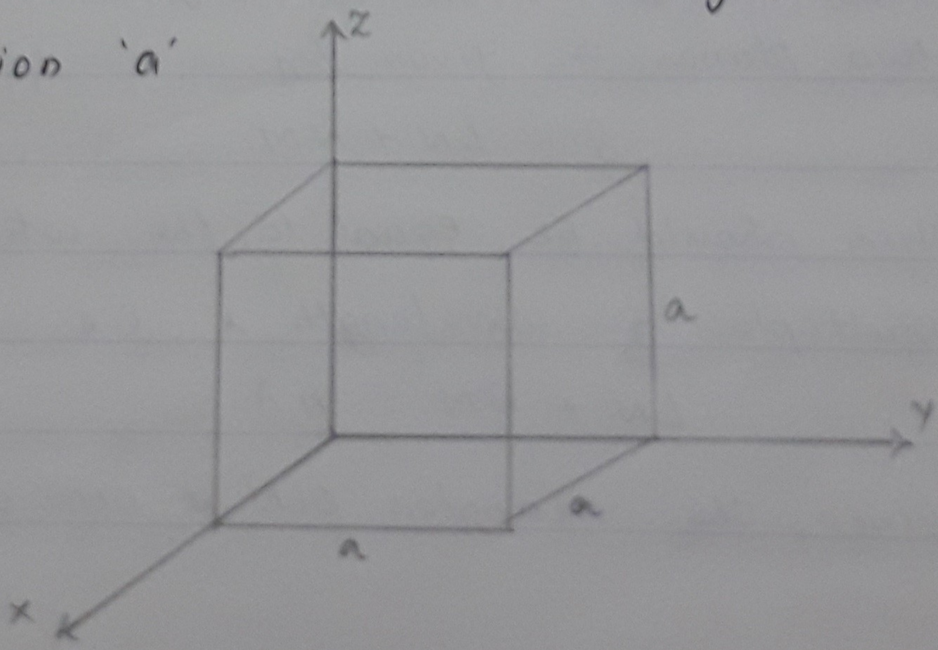
or $\quad 2d\sin\theta = n\lambda$.

This is the Bragg equation. knowing θ, n & λ, d can be calculated.

Miller Indices (hkl)

The orientation of a crystal plane is defined by considering how the plane intersects the main crystallographic axes of the solid. The application of a set of rules leads to the assignment of the Miller indices. (hkl); a set of numbers which quantify the intercepts and thus may be used uniquely to identify the plane or surface.

If we consider a cubic system with dimension 'a'



Miller Indices

The crystal lattice may be regarded as made up of infinite set of equidistant planes passing through lattice points which are known as lattice planes.

The orientation of planes in a crystal can be described interms of their intercepts on the three axes.

Miller introduced a system to ~~investigate~~ designate a plane in a crystal. He introduced a set of three numbers to specify a plane in a crystal. These set of 3 numbers are known as Miller indices of the concerned plane. These are used to express lattice planes and directions.

Significance:

Miller indices are group of three numbers that indicate the orientation of a plane or set of parallel planes of atoms in a crystal It has the advantage of eliminating all fractions from the notation for a plane.

Definition :-

Miller indices of a plane indicated by hkl, are given by the reciprocal of the intercepts of the plane on the three axes.

It usually refers to the plane nearest to the origin.

Family of planes :-

Infinite set of parallel lattice planes.

Unit cell :-

Most basic and least volume consuming repeating structure of any solid.

Lattice :-

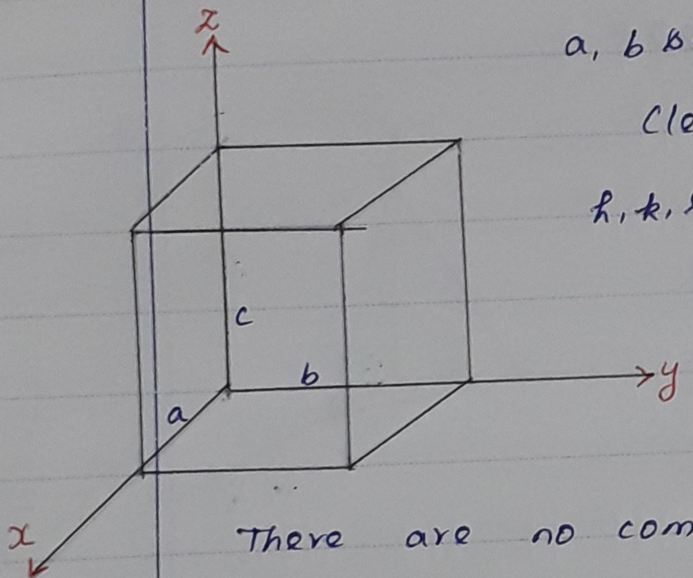
When the unit cell repeats, the network is called lattice.

