

AIM:

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

APPARATUS REQUIRED:

XRD pattern (upload in the course page)

Peak fitting program (Open Source / free software like fitlyk, guplot and qtiplot is preferable)

Usage of any pirated or cracked software is strictly prohibited.

FORMULA:

The scherrer is used to calculate crystalline size here,

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

DATA GIVEN:

Instrumental broadening = 0.01

$\lambda = 1.546 \text{ \AA}$

Scherrer constant $K = 0.94$

OBSERVATION TABLE:

Peak Centre	FWMM	FWMM after instrumental broadening correction	$\frac{FWMM}{2}$	Avg. crystal size (Å)
28.57	0.234	$0.224 = 0.00390$	0.00195	848.57
47.54	0.276	$0.266 = 0.0046$	0.00232	927.89
56.37	0.298	$0.288 = 0.00502$	0.00251	1045.41
33.13	0.248	$0.238 = 0.00415$	0.002075	1836.31
59.13	0.305	$0.295 = 0.00514$	0.00257	1102.06

CALCULATIONS:

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

$$D_1 = \frac{0.94 \times 1.546}{0.00195 \times \cos(28.57)} = 848.57 \text{ Å}$$

$$D_2 = \frac{0.94 \times 1.546}{0.00232 \times \cos(47.94)} = 927.89 \text{ Å}$$

$$D_3 = \frac{0.94 \times 1.546}{0.00251 \times \cos(56.37)} = 1045.4 \text{ Å}$$

$$D_4 = \frac{0.94 \times 1.546}{0.002079 \times \cos(33.13)} = 1836.31 \text{ Å}$$

$$D_5 = \frac{0.94 \times 1.546}{0.00297 \times \cos(59.3)} = 1102.06 \text{ Å}$$

$$\text{Average} = \frac{D_1 + D_2 + D_3 + D_4 + D_5}{5} = 952.048 \text{ Å}$$

Too long

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02/11/14

RESULT:

The average crystalline size by scherrer formula of poly-crystalline using is 952.098 \AA