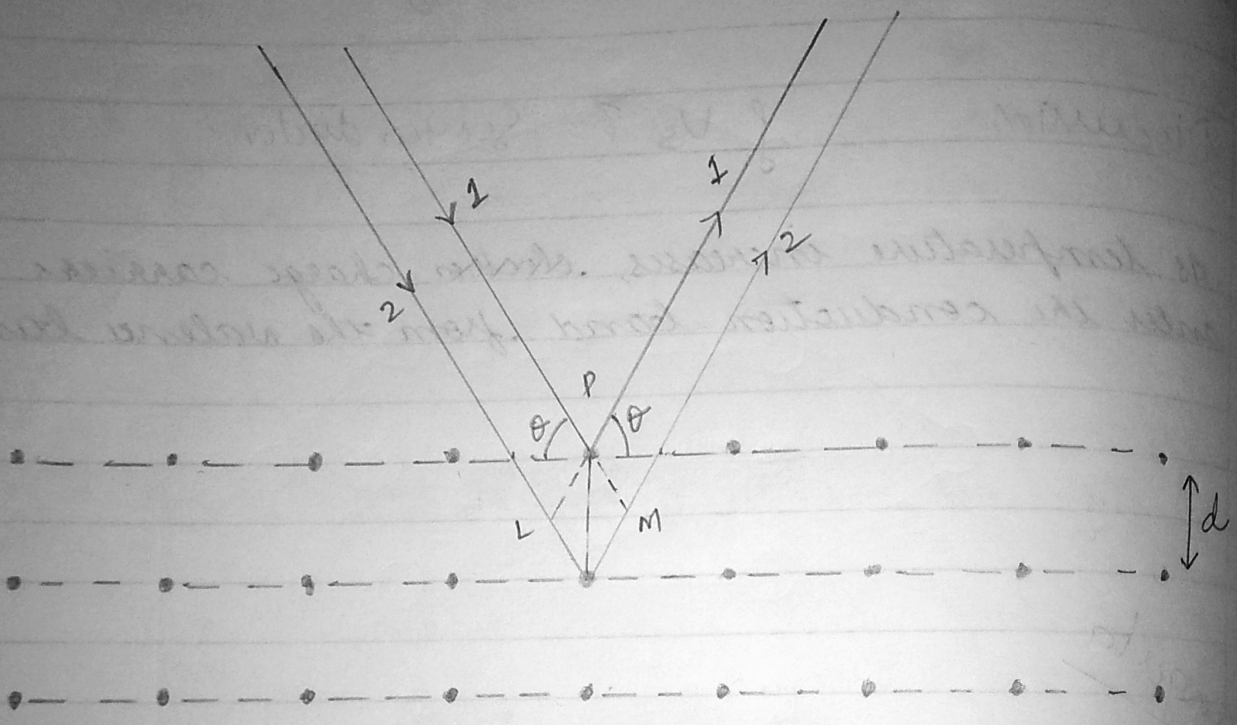

Bragg's Reflection of x-rays from atomic planes

Date 9/9/22

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Experiment - 2
X-Ray Diffraction

Aim:

To find the lattice parameters and grain size of different samples containing Magnesium doped ZnO, using X-Ray diffraction data

Apparatus Required

- Software used: Python

Working Formula:

1. Bragg's Cond^n: $\boxed{2d\sin\theta = n\lambda}$

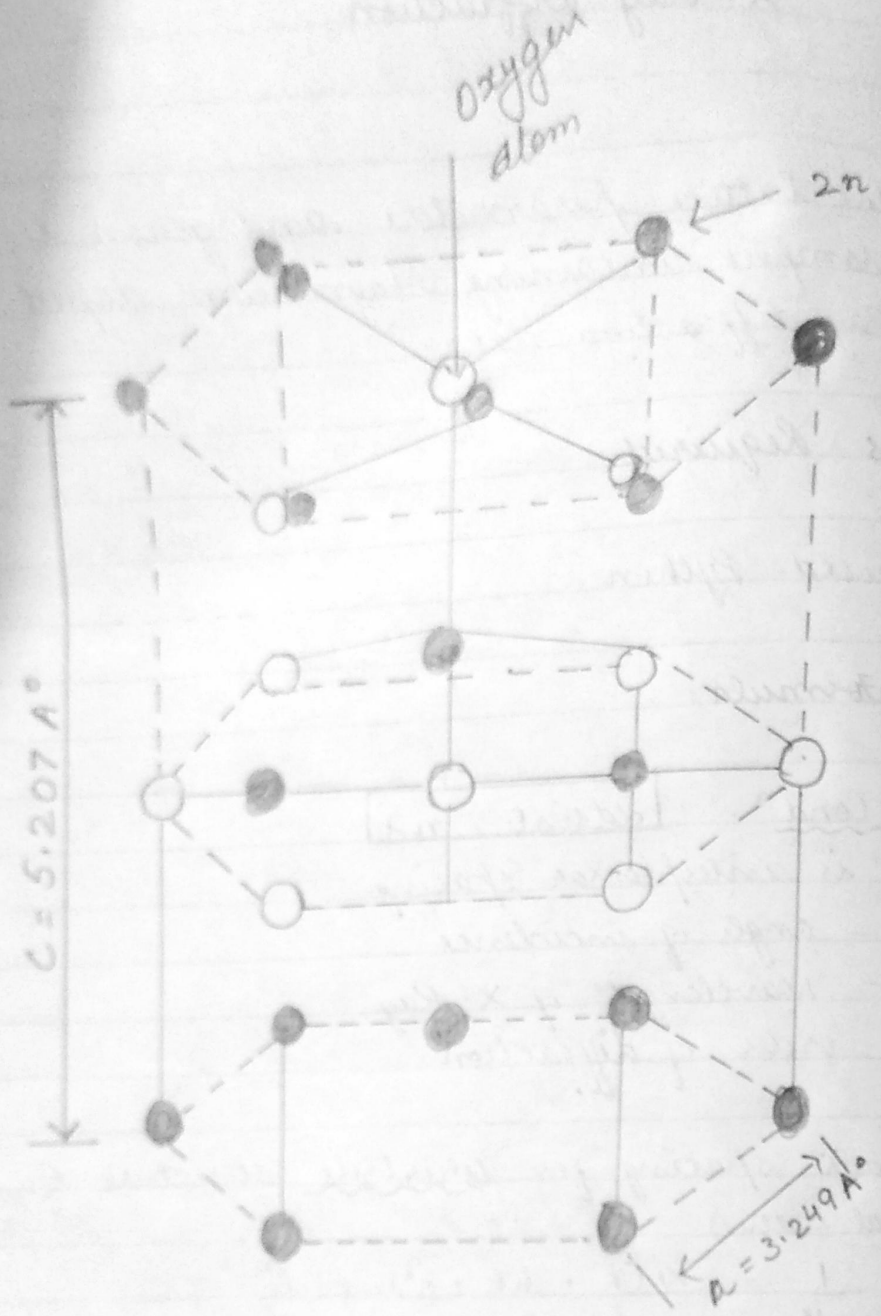
Where 'd' is interplanar spacing
θ - angle of incidence
λ - wavelength of X-Ray
n - order of diffraction

