

Nitride film 3**MT-455**

Aim: To determine crystallite size and lattice strain for the given data.

Procedure:

Given the instrumental broadening value, $B_i = 0.045^\circ$

Gaussian equation $B_R^2 = B_o^2 - B_i^2$

$$B_R \cos \theta = \frac{k\lambda}{L} + \eta \sin \theta \quad \text{where, } \eta = \text{Strain in the material}$$

L = Crystallite Size

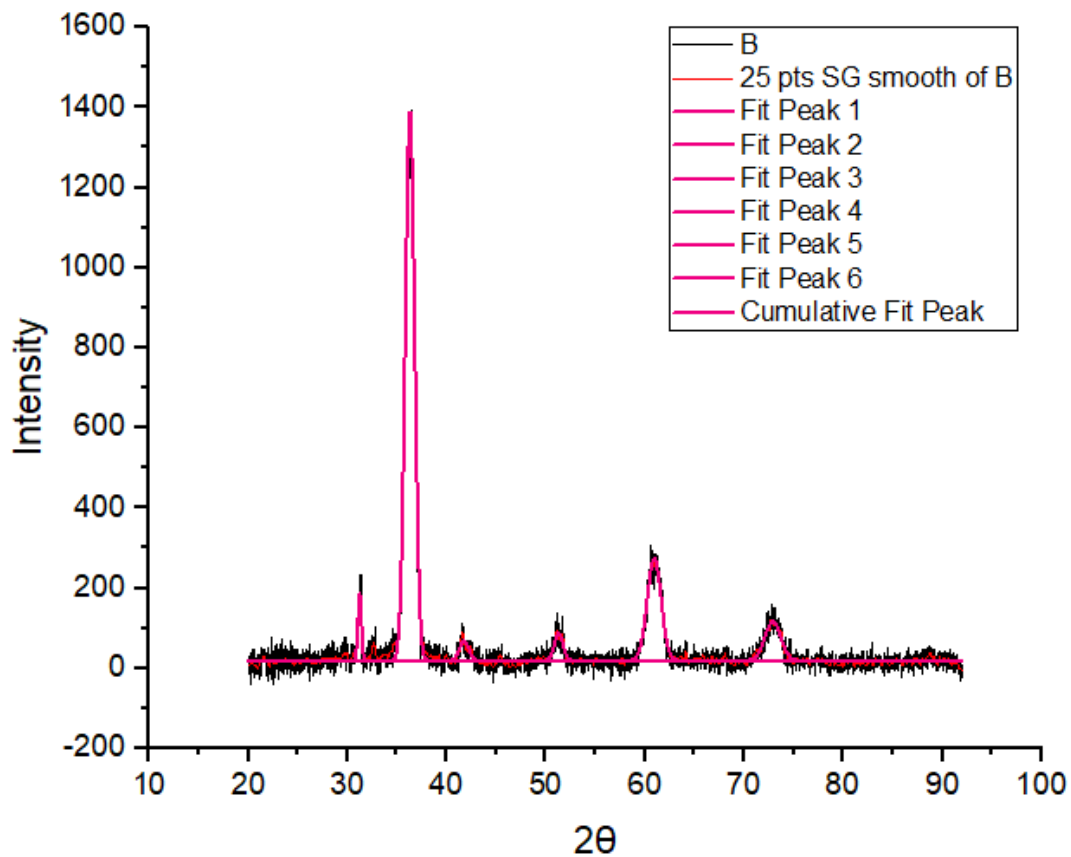
$k=0.94$

$\lambda = 0.154\text{nm}$

$b = \text{Slope} = \eta$

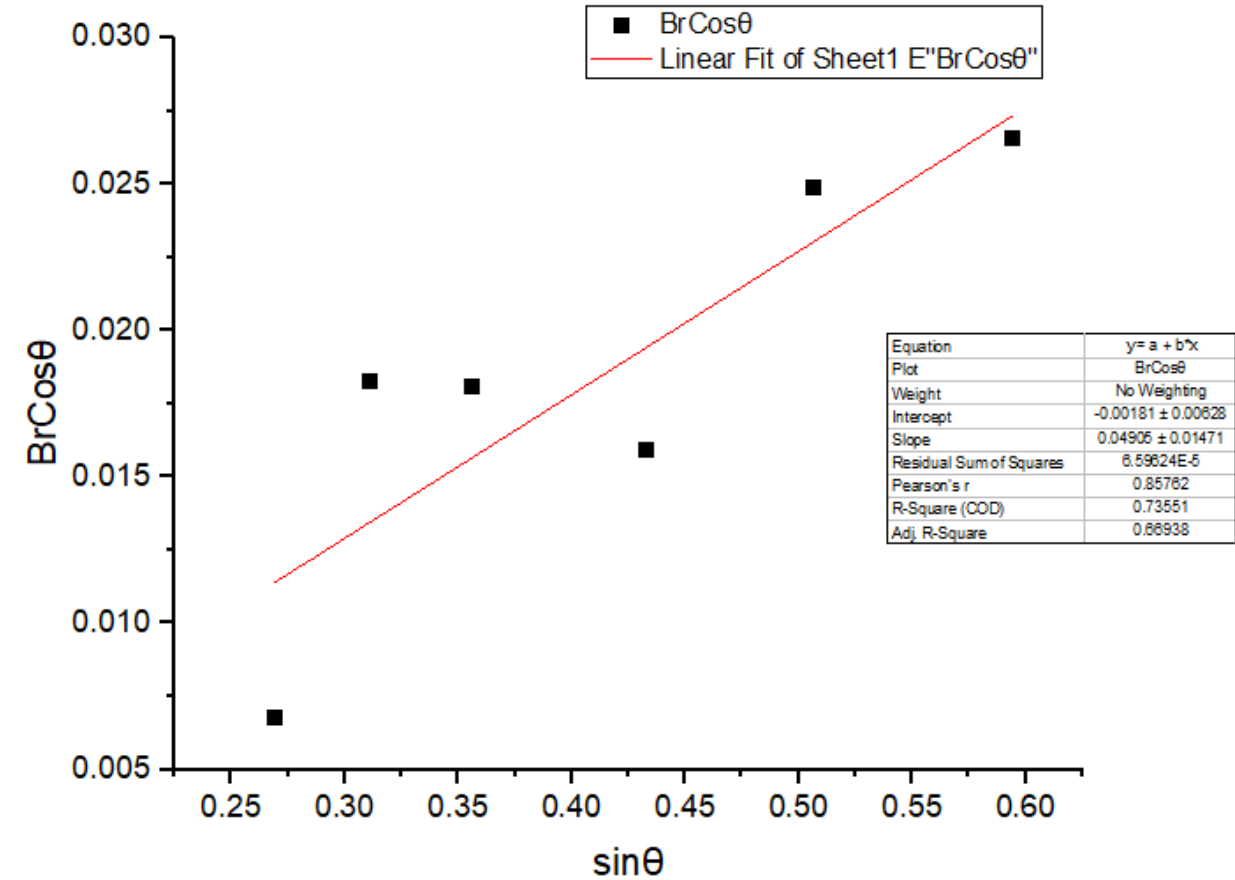
Comparing the above equation with $y = bx + a$

Where, $a = \text{Intercept} = \frac{k\lambda}{L}$



2θ	θ(rad)	B _o (fwhm)	B _o (rad)	B _o ²	B _i (deg)	B _i (rad)	B _i ²
31.23024	0.272535	0.40573	0.007081	5.01E-05	0.045	0.000785	6.17E-07
36.29897	0.316768	1.10047	0.019207	0.000369	0.045	0.000785	6.17E-07
41.76266	0.364448	1.10718	0.019324	0.000373	0.045	0.000785	6.17E-07
51.3042	0.447714	1.01079	0.017642	0.000311	0.045	0.000785	6.17E-07
