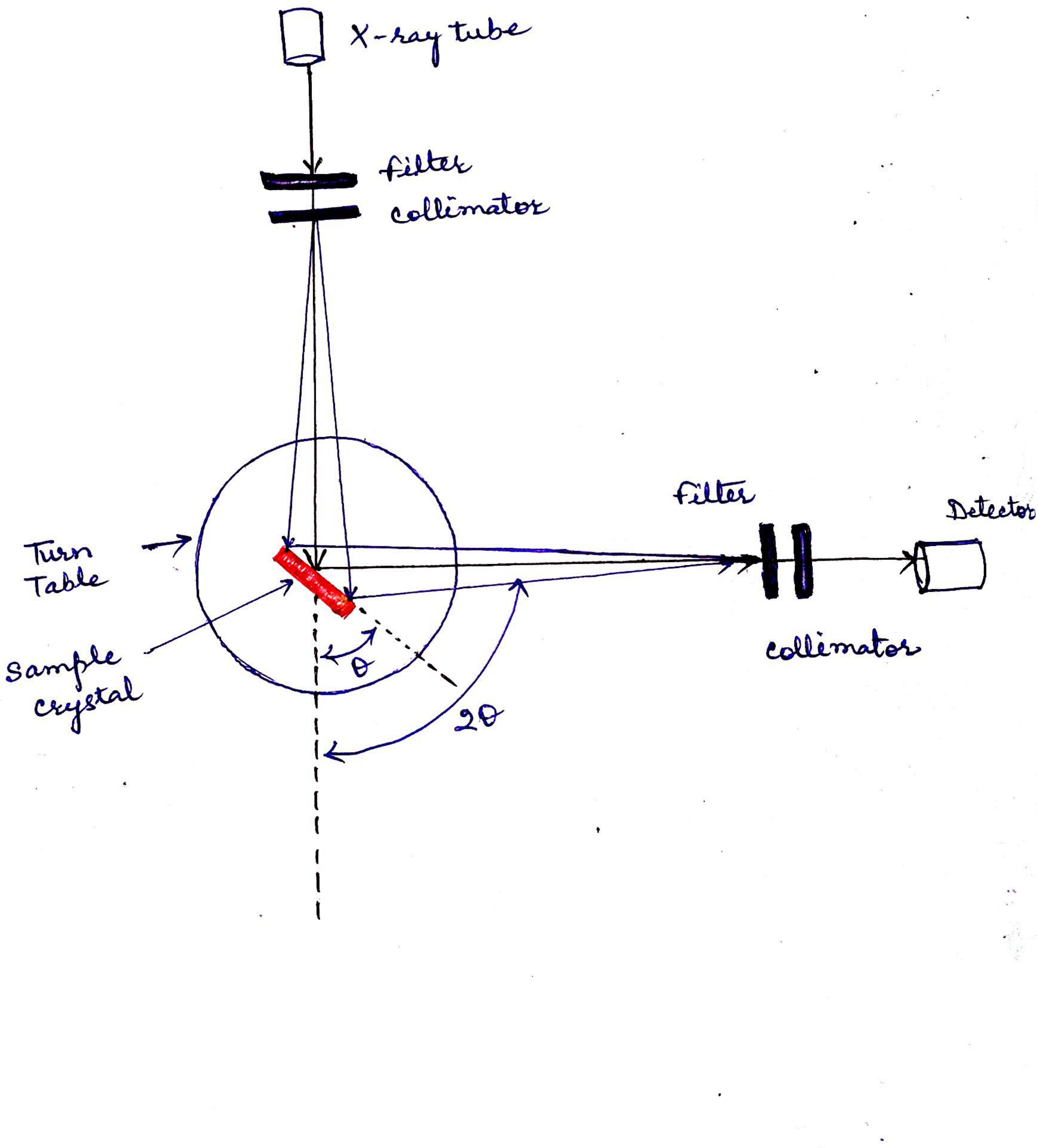
An X-ray Spectrometer



Date ___
Page ___

X-ray diffraction

German Physicist M. von Laue suggested the possibility of diffraction of X-rays by crystals since the wavelength of X-rays was of about the same order as the interatomic distances in a crystal. In fact, W. H. Bragg succeeded in diffracting X-rays from NaCl crystal.

