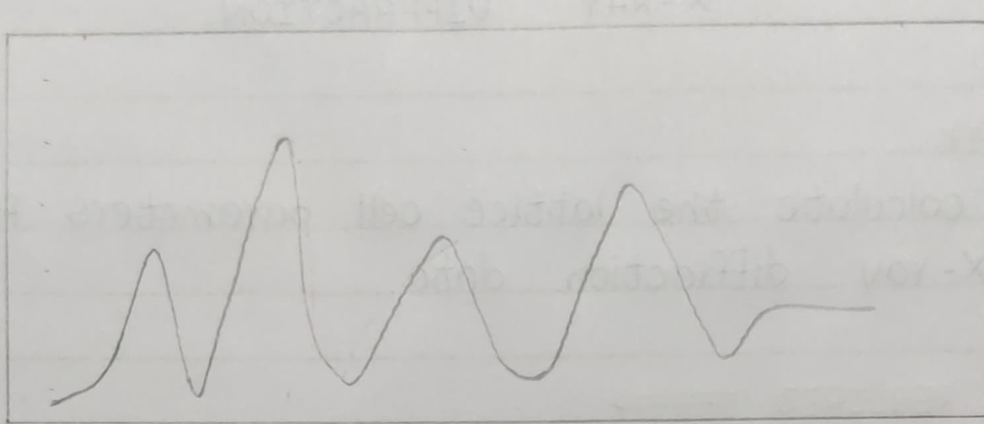
DIAGRAM ⟹



XRD Pattern

The problem of indexing lies in fixing the correct value of a by inspection of the $\sin^2\theta$ values.

OBSERVATIONS ⟹

	2θ	$\sin^2\theta$	$1\times\frac{\sin^2\theta}{\sin^2\theta_{min}}$	$2\times\frac{\sin^2\theta}{\sin^2\theta_{min}}$	$3\times\frac{\sin^2\theta}{\sin^2\theta_{min}}$	$h^2+k^2+l^2$	hkl	a	d
								A°	A°
1)	27.137	0.0550	1	2	3	3	1,1,1	5.6900	3.285
2)	45.077	0.1469	3	5	8	8	2,2,0	5.6837	2.009
3)	53.415	0.2019	4	7	11	11	3,1,1	5.6845	1.713
4)	65.677	0.2940	5	11	16	16	4,0,0	5.6818	1.420
5)	83.189	0.4407	8	16	24	24	-	5.6841	1.160
6)	106.540	0.6423	12	23	35	35	-	5.6857	0.961
							MEAN ⟶	5.6849	1.758

Date 05/01/2021

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CALCULATION OF LATTICE CELL PARAMETERS - X-RAY DIFFRACTION.

AIM ⟹

To calculate the lattice cell parameters from the powder X-ray diffraction data.

APPARATUS REQUIRED ⟹

Powder X-ray diffraction diagram.

FORMULAE ⟹

1) For a cubic crystal:

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

2) For a tetragonal crystal:

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

3) For a orthorhombic crystal:

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

4) The lattice parameter and interplanar distance are given, for a cubic crystal as:

$$a = \frac{\lambda}{2\sin\theta}\sqrt{h^2+k^2+l^2} \ \text{Å}$$

$$d = \frac{a}{\sqrt{h^2+k^2+l^2}} \ \text{Å}$$

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CALCULATIONS $\Longrightarrow$

- For calculating 'a' :