60.93761	0.531781	1.65249	0.028841	0.000832	0.045	0.000785	6.17E-07
72.90834	0.636245	1.89106	0.033005	0.001089	0.045	0.000785	6.17E-07

$B_r^2=B_o^2-B_i^2$	B_r	$B_r\cos\theta$	$\sin\theta$
4.95E-05	0.007038	0.006778	0.269174
0.000368	0.019191	0.018236	0.311497
0.000373	0.019308	0.01804	0.356434
0.000311	0.017624	0.015887	0.432906
0.000831	0.028831	0.024849	0.507069
0.001089	0.032996	0.02654	0.59418



Equation	$y = a + b \cdot x$
Plot	BrCos θ
Weight	No Weighting
Intercept	-0.00181 ± 0.00628
Slope	0.04905 ± 0.01471
Residual Sum of Squares	6.59624E-5
Pearson's r	0.85762
R-Square (COD)	0.73551
Adj. R-Square	0.66938

$$b = \text{Slope} = \eta$$

$$a = \text{Intercept} = \frac{k\lambda}{L}$$

$$\text{Therefore, } \eta = 0.04905$$

$$\frac{k\lambda}{L} = 0.00447$$

$$L = \frac{k\lambda}{0.00447}$$

$$L = \frac{0.94 \times 0.154}{0.00447}$$

$$L = 32.3847 \text{ nm}$$

Result

$$\eta = \text{Strain in the material} = 0.04905$$

$$L = \text{Crystallite Size} = 32.3847 \text{ nm}$$