The Bragg equation Bragg pointed out that the reflection of X-rays can take place only at certain angles (unlike ordinary light) which are determined by the wavelength of the X-rays and the distance between the planes in the crystal. The fundamental equation representing their relation is called as the Bragg equation.

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

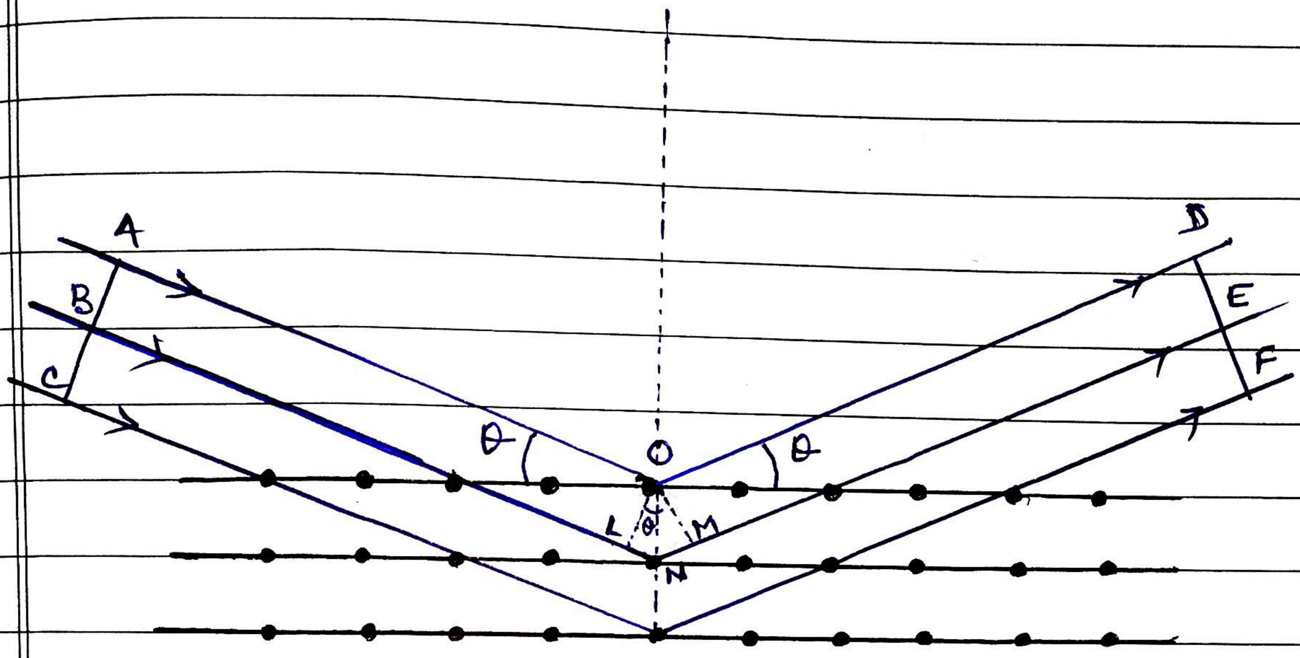
where n = an Integer (1, 2, 3 ....)

λ = wave length of X-rays

d = interplanar distance

θ = glancing angle

Derivation



X-ray reflections from a crystal

In this figure, horizontal lines 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 rays be reflected from the upper planes at the same angle θ while some others will be absorbed and get reflected from the successive layers.

Let the planes ABC and DEF be drawn perpendicular to the incident and reflected beams respectively.

The waves reflected by different layer planes will be "in phase" with one another only if the difference in the path lengths of the waves reflected from the successive layers is equal to an integral number of wavelengths.

