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PHY 1701 (Engineering Physics). Lab Manual and Records.

OBJECTIVE OF THE EXPERIMENT:

ENGINEERING APPLICATIONS OF NANOMATERIALS

Tools Required:-

- XRD pattern
- Peak fitting program (fityk, gnuplot or qtiplot)
- Usage of

SLO :-

To determine the average crystallite size from the X-ray diffraction (XRD) pattern of a polycrystalline materials.

Formula to Use:-

The scherrer equation is to calculate the crystallite size. This method gives qualitative results. The Scherrer Equation is:-

$$D = \frac{K\lambda}{\beta \cos\theta}$$

Here,

- Peak width (β in radians).
- Crystallite size (D)
- Scherrer Constant (K).
- X-ray wavelength (λ).
- Peak-position (θ).

DATA GIVEN:

Instrumental Broadening : 0.01°

Wavelength of X-ray Used : 1.546 Å

Scherrer Constant: 0.94 (assuming the crystallites are spherical in shape).

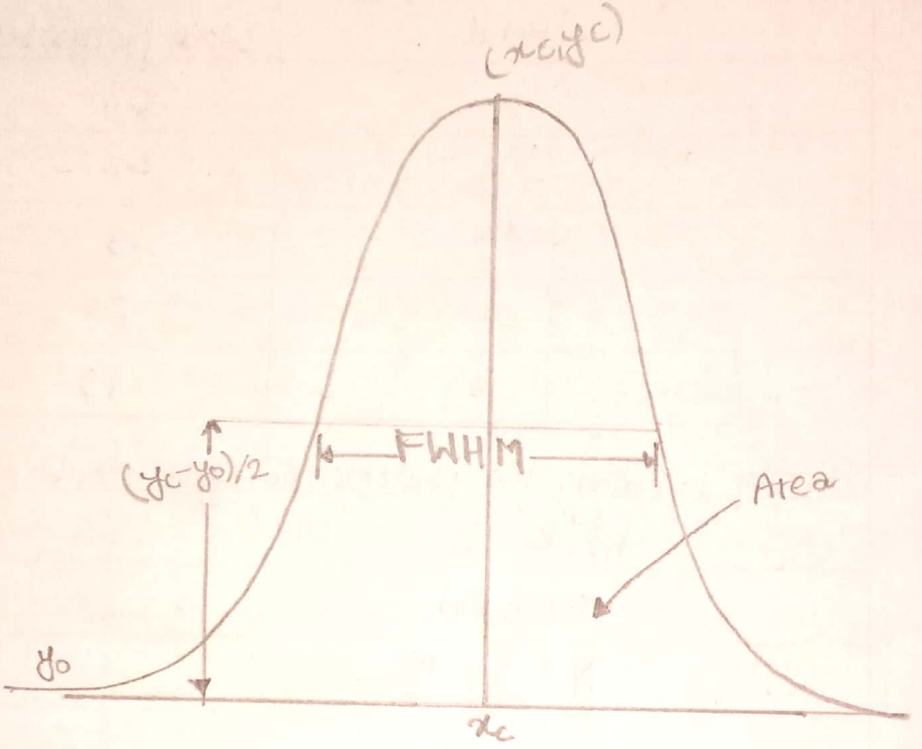

Fig:- Peak Fitting Using Gaussian/Pseudovoigt function.

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Tabulation:-

Peak Center (degree)	FWHM (degree)	FWHM after instrumental broadening correction. (degree)	FWHM (in radian)	Average Crystallite Size (Å)
28.57	0.33	0.320	0.00558	267.81
47.540	0.390	0.380	0.00663	238.67
56.370	0.389	0.379	0.0066	248.93
33.130	0.420	0.410	0.00716	211.01
59.13	0430	0.420	0.00733	227.14

Sample Calculation:-

For 1st order maxima, $K = 0.94$, $\lambda = 1.06 \text{ Å}$

Peak Center (θ) = 14.285°

FWHM (β) = 0.00558^c

$$\therefore \text{Crystallite size} = \frac{K\lambda}{\beta \cos\theta} = \frac{0.94 \times 1}{0.00558 \times \cos(14.285)^c} \text{ Å}$$

$$D_1 = 267.81 \text{ Å}$$

$$\approx 268 \text{ Å}$$

Similarly, $D_2 = 238$ Å, $D_3 = 248$ Å, $D_4 = 211$ Å, $D_5 = 227$ Å

Now, Average of all values is $D = \frac{D_1 + D_2 + D_3 + D_4 + D_5}{5}$

$= 238.8$ Å

≈ 23.8 nm

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Inference:-

The Crystallite Size was calculated to be 23.8 nm.