Crystal planes :-

Some imaginary planes inside a crystal in which large concentration of atoms exist in certain directions. These directions are called crystal directions.

Crystallography :

It is the experimental science of determining the arrangement of atoms in crystalline solids.



x, y & z are the axes.

a, b & c are lattice parameters.

(length of the unit cell along a side).

h, k, l are Miller indices for planes and directions.

Expression of planes (hkl)

Expression of direction [hkl]

There are no commas between the numbers.

Determination of Miller Indices :

Find the Miller indices for the parameters $a = 2$; $b = 3$; $c = 2$.

Step 1 : The intercepts are 2, 3, 2 on three axes.

Step 2 : The reciprocals are $1/2$, $1/3$, $1/2$.

Step 3 : The least common denominator is 6.

Multiplying each reciprocal by 6, we get

$1/2 \times 6$, $1/3 \times 6$, $1/2 \times 6$.

3 2 3

Step 4 : Miller Indices for the plane is (3 2 3)

Problems:

1)

	a	b	c
Intercept length	$\frac{1}{4}$	1	$\frac{1}{2}$
Reciprocal	$\frac{1}{1/4}$	$\frac{1}{1}$	$\frac{1}{1/2}$.
Cleared fraction	4	1	2

∴ Miller Indices (412)

2)

a	b	c
1	0	2
1	∞	2
$\frac{1}{1}$	$\frac{1}{\infty}$	$\frac{1}{2}$
1	0	2

M. I (102)

3)

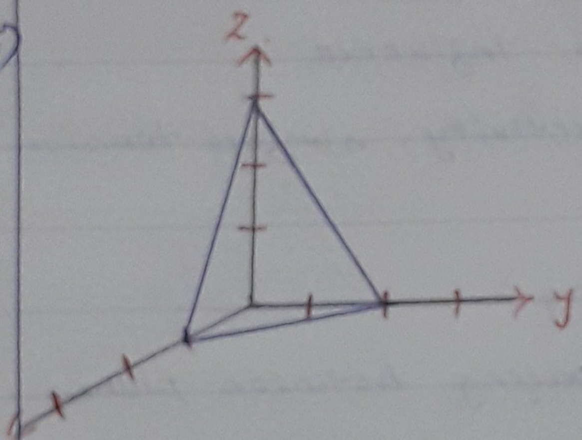
a	b	c
3	1	2
$\frac{1}{3}$	$\frac{1}{1}$	$\frac{1}{2}$
$\frac{1}{3} \times 6$	$\frac{1}{1} \times 6$	$\frac{1}{2} \times 6$
2	6	3

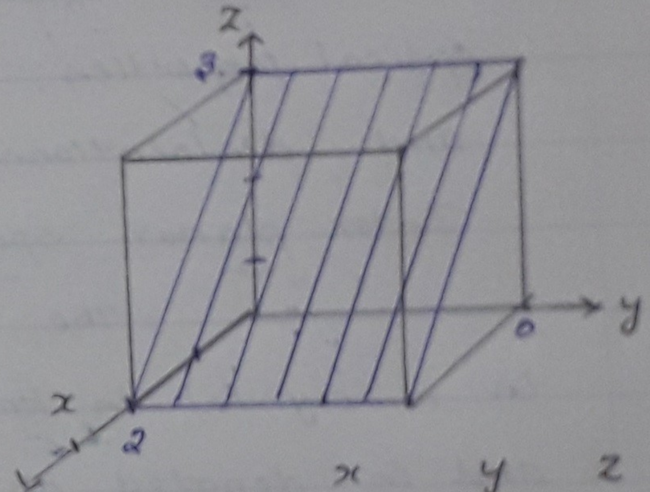
M. I (263)

	x	y	z
4)	1	2	3
	$\frac{1}{1}$	$\frac{1}{2}$	$\frac{1}{3}$
	$\frac{1}{1}\times 6$	$\frac{1}{2}\times 6$	$\frac{1}{3}\times 6$
	6	3	2