Hence,

difference in the path length $\delta = LN + NM = n\lambda$

Since, the triangles OLN and OMN are congruent

hence, $LN = NM$

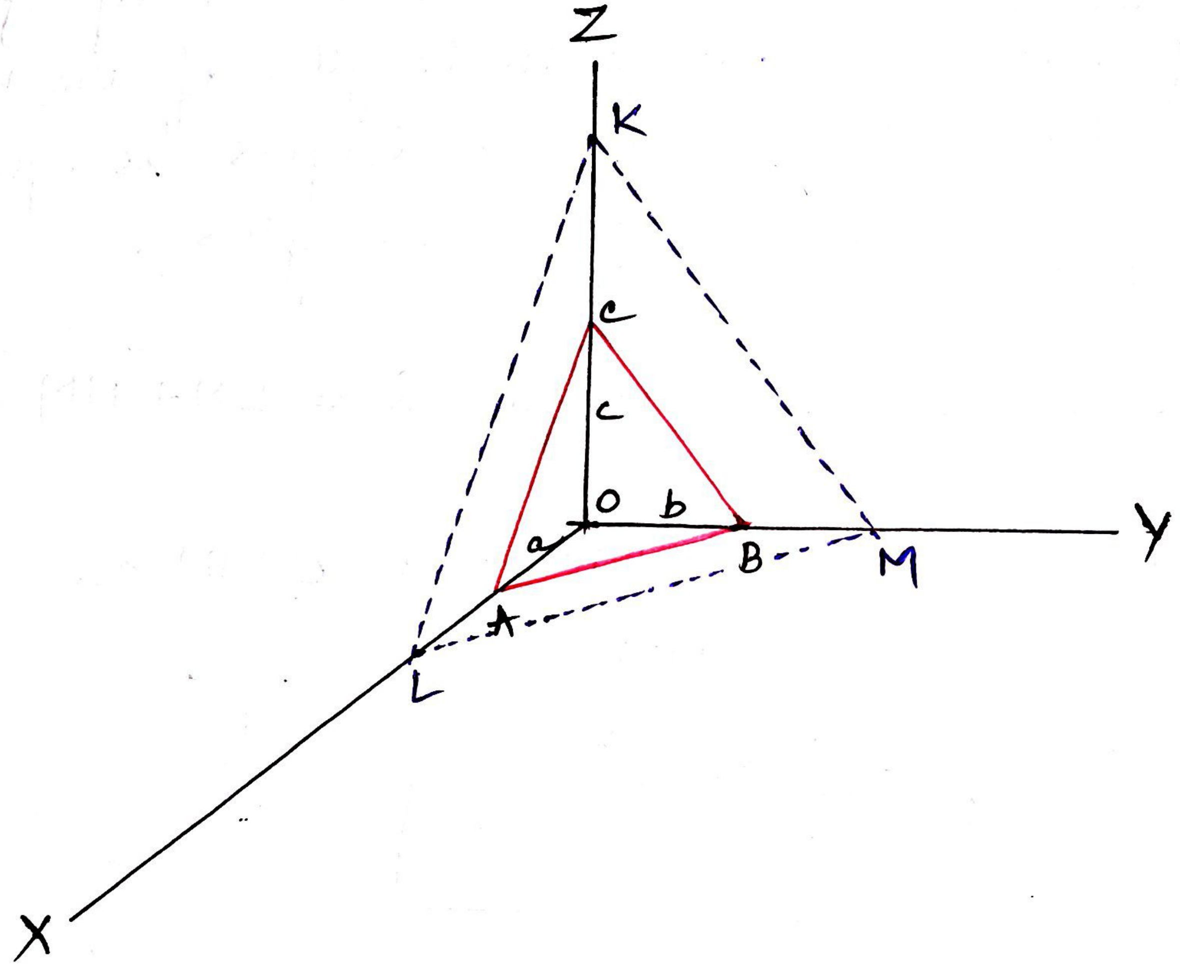
$\therefore \quad 2LN = n\lambda$

or $\boxed{2d \sin\theta = n\lambda}$

Thus, if λ is known, d can be determined by determining θ experimentally. On the other hand, if d is known, λ can be evaluated.