2. Interplanar spacing for Wurtzite structure of ZnO (hexagonal lattice)

$$\frac{1}{d^2} = \frac{4(h^2+hk+k^2)}{3a^2} + \frac{l^2}{c^2}$$

where h, k, l - miller indices of plane
a, c - lattice parameters
d - interplanar spacing

Teacher's Signature :



Hexagonal Wurtzite Structure of ZnO.

3 Scherrer's Formula:

$$t = \frac{k\lambda}{B\cos\theta_B}$$

$k = 0.94$ - Scherrer's constant

λ - wavelength of monochromatic x-ray

θ_B - Bragg's diffraction angle

B - FWHM of the peaks obtained in Intensity vs 2θ graph.

k depends on grain size distribution, grain shape, and how the peak width is defined. Generally it is given as $k = 2\sqrt{\ln(2)/\pi} \approx 0.9394$. It is correct for spherical crystals with cubic symmetry where the peak width is defined using FWHM. If we use Integral Breadth, then $k = 0.89$.

Precautions:

- Use finite-grained powder to ensure a random distribution of lattice orientations. Powder less than 10μm in size is preferred.
- Very small amount of the sample limits the no. of crystallites that can contribute to the measurement.
- Make the upper surface of the sample flat to achieve homogenity.
- Make sure there is no direct exposure to X-Rays.

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Observations :

- Wavelength of X-rays = 1.54 Å [These x-rays are produced due to K_α lines (transition from L to K shell), with Cu as target. ~~Inner shell e⁻ accelerated e⁻ strike target~~ ie inner shell e⁻].

- Data for 2θ vs intensity was provided for different concentration of Mn impurity in ZnO sample has been attached.

Calculations : ~~And Result~~.

Sample	hkl	2θ (in°)	d_{hkl} (in Å)	t (grain size (in Å)	Lattice parameters a (in Å)	c (in Å)
ZnO	100	31.88631	2.80322	498.495	3.23689	
	002	34.57750	2.59096	439.577		5.18191
	101	36.38353	2.46638	460.685		
Zn Mn (3%) O	100	31.92750	2.79970	498.547	3.23281	
	002	34.59830	2.58945	439.599		5.17889
	101	36.41287	2.46446	460.724		
Zn Mn (6%) O	100	31.87244	2.80441	414.629	3.23826	
	002	34.54751	2.59314	407.380		5.18627
	101	36.36989	2.46727	398.164		
Zn Mn (10%) O	100	31.90702	2.80145	434.381	3.23484	
	002	34.57813	2.59091	423.476		5.18182
	101	36.40167	2.46519	380.074		

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The graphs related to Gaussian fitting & the trends of FWHM, 2θ, t, a and c with varying impurity concentration have been attached.

Sources of Error:

- The choice of parameters like max. intensity, 2θ value at peak position, and the spread of function can alter our results due to fitting.
- The choice of function to be fitted (here Gaussian model) induces error in fitting & further measurements

Discussion

1. After analysing 2θ vs. Mn concentration graph, an t (grainsize) v/s Mn concentration graph ~~and c v/s~~ we understand that we obtain maximum 2θ at the maximum grainsize. This trend is observed for all the three peaks.
2. There is not much interpolation that we can get from a v/s Mn concentration graph, as well as c vs Mn concentration graph. This is because they do not seem to follow any particular trend.
3. The lattice parameters a & c for ZnO sample with different concentration of impurity (Mn) are very close to each other.

16/9/22

Teacher's Signature: 23/9/22