Ragula Bhoopal

20ETMM11

Group-2

Nitride film 0 **MT-455**

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

Procedure:

Given the instrumental broadening value, $\mathbf{B_i} = 0.045^{o}$

Gaussian equation $\mathbf{B_R^2} = \mathbf{B_O^2} - \mathbf{B_i^2}$

$\mathbf{B_R Cos\theta} = \frac{\mathbf{k\lambda}}{\mathbf{L}} + \eta \mathbf{Sin\theta}$ where, $\eta = S$train in the material

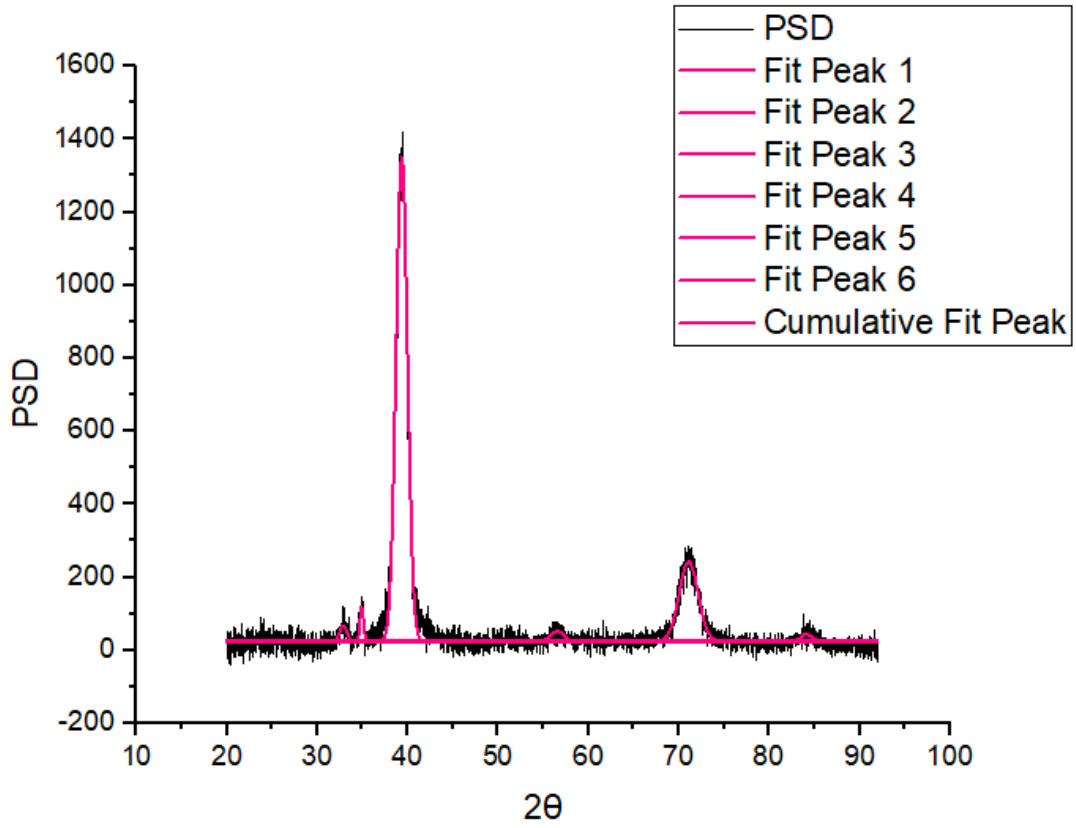
L= Crystallite Size

k=0.94

$\lambda = 0.154$nm

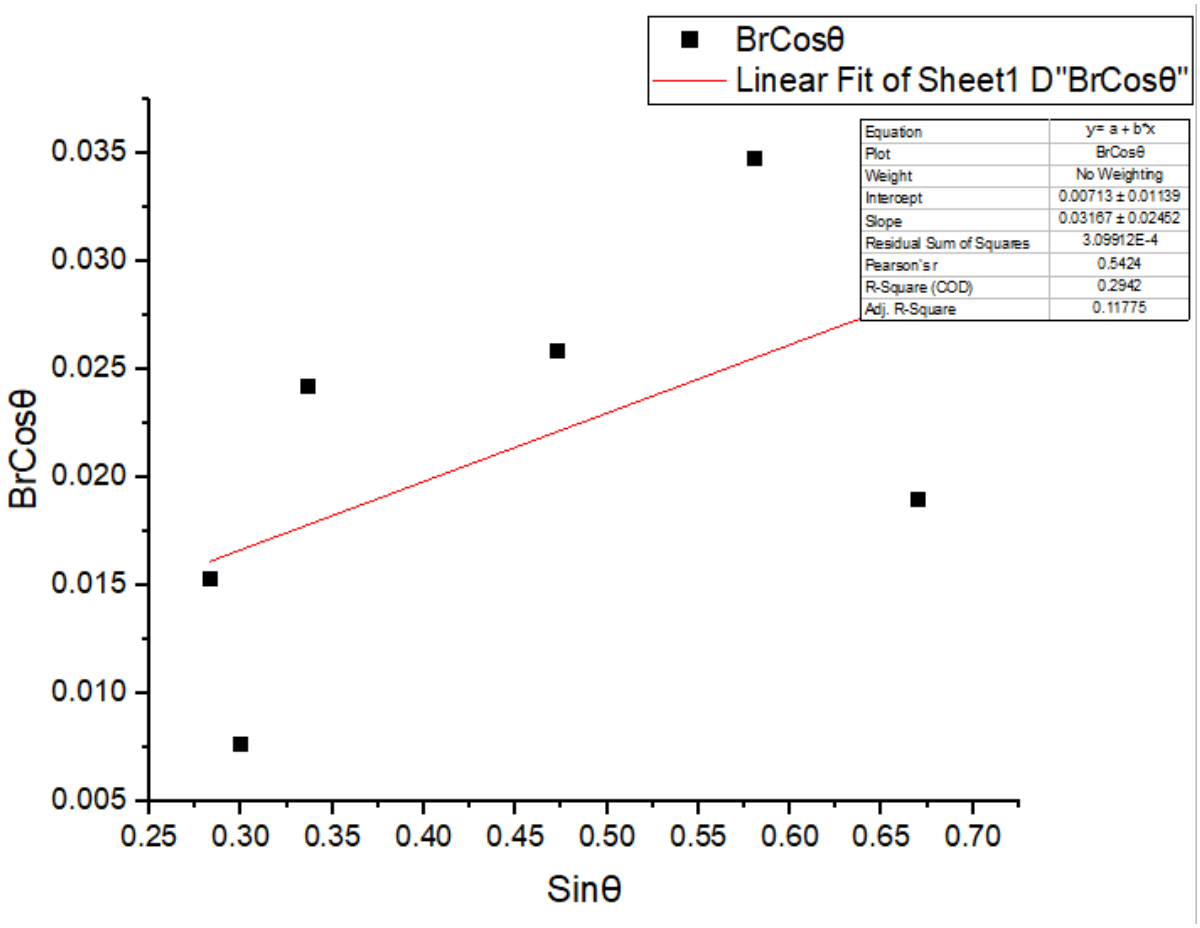
Comparing the above equation with $y = bx + a$ Where, $b = \text{Slope} = \eta$

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



2θ	θ(rad)	B_o(fwhm)	B_o(rad)	B_o^2	B_i(deg)	B_i(rad)	B_i^2
32.89235	0.28704	0.91439	0.015959	0.000255	0.045	0.000785	6.1685E-07
34.91805	0.304717	0.45754	0.007986	6.38E-05	0.045	0.000785	6.1685E-07
39.34331	0.343335	1.47026	0.025661	0.000658	0.045	0.000785	6.1685E-07
56.53556	0.493366	1.68187	0.029354	0.000862	0.045	0.000785	6.1685E-07
71.0858	0.620341	2.44668	0.042703	0.001824	0.045	0.000785	6.1685E-07
84.1166	0.734056	1.46242	0.025524	0.000651	0.045	0.000785	6.1685E-07