Applications (i) X-ray diffraction is highly useful in determining structures and dimensions of crystals

(ii) It is also useful in the study of a number of properties of X-rays themselves.


Z
K
C
c
O
b
Y
a
B
M
A
L
X

Law of Rational Indices :- It states that the intercepts of any face of a crystal along the crystallographic axes are either equal to the unit intercepts (a, b, c) or some simple whole number multiples of them.

Miller Indices

Miller indices are a set of integers (h, k, l) which are used to describe a given plane in a crystal.

The Miller indices of a face of a crystal are inversely proportional to the intercepts of that face on the various axes.

Procedure for determining Miller indices

(i) Prepare a 3-column table with the unit cell axes at the tops of the column.
(ii) Enter in each column the intercept (expressed as a multiple of a, b or c) of the plane with these axes.
(iii) Invert all numbers
(iv) clear fractions to obtain h, k, l.
(v) Negative sign is shown by a bar on the integer

Interplanar spacing in a crystal system.

In a crystal, the interplanar distance d_{hkl} is given by

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

where h, k, l are the Miller indices of the planes and a, b, c are the dimensions of the cell.

Hence; for cubic systems :-

$(a=b=c)$

$$\boxed{d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}} \quad \text{(cubic systems)}}$$

Q. Calculate the Miller indices of crystal planes which cut through the crystal axes at

(i) $(2a, 3b, c)$ (ii) (a, b, c) (iii) $(6a, 3b, 3c)$

(iv) $(2a, -3b, -3c)$

Solution:-

(i)

a	b	c	
2	3	1	intercepts
$\frac{1}{2}$	$\frac{1}{3}$	1	reciprocals
3	2	6	clear fractions

Miller indices are (326)

(ii)

a	b	c	
1	1	1	intercepts
1	1	1	reciprocals
1	1	1	clear fractions

Miller indices are (111)

(iii)

a	b	c	
6	3	3	intercepts
$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$	reciprocals
1	2	2	clear fractions

Miller indices are (122)

(iv)

	a	b	c	
	2	−3	−3	intercepts
	1/2	−1/3	−1/3	reciprocals
	3	−2	−2	clear fractions

Miller indices are $(3\bar{2}\bar{2})$

Q. The parameters of an orthorhombic unit cell are a = 50 pm, b = 100 pm, c = 150 pm. Determine the spacing between the (123) planes.

Ans:-

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

$$\left(\frac{1}{d_{hkl}}\right)^2 = \left(\frac{1}{d_{123}}\right)^2 = \left(\frac{1}{50}\right)^2 + \left(\frac{2}{100}\right)^2 + \left(\frac{3}{150}\right)^2$$

$$= 3\left(\frac{1}{50}\right)^2$$

$$\frac{1}{d_{123}} = \sqrt{3} \times \frac{1}{50}$$

$$d_{123} = \frac{50}{\sqrt{3}} = 29 \text{ pm.}$$

Q. Calculate the length of the unit cell of cubic lattice of Li metal in which the separation of the (100) planes of the metal is 350 pm.

