TOPIC :	Engineering Application of Nanomaterials
Tools Reqd.:	• XRD pattern • Peak fitting program (open source / free software like fityk, gnuplot and qtiplot is preferable)
Objective :	To determine the average crystallite size from the given x-ray diffraction (XRD) pattern of a polycrystalline material.
Formula to Use :	The Scherrer equation is to calculate the crystallite size. This method gives qualitative results.

The Scherrer Equation is :

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

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 the x-ray used : 1.546 Å
- Scherrer constant : 0.94 (assuming that crystallites are spherical in shape)

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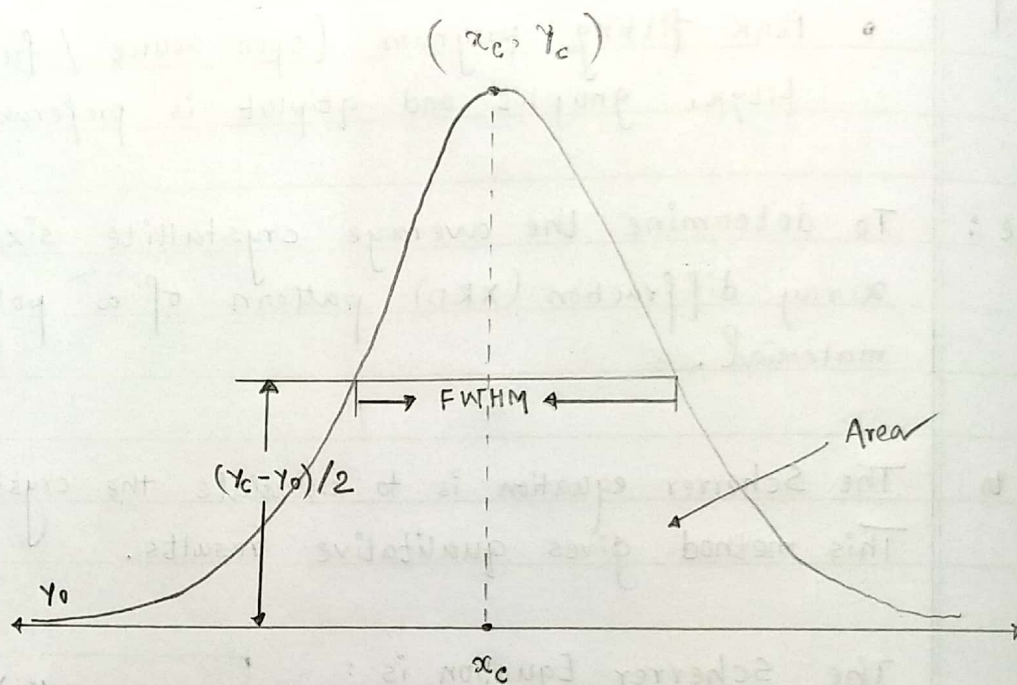**Fig.** Peak fitting using Gaussian / Pseudovoigt function

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TABULATION:	Peak center (in degree) 2θ	FWHM (in degree)	FWHM after instrumental correction	FWHM (in radian)	Avg. Crystallite size (in nm)
	28.57	0.33	0.32	0.0055	27.267
	47.54	0.39	0.38	0.0066	24.064
	56.37	0.42	0.41	0.0071	23.259
	33.13	0.35	0.34	0.0059	25.927
	59.13	0.43	0.42	0.0073	22.908

Mean = 24.685 nm

RESULT :

The average crystallite size from the given x-ray diffraction (XRD) pattern of a polycrystallite material is 24.685 nm.

Himani
05/09/19
19 BCE 2105

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Teacher's Signature _____