$B_r^2=B_o^2-B_i^2$	B_r	$B_r\cos\theta$	sinθ
0.000254077	0.01594	0.015288	0.283114
6.31526E-05	0.007947	0.007581	0.300024
0.000657864	0.025649	0.024152	0.336629
0.00086105	0.029344	0.025844	0.473593
0.001822897	0.042695	0.03474	0.581312
0.00065086	0.025512	0.018942	0.669886



Equation	y = a + b*x
Plot	BrCosθ
Weight	No Weighting
Intercept	0.00713 ± 0.01139
Slope	0.03167 ± 0.02452
Residual Sum of Squares	3.09912E-4
Pearson's r	0.5424
R-Square (COD)	0.2942
Adj. R-Square	0.11775

$$\mathrm{b} = \mathrm{Slope} = \eta$$
$$\mathbf{a} = \mathrm{Intercept} = \frac{\mathbf{k}\lambda}{\mathbf{L}}$$
$$\mathrm{Therefore}, \eta = 0.03167$$
$$\frac{\mathbf{k}\boldsymbol{\lambda}}{\mathbf{L}} = 0.00713$$
$$\mathbf{L} = \frac{\mathbf{k}\lambda}{0.00713}$$
$$\mathbf{L} = \frac{0.94 \times 0.154}{0.00713}$$
$$\mathbf{L} = 20.3029 \text{ nm}$$

Result

$\eta = S$train in the material=0.0316

L= Crystallite Size $= 20.3029$ nm

Ragula Bhoopal

20ETMM11

Group-2

Nitride film 1 **MT-455**

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

Procedure:

Given the instrumental broadening value, $\mathbf{B_i} = 0.045^{o}$

Gaussian equation $\mathbf{B_R^2 = B_O^2 - B_i^2}$

$\mathbf{B_R Cos\theta} = \frac{\mathbf{k\lambda}}{\mathbf{L}} + \eta \mathbf{Sin\theta}$ where, $\eta = S$train in the material