1) $\theta = 13.5685 \quad , \quad h^2+k^2+l^2 = 3$

$$\therefore \quad a = \frac{\lambda}{2\sin\theta} \cdot \sqrt{h^2+k^2+l^2}$$

$$= \frac{1.5405}{2 \times \sin(13.5685)} \cdot \sqrt{3}$$

$$= \frac{1.5405}{2 \times 0.2346} \times 1.73$$

$$= 3.2832 \times 1.73 \quad = 5.6900 \text{ A}^\circ$$

2) $\theta = 22.5385 \quad , \quad h^2+k^2+l^2 = 8$

$$\therefore \quad a = \frac{\lambda}{2\sin\theta} \cdot \sqrt{h^2+k^2+l^2}$$

$$= \frac{1.5405}{2 \times \sin(22.5385)} \cdot \sqrt{8}$$

$$= \frac{1.5405}{2 \times 0.3833} \times 2.82$$

$$= 2.0095 \times 2.82 \quad = 5.6837 \text{ A}^\circ$$

3) $\theta = 26.7075 \quad , \quad h^2+k^2+l^2 = 11$

$$\therefore \quad a = \frac{\lambda}{2\sin\theta} \cdot \sqrt{h^2+k^2+l^2}$$

$$= \frac{1.5405}{2 \times \sin(26.7075)} \cdot \sqrt{11}$$

$$= \frac{1.5405}{2 \times 0.4494} \times 3.31$$

$$= 1.7139 \times 3.31 \quad = 5.6845 \text{ A}^\circ$$

where,

a = lattice parameter
d = interplanar distance
λ = wavelength of the CuKα radiation (1.5405)
h, k, l = miller integers

PRINCIPLE ⟹

Bragg's law is the theoretical basis for X-ray diffraction.

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

Each of the miller indices can take values 0, 1, 2, 3, ... Thus, the factor $(h^2+k^2+l^2)$ takes the values given in the table below.

h, k, l	$h^2+k^2+l^2$	h, k, l	$h^2+k^2+l^2$
100	1	300	9
110	2	310	10
111	3	311	11
200	4	322	12
210	5	320	13
211	6	321	14
220	8	400	16
221	9	410	17

LATTICE DETERMINATION ⟹

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4) $\theta = 32.8385$, $h^2 + k^2 + l^2 = 16$

$$\therefore \ a = \frac{\lambda}{2\sin\theta} \cdot \sqrt{h^2 + k^2 + l^2}$$

$$= \frac{1.5405}{2 \times \sin(32.8385)} \cdot \sqrt{16}$$

$$= \frac{1.5405}{2 \times 0.5422} \times 4$$

$$= 1.4206 \times 4 = 5.6818 \ A^\circ$$

5) $\theta = 41.5945$, $h^2 + k^2 + l^2 = 24$

$$\therefore \ a = \frac{\lambda}{2\sin\theta} \cdot \sqrt{h^2 + k^2 + l^2}$$

$$= \frac{1.5405}{2 \times \sin(41.5945)} \cdot \sqrt{24}$$

$$= \frac{1.5405}{2 \times 0.6638} \times 4.89$$

$$= 1.1603 \times 4.89 = 5.6841 \ A^\circ$$

6) $\theta = 53.2700$, $h^2 + k^2 + l^2 = 35$

$$\therefore \ a = \frac{\lambda}{2\sin\theta} \cdot \sqrt{h^2 + k^2 + l^2}$$

$$= \frac{1.5405}{2 \times \sin(53.2700)} \cdot \sqrt{35}$$

$$= \frac{1.5405}{2 \times 0.8014} \times 5.91$$

$$= 0.9611 \times 5.91 = 5.6857 \ A^\circ$$

Lattice Type	Rule for reflection to be observed
Primitive (P)	None
Body Centered (I)	hkl: $h + k + l = 2n$
Face Centered (F)	hkl: h, k, l either all odd or all even.

Depending on the nature of the h, k, l values the lattice type can be determined.

- For calculating 'd' :

1) $a = 5.6900$, $\sqrt{h^2+k^2+l^2} = 1.73$

$$\therefore d = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

$$= \frac{5.6900}{1.73} = 3.285 \text{ A}^\circ$$

2) $a = 5.6837$, $\sqrt{h^2+k^2+l^2} = 2.82$

$$\therefore d = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

$$= \frac{5.6837}{2.82} = 2.009 \text{ A}^\circ$$

3) $a = 5.6845$, $\sqrt{h^2+k^2+l^2} = 3.31$

$$\therefore d = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

$$= \frac{5.6845}{3.31} = 1.713 \text{ A}^\circ$$

4) $a = 5.6818$, $\sqrt{h^2+k^2+l^2} = 4$

$$\therefore d = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

$$= \frac{5.6818}{4} = 1.420 \text{ A}^\circ$$

5) $a = 5.6841$, $\sqrt{h^2+k^2+l^2} = 4.89$

$$\therefore d = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

$$= \frac{5.6841}{4.89} = 1.160 \text{ A}^\circ$$

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RESULT ⟹

The lattice parameters are calculated theoretically from the powder X-Ray diffraction pattern.

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