Experiment

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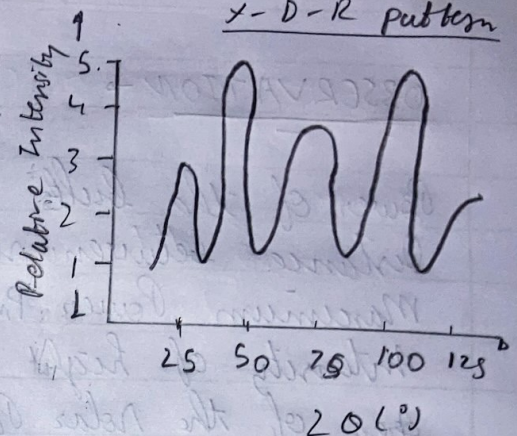
Value of $h^2+k^2+l^2$ for diff. planes.

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	320	12
210	5	321	13
211	6	322	14
220	8	400	16
221	9	410	17

X-D-R pattern



OBSERVATION TABLE

2θ	θ	$\sin^2\theta$	$\frac{\sin^2\theta}{\sin^2\theta_{min}}$	$2\times\frac{\sin^2\theta}{\sin^2\theta_{min}}$	$3\times\frac{\sin^2\theta}{\sin^2\theta_{min}}$	$h^2+k^2+l^2$	h,k,l	a	d
27.137	13.5685	0.055	1	2	3	3	1,1,1	5.6900	3.285
45.077	22.5385	0.1469	2.6713	5.3426	8.0139	8	2,2,0	5.6553	1.999
53.415	26.7075	0.2019	3.6725	7.3451	11.0177	11	3,1,1	5.7001	1.718
65.677	32.8385	0.2940	5.3465	10.6930	16.0396	16	4,0,0	5.6551	1.413
83.189	41.5945	0.4407	8.0127	16.0255	24.0383	24	4,2,2	5.6872	1.610
106.54	53.27	0.6423	11.6781	23.3563	35.0345	35	5,3,1	5.7034	0.964

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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

FORMULA

For a cubic crystal.

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

For a tetragonal crystal

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

For a osthographic crystal

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

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Experiment

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CALCULATION :-

w.r.t $a = \frac{\lambda}{2\sin\theta}\sqrt{h^2+k^2+l^2}$

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

(i) $a = \frac{1.5405 \times 1.732}{0.46291} = \boxed{5.686}$

$d = \frac{5.686}{1.732} = \boxed{3.28}$

(ii) $a = \frac{1.5405 \times 2.8284}{0.7666} = \boxed{5.683}$

$d = \frac{5.683}{2.8284} = \boxed{2}$

(iii) $a = \frac{1.5405 \times 3.31662}{0.89887} = \boxed{5.684}$

$d = \frac{5.684}{3.3162} = \boxed{1.71}$

(iv) $a = \frac{1.5405 \times 4}{1.08485} = \boxed{5.681}$

$d = \frac{5.631}{4} = \boxed{1.16}$

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

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

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

where,

a = lattice parameter
d = Interplanner distance
λ = Wavelength of Cu Kα radiation (1.5405 Å)
h, k, l = Miller integers

Experiment

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(v) $a = \frac{1.5405 \times 4.8989}{1.3277} = \boxed{5.684}$

$d = \frac{5.684}{4.8989} = \boxed{1.16}$

(vi) $a = \frac{1.5405 \times 5.9160}{1.60292} = \boxed{5.685}$

$d = \frac{5.685}{5.916} = \boxed{0.96}$

PRINCIPLE :-

Bragg law is the thoritical basis for x-ray diffraction.

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

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

RESULT :

The lattice cell parameters are calculated theoritically from the powder x-ray diffraction pattern and values are tabulated.

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