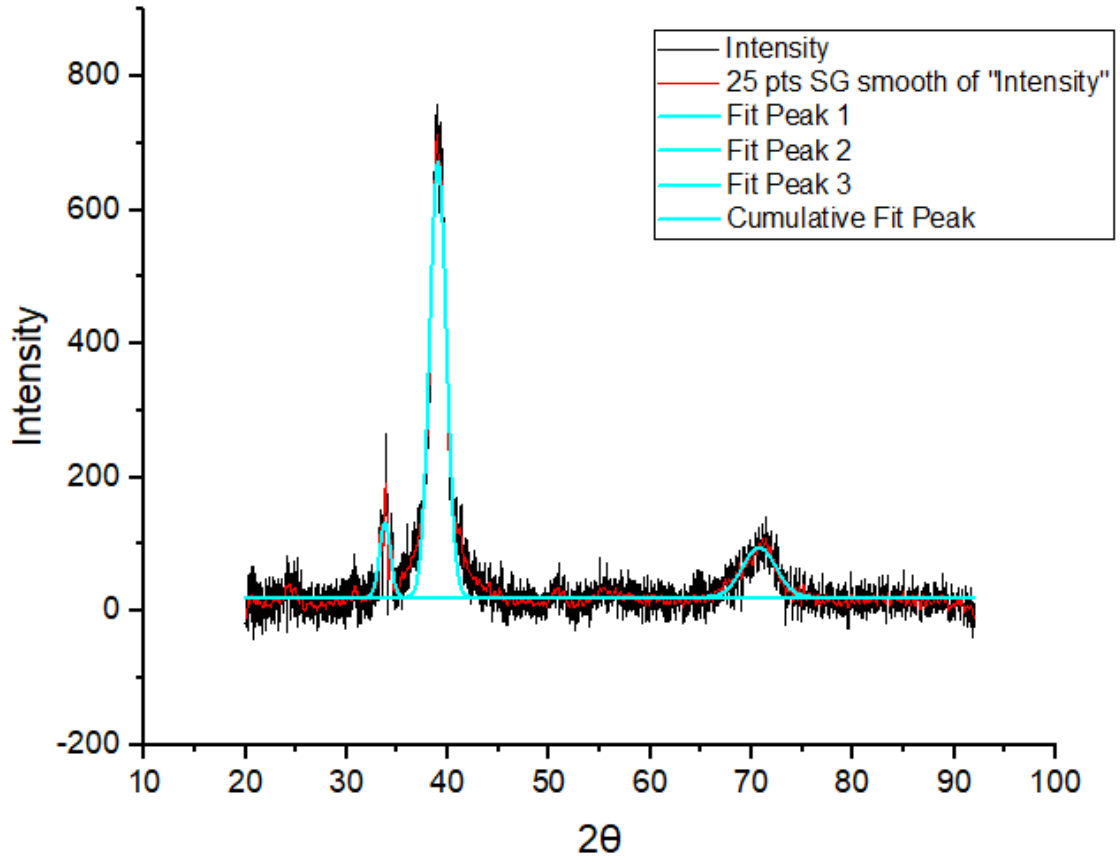
L= Crystallite Size

k=0.94

$\lambda = 0.154$nm

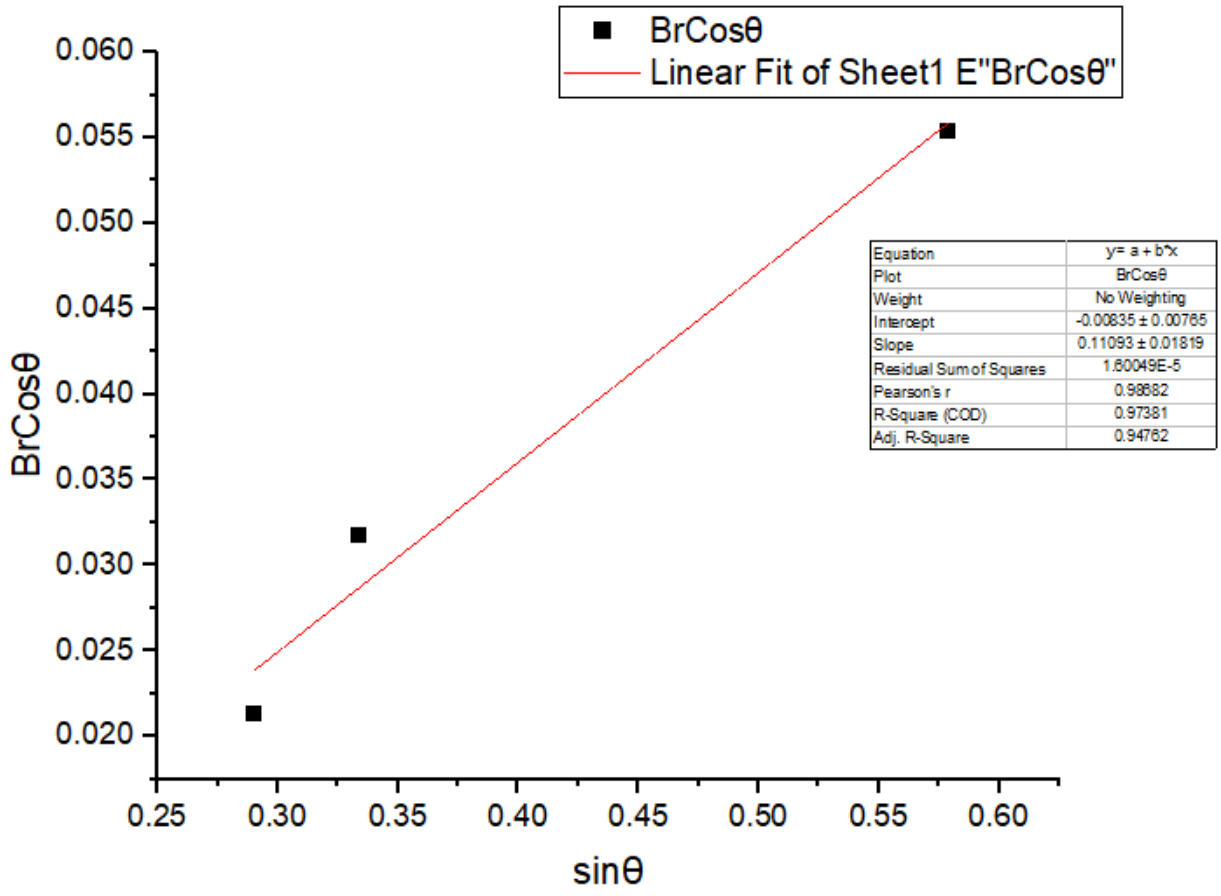
Comparing the above equation with $y = bx + a$ Where, $b = \text{Slope} = \eta$