M. I (6 3 2)

↓

5) 



x	y	z
2	0	3
$\frac{1}{2}$	0	$\frac{1}{3}$
$\frac{1}{2}\times 6$	0×6	$\frac{1}{3}\times 6$
3	0	2

[hkl] - represents a direction.

<hkl> - represents a ~~fam~~ family of directions.

(hkl) - represents a plane

{hkl} - represents a family of planes.

Applications of Miller Indices :

Miller Indices influence optical properties, reactivity, surface tension and dislocations.

Inter planar spacing :

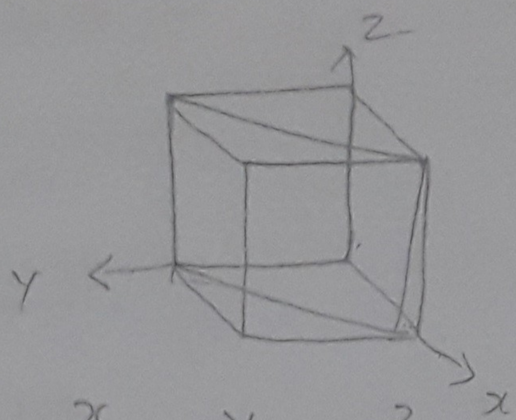
The spacing between planes in a crystal is known as interplanar spacing and is denoted as d_{hkl}.

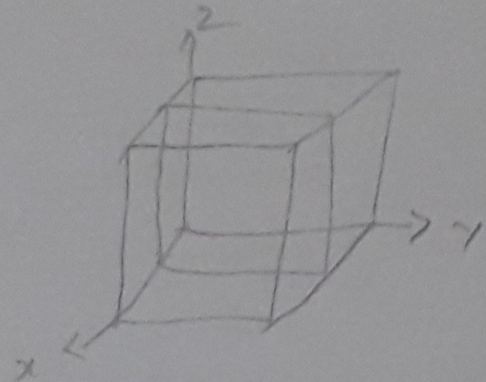
For cubic $\frac{1}{d^2_{hkl}} = \frac{1}{a^2}(h^2 + k^2 + l^2)$

For Tetragonal $\frac{1}{d^2_{hkl}} = \frac{1}{a^2}(h^2 + k^2) + \frac{1}{c^2} l^2$

For Orthorhombic $\frac{1}{d^2_{hkl}} = \frac{1}{a^2} h^2 + \frac{1}{a^2} k^2 + \frac{1}{c^2} l^2$

For Hexagonal $\frac{1}{d^2_{hkl}} = \frac{4}{3a^2}(h^2 + k^2 + l^2) + \frac{1}{c^2} l^2$.

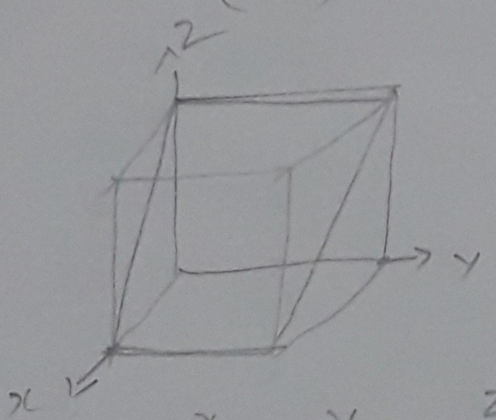


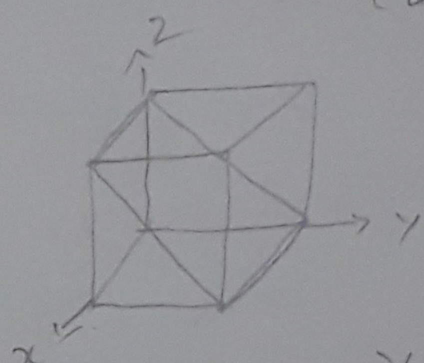


	x	Y	Z
Intercept	1	1	∞
Reciprocal	$\frac{1}{1}$	$\frac{1}{1}$	$\frac{1}{\infty}$
Reduction	1	1	0
M. I	(110)		

x	Y	Z
$\frac{1}{2}$	∞	∞
$\frac{1}{1/2}$	$\frac{1}{\infty}$	$\frac{1}{2}$
2	0	0

(200)