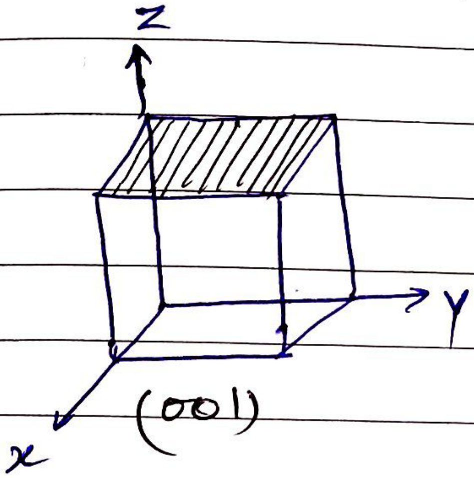
Ans:-

For the cubic system

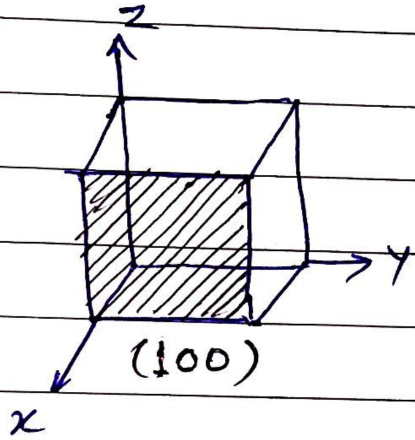
$$d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

$$d_{100} = \frac{a}{\sqrt{1^2+0^2+0^2}} = 350 \text{ pm}$$

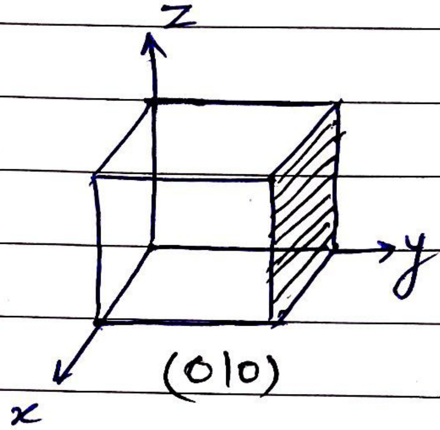
$$a = 350 \text{ pm} = 350 \times 10^{-12} \text{ m}.$$



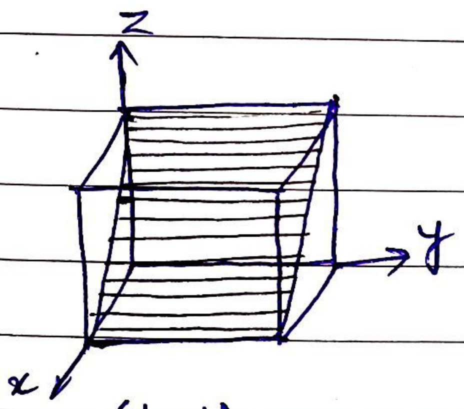
(001)



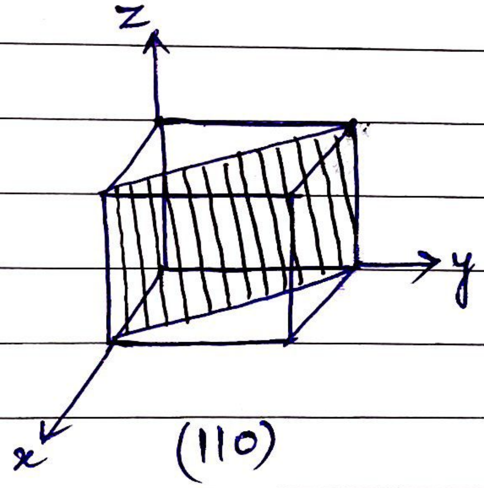
(100)



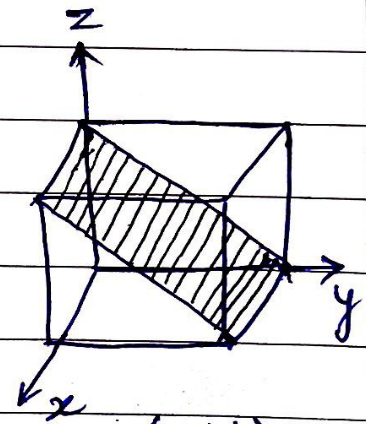
(010)



