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Apparatus :- (i) xRD pattern
(ii) Peak fitting program
(iii) Usage of any pirated or cracked software is strictly prohibited.

Formulae :- The scherror equation is to calculate the crystallite size. This method gives qualitative results.

$$D = \frac{k\lambda}{\beta \cos\theta)}$$

Here $\beta \rightarrow$ peak ~~voltage~~ width
$D \rightarrow$ crystallite size
$k \rightarrow$ Scherror constant
$\lambda \rightarrow$ x-ray wavelength
$\theta \rightarrow$ peak position

Data given :- instrumental broadening : 0.01°
wavelength of the x-ray used : 1.546 Å
Scherror constant : 0.44 (assuming that crystallite is spherical)

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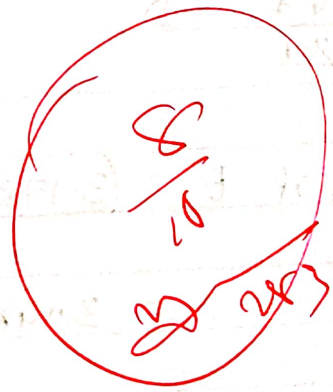
Peak (center) 2θ	FWHM (deg)	FWHM after instrumental broadening correction (rad)	$\frac{\text{FWHM}}{2}$ (deg)	D (nm)
28.57	0.31	$2\times 2.703\times 10^{-3}$	2.703×10^{-3}	55.4
33.11	0.325	$2\times 2.834\times 10^{-3}$	2.834×10^{-3}	53.4
47.52	0.356	$2\times 3.105\times 10^{-3}$	3.105×10^{-3}	51.1
56.38	0.394	$2\times 3.436\times 10^{-3}$	3.436×10^{-3}	47.9
59.14	0.427	$2\times 3.724\times 10^{-3}$	3.724×10^{-3}	44.8



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Calculation :-

$$D_1 = \frac{K\lambda}{\beta \cos\theta} = \frac{0.94 \times 1.546 \times 10^{-10}}{2.703 \times 10^{-3} \times \cos(14.285)} = 55.4 \times 10^{-9} m$$

$$D_2 = \frac{0.94 \times 1.546 \times 10^{-10}}{2.834 \times 10^{-3} \times \cos(16.555)} = 53.4 \times 10^{-9} m$$

$$D_3 = \frac{0.94 \times 1.546 \times 10^{-10}}{3.105 \times 10^{-3} \times \cos(23.76)} = 51.1 \times 10^{-9} m$$

$$D_4 = \frac{0.94 \times 1.546 \times 10^{-10}}{3.436 \times 10^{-3} \times \cos(28.19)} = 47.9 \times 10^{-9} m$$

$$D_5 = \frac{0.94 \times 1.546 \times 10^{-10}}{3.72 \times 10^{-3} \times \cos(29.57)} = 44.8 \times 10^{-9} m$$

$$\text{Average } D = \frac{D_1 + D_2 + D_3 + D_4 + D_5}{5} = 50.52 \times 10^{-9} m$$

$$= 50.52 \text{ nm}$$

Inference :-

The average crystallite size of the given poly-crystallite material is 50.52 nm

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