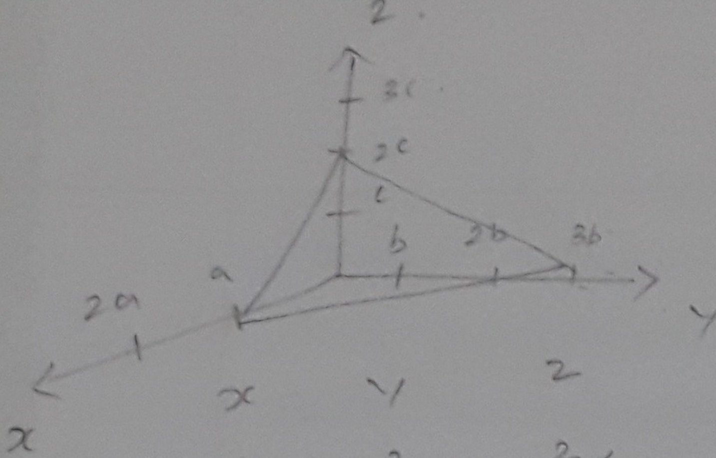




x	Y	Z
∞	1	1
$\frac{1}{\infty}$	$\frac{1}{1}$	$\frac{1}{1}$
0	1	1

x	Y	Z
1	∞	1
$\frac{1}{1}$	$\frac{1}{\infty}$	$\frac{1}{1}$
1	0	1

(101)



x y z

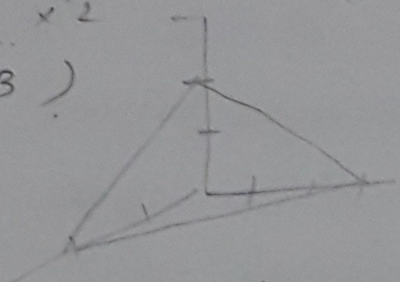
$1/3$ $3/3$ $2/3$

$\frac{1}{1/3}$ $1/1$ 1 $1/3$ $1/2$ $\frac{1}{2/3}$.

6 2 3.

3 1 $3/2$ $\times 2$

(6 2 3)

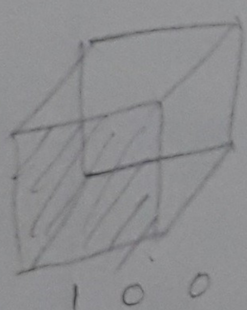


x y z

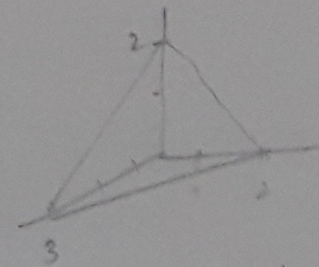
2 3 2

$1/2$ $1/3$ $1/2$

3 2 3



1 0 0



x y z

3 2 2

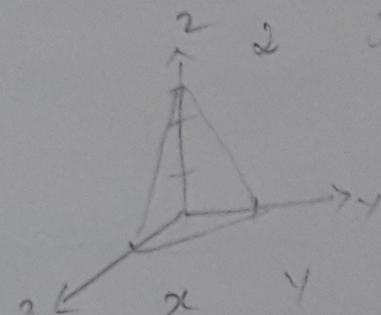
$\frac{1\times 2}{3\times 2}$ $\frac{1\times 3}{2\times 3}$ $\frac{1\times 2}{2\times 3}$

$\times$

$2/6$ $3/6$ $3/6$

~~3 2 2~~

2 3 3



x y z

1 1 3

$1/1$ $1/1$ $1/3$

3 3 1

$1/3$ $1/3$ $3/3$

$\frac{1}{1/3}$ $\frac{1}{1/3}$ 1

(3 3 1)