Assignment-12 Experiment-12

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 orthorhombic crystal

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

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

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

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

Where, a = Lattice parameter
d = Interplanner distance
λ = Wavelength of the CuKα radiation (1.5405 Å)
h, k, l = Miller integers

Principle

Braggs law is the theoretical 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 the values given in Table 6.7.1.

Value of $h^2 + k^2 + l^2$ for different 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	322	12
210	5	320	13
211	6	321	14
220	8	400	16
221	9	410	17

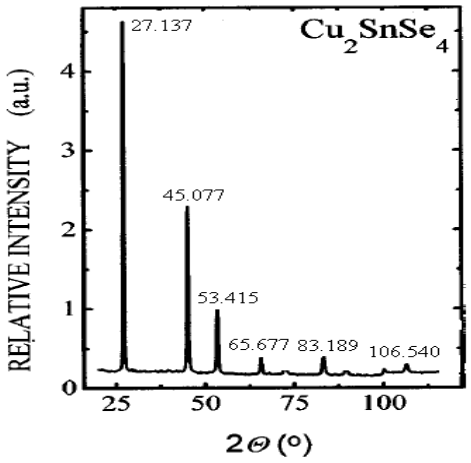

Fig. XRD pattern

Procedure:

From the 2θ values on a powder photograph, the θ values are obtained. The $\sin^2\theta$ values are tabulated. From that the values of $1 \times \frac{\sin^2\theta}{\sin^2\theta_{min}}, 2 \times \frac{\sin^2\theta}{\sin^2\theta_{min}}, 3 \times \frac{\sin^2\theta}{\sin^2\theta_{min}}$ are determined and are tabulated. The values of $3 \times \frac{\sin^2\theta}{\sin^2\theta_{min}}$ are rounded to the nearest integer. This gives the value of $h^2+k^2+l^2$ .From these the values of h,k,l are determined from the Table.

2θ	θ	$\sin^2\theta$	$1 \times \frac{\sin^2\theta}{\sin^2\theta_{min}}$	$2 \times \frac{\sin^2\theta}{\sin^2\theta_{min}}$	$3 \times \frac{\sin^2\theta}{\sin^2\theta_{min}}$	$h^2+k^2+l^2$	*hkl*	**a** Å	**d** Å
27.137	?	?	?	?	?	?	?	?	?
45.077	?	?	?	?	?	?	?	?	?
53.415	?	?	?	?	?	?	?	?	?
65.677	?	?	?	?	?	?	?	?	?
83.189	?	?	?	?	?	?	?	?	?
106.54	?	?	?	?	?	?	?	?	?

Assignment Question:

1. From the 2θ values in the tabular coloum find out θ & $Sin^2\theta$ and tabulate the values in four decimal points. Let us assume that first reading in the coloum $Sin^2\theta$ is $Sin^2\theta_{min}$.
2. From that value calculate $1 \times \frac{sin^2\theta}{sin^2\theta_{min}}, 2 \times \frac{sin^2\theta}{sin^2\theta_{min}}, 3 \times \frac{sin^2\theta}{sin^2\theta_{min}}$ and tabulate the values in four decimal points in respective coloums.
3. The values of $3 \times \frac{sin^2\theta}{sin^2\theta_{min}}$ are rounded to the nearest integer and assume that $h^2+k^2+l^2$.
4. From that value identify h,k,l and tabulate in respective coloum.
5. By using the values of λ, Sinθ and h, k, l, calculate the lattice cell parameter (a) and tabulate the values in four decimal points.
6. Also calculate and tabulate the inter planer distance (d) in four decimal points by using the values of a and h,k,l.
7. Write the result in the following order

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

   Finally, submit the scanned copy of your observation note book in GCR on (or) before THREE working days from the date of experiment.