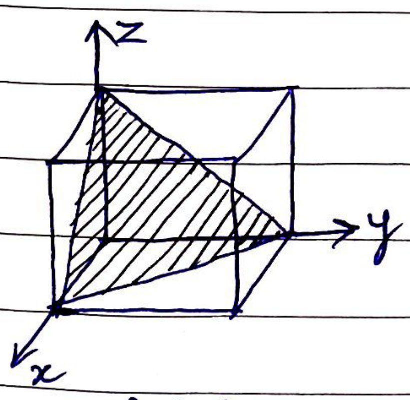
(101)



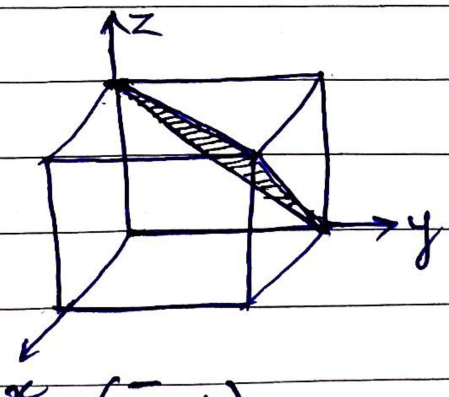
(110)



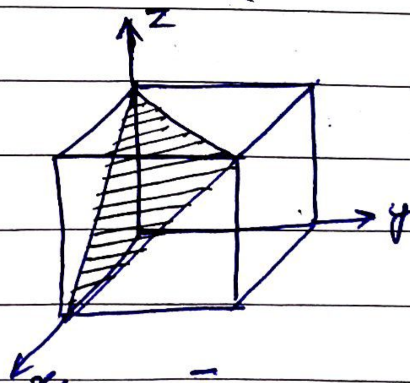
(011)



(111)



$(\bar{1}11)$



$(1\bar{1}1)$

classmate

Date ____

Page ____

Q. Calculate the angle at which (a) first order reflection and (b) second order reflection will occur in an X-ray spectrometer when X-rays of wave length 1.54 Å are diffracted by the atoms of a crystal, given that the interplanar distance is 4.04 Å.

Solution:- (a) for first order reflection ($n=1$)

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

$$\theta = \sin^{-1}(\lambda/2d) = \sin^{-1}(1.54\,Å/8.08\,Å)$$

$$= \sin^{-1}(0.191) = 10^\circ 59'$$

(b) for second order reflection ($n=2$), the Bragg equation is

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

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

$$\theta = \sin^{-1}(\lambda/d) = \sin^{-1}(1.54/4.04)$$

$$= \sin^{-1}(0.381) = 22^\circ 24'$$

Q. KNO_3 crystallizes in orthorhombic system with the unit cell dimensions $a = 542$ pm, $b = 917$ pm, and $c = 645$ pm. Calculate the diffraction angles for first order X-ray reflections from (100), (010) & (111) planes using radiation with wavelength $= 154.1$ pm classmate

Date ______
Page ______

Solution :- $n\lambda = 2d \sin\theta$

For an orthorhombic system

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

$$\left(\frac{1}{d_{100}}\right)^2 = \left(\frac{1}{542}\right)^2 + \left(\frac{0}{917}\right)^2 + \left(\frac{0}{645}\right)^2$$

$$= \left(\frac{1}{542}\right)^2$$

$d_{100} = a = 542$ pm

Similarly $d_{010} = b = 917$ pm

$d_{111} = c = 378$ pm

For first order reflections, $n = 1$

$\lambda = 154.1$ pm

$$\sin\theta_{100} = \frac{\lambda}{2d_{100}} = \frac{154.1}{2 \times 542} = 0.142$$

whence $\theta_{100} = 8^\circ 10'$

$$\sin\theta_{010} = \frac{\lambda}{2d_{010}} = \frac{154.1}{2 \times 917} = 0.084$$

whence $\theta_{010} = 4^\circ 49'$

$$\sin\theta_{111} = \frac{\lambda}{2d_{111}} = \frac{154.1}{2 \times 378} = 0.204$$

whence $\theta_{111} = 11^\circ 46'$