

Date:Reg. No.

ENGINEERING APPLICATION OF NANOMATERIALS

Tools Required:

- XRD pattern (uploaded in the course page)
- Peak fitting program (Open source/free software like `fityk`, `gnuplot` and `qtplot` is preferable)
- **Usage of any pirated or cracked software is strictly prohibited**

SLO:

- ✓ 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:

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

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 \AA

Scherrer constant: 0.94 (assuming that crystallites are spherical in shape)

[IMPORTANT - Use "PseudoVoigt" function for fitting in `fityk`]

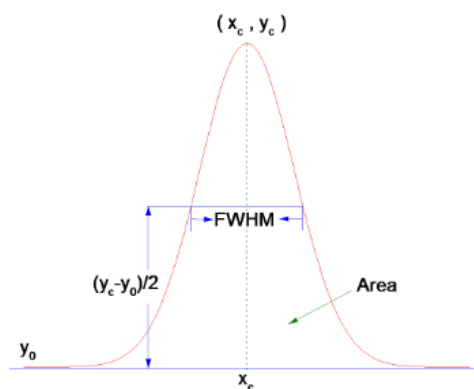


Fig 1 Peak fitting using Gaussian/PseudoVoigt function

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Tabulation

Peak Center ()	FWHM ()	FWHM after instrumental broadening correction ()	<i>FWHM</i> (in Radian)	Average crystallite size ()

Inference:

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