20BDS0406

Name of the Experiment

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Engineering Application of Nanomaterials

* Tools Required
  - i) XRD pattern
  - ii) Peak fitting Program (Open source / free software like 'fityk', 'gnuplot', 'qtiplot')

*) SLO

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

Formula to Use:

The Scherrer equation is used to calculate the crystallite size. This method gives qualitative result.

The Scherrer's equation is:

$$D = \frac{K \lambda}{\beta \sin \theta}.$$

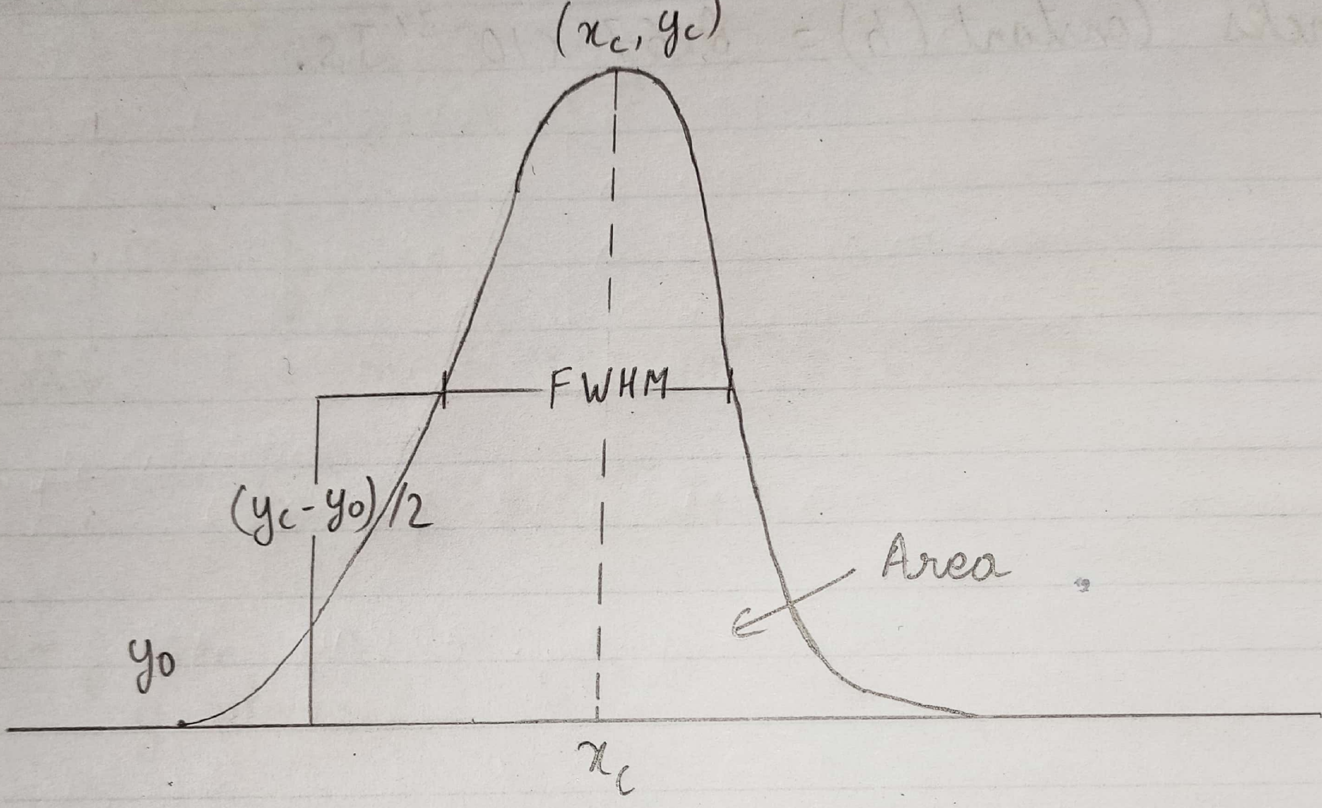

Fig 1. Peak fitting using Gaussian/Pseudovoigt Function

Here, •) Peak Width (β in radians)
•) Crystallite size (D)
•) Scherrer's constant (K)
•) X-Ray Wavelength (λ)
•) Peak position (θ)

Data Given

i) Instrumental broadening : 0.01°
ii) Wavelength (λ) of X-Ray used : $1.5406\ \mathring{A}$
iii) Scherrer's constant (K) = 0.94
(assuming crystallite are spherical in shape)

Inference

The average crystallite size is 23.74 nm.

Tabulation

Peak Centre (2θ) (deg)	θ (deg)	FWHM(β) (deg)	FWHM(β) (rad)	Average Crystallite Size (nm)
28.57	14.285	0.33	5.76×10^{-3}	25.94
47.54	23.77	0.389	6.79×10^{-3}	23.3
56.37	28.185	0.419	7.31×10^{-3}	22.48
33.13	16.565	0.349	6.09×10^{-3}	24.81
59.13	29.565	0.43	7.5×10^{-3}	22.19

Sample Calculation

here $K = 0.94$, $\lambda = 1.5406 \times 10^{-10}$ m.

$\theta = 14.285$ and $\beta = 5.76 \times 10^{-3}$

So, $$D_1 = \frac{K\lambda}{\beta \cos\theta} = \frac{0.94 \times 1.5406 \times 10^{-10}}{5.76 \times 10^{-3} \times \cos(14.285)}$$

$\therefore D_1 = 25.94$ nm

Similarly, $D_2 = 23.3$ nm ; $D_3 = 22.48$ nm ; $D_4 = 24.81$ nm
$D_5 = 22.19$ nm

Then, $D_{avg} = (D_1 + D_2 + D_3 + D_4 + D_5)/5$

$$= \frac{25.94 + 23.3 + 22.48 + 24.81 + 22.19}{5}$$

$\therefore D_{avg} = 23.74$ nm