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



2θ	θ(rad)	B_o(fwhm)	B_o(rad)	B_o^2	B_i(deg)	B_i(rad)	B_i^2
33.76656	0.294669	1.27552	0.022262	0.000496	0.045	0.000785	6.17E-07
39.00728	0.340403	1.928	0.03365	0.001132	0.045	0.000785	6.17E-07
70.73872	0.617312	3.89281	0.067942	0.004616	0.045	0.000785	6.17E-07

$B_r^2=B_o^2-B_i^2$	B_r	$B_r\cos\theta$	sinθ
0.000495	0.022248	0.021289	0.290423
0.001132	0.033641	0.03171	0.333867
0.004616	0.067938	0.055399	0.578845



Equation	y = a + b*x
Plot	BrCosθ
Weight	No Weighting
Intercept	-0.00835 ± 0.00765
Slope	0.11092 ± 0.01819
Residual Sum of Squares	1.6005E-5
Pearson's r	0.98682
R-Square (COD)	0.97381
Adj. R-Square	0.94762

$$\mathrm{b} = \mathrm{Slope} = \eta$$
$$\mathbf{a} = \mathrm{Intercept} = \frac{\mathbf{k}\lambda}{\mathbf{L}}$$
$$\mathrm{Therefore}, \eta = 0.11092$$
$$\frac{\mathbf{k}\boldsymbol{\lambda}}{\mathbf{L}} = 0.00835$$
$$\mathbf{L} = \frac{\mathbf{k}\lambda}{0.00835}$$
$$\mathbf{L} = \frac{0.94 \times 0.154}{0.00835}$$
$$\mathbf{L} = 17.3365 \text{ nm}$$

Result

$\eta = S$train in the material=0.11092
L= Crystallite Size $= 17.3365$ nm

Ragula Bhoopal
20ETMM11
Group-2

Nitride film 2 **MT-455**

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

Procedure:

Given the instrumental broadening value, $\mathbf{B_i} = 0.045^{o}$

Gaussian equation $\mathbf{B_R^2} = \mathbf{B_O^2} - \mathbf{B_i^2}$

$\mathbf{B_R Cos\theta} = \frac{\mathbf{k\lambda}}{\mathbf{L}} + \eta \mathbf{Sin\theta}$ where, $\eta = S$train in the material

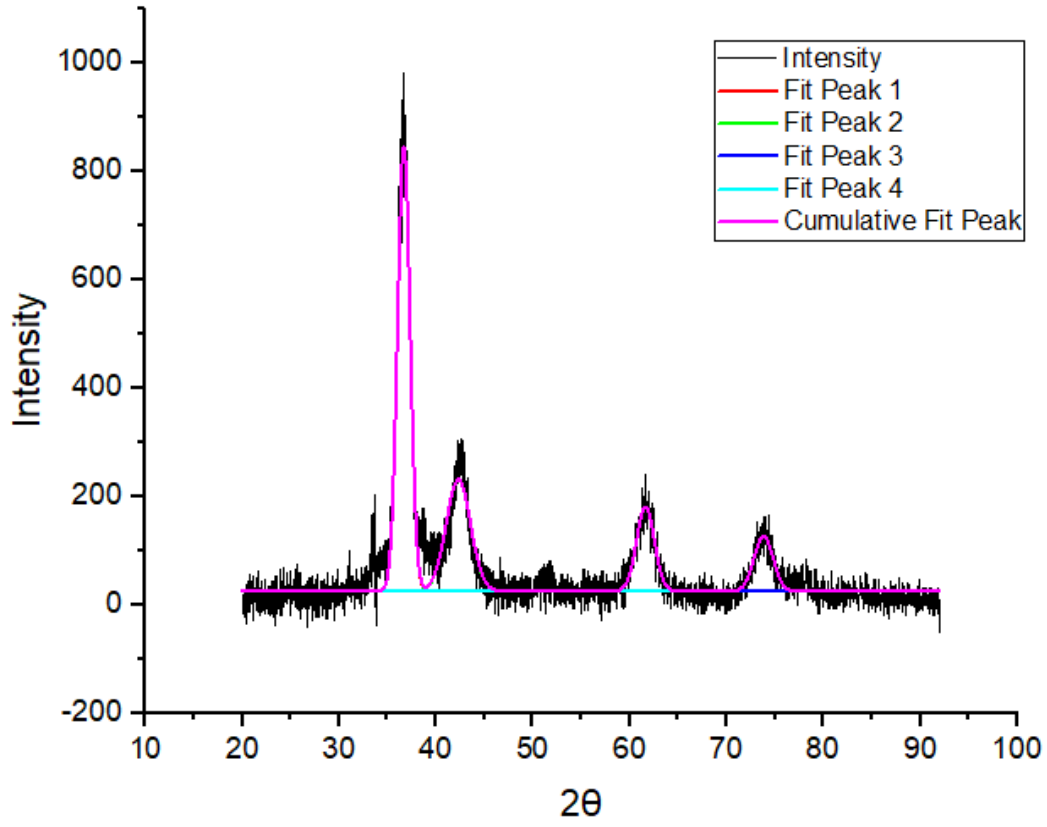
L= Crystallite Size

k=0.94

$\lambda = 0.154$nm

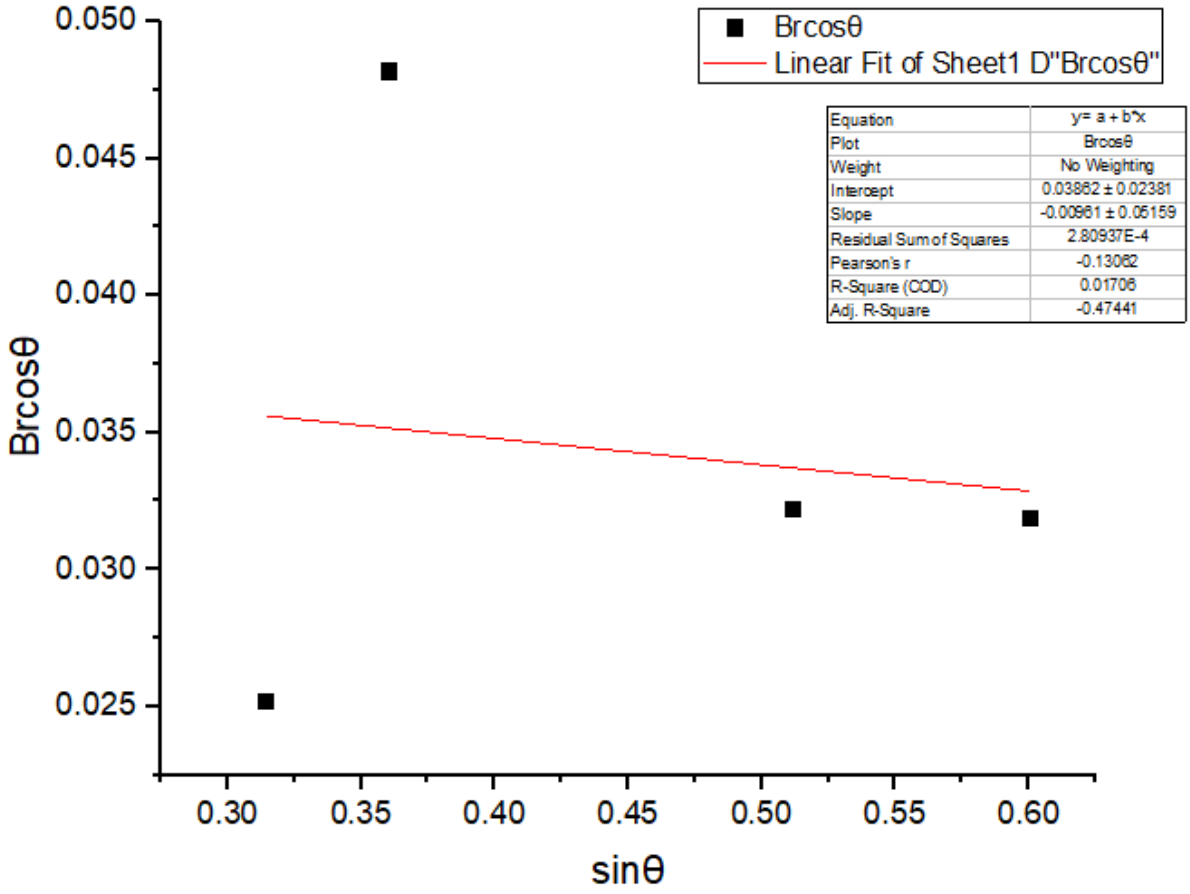
Comparing the above equation with $y = bx + a$ Where, $b = \text{Slope} = \eta$

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



2θ	θ(rad)	B_o(fwhm)	B_o(rad)	B_o^2	B_i(deg)	B_i(rad)	B_i^2
36.67767	0.320073	1.52066	0.026541	0.000704	0.045	0.000785	6.17E-07
42.30679	0.369196	2.95861	0.051637	0.002666	0.045	0.000785	6.17E-07
61.62263	0.537759	2.14505	0.037438	0.001402	0.045	0.000785	6.17E-07
73.8236	0.644232	2.28072	0.039806	0.001585	0.045	0.000785	6.17E-07

$B_r^2=B_o^2-B_i^2$	B_r	$B_r\cos\theta$	sinθ
0.000704	0.026529	0.025182	0.314636
0.002666	0.051632	0.048152	0.360866
0.001401	0.03743	0.032147	0.512212
0.001584	0.039798	0.031821	0.600585



Equation	y = a + b*x
Plot	Brcosθ
Weight	No Weighting
Intercept	0.03862 ± 0.02381
Slope	-0.00961 ± 0.05159
Residual Sum of Squares	2.80937E-4
Pearson's r	-0.13062
R-Square (COD)	0.01706
Adj. R-Square	-0.47441

$$\mathrm{b} = \mathrm{Slope} = \eta$$
$$\mathbf{a} = \mathrm{Intercept} = \frac{\mathbf{k}\lambda}{\mathbf{L}}$$
$$\mathrm{Therefore}, \eta = 0.00961$$
$$\frac{\mathbf{k}\boldsymbol{\lambda}}{\mathbf{L}} = 0.03862$$
$$\mathbf{L} = \frac{\mathbf{k}\lambda}{0.03862}$$
$$\mathbf{L} = \frac{0.94 \times 0.154}{0.03862}$$
$$\mathbf{L} = 3.7483 \text{ nm}$$

Result

$\eta = S$train in the material=0.00961

L= Crystallite Size $= 3.7483$ nm

Ragula Bhoopal

20ETMM11

Group-2

Nitride film 3 **MT-455**

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

Procedure:

Given the instrumental broadening value, $\mathbf{B_i} = 0.045^{o}$

Gaussian equation $\mathbf{B_R^2} = \mathbf{B_O^2} - \mathbf{B_i^2}$

$\mathbf{B_R Cos\theta} = \frac{\mathbf{k\lambda}}{\mathbf{L}} + \eta \mathbf{Sin\theta}$ where, $\eta = S$train in the material

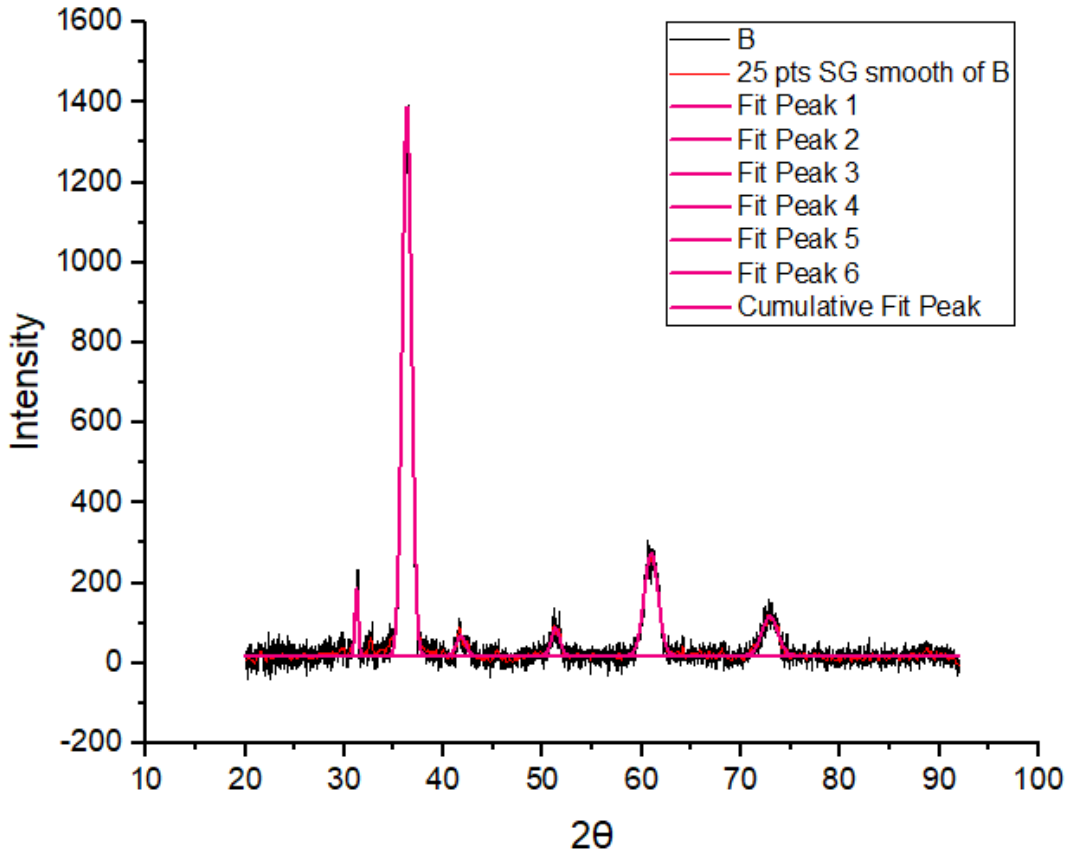
L= Crystallite Size

k=0.94

$\lambda = 0.154$nm

