Engineering Applications of Nanomaterials

Tools Required :
- XRD pattern
- Peak fitting program (Open source / free software like fityk, gnuplot and gfiplot)
- Usage of cracked software is prohibited

Aim :
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.
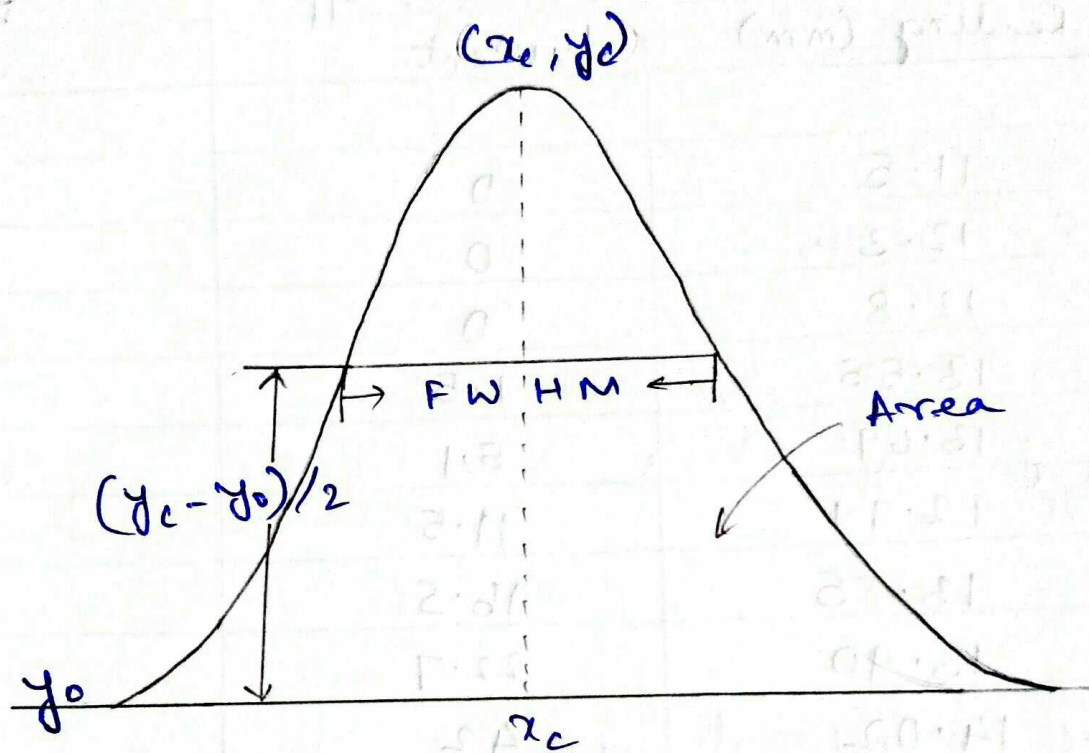
The Scherrer Equation is :

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

Here,
- Peak width (β in radians)
- Crystallite size (D)
- Scherrer constant (k)
- X-ray wavelength (λ)
- Peak position (θ)

Peak fitting using Gaussian function

Data Given :

Instrumental broadening : 0.01°

Wavelength of the X-ray used : 1.546Å

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

Tabulation :

Peak Center ( )	FWHM ( )	FWHM after instrumental correction	FWHM (in Radian)	Avg. crystallite size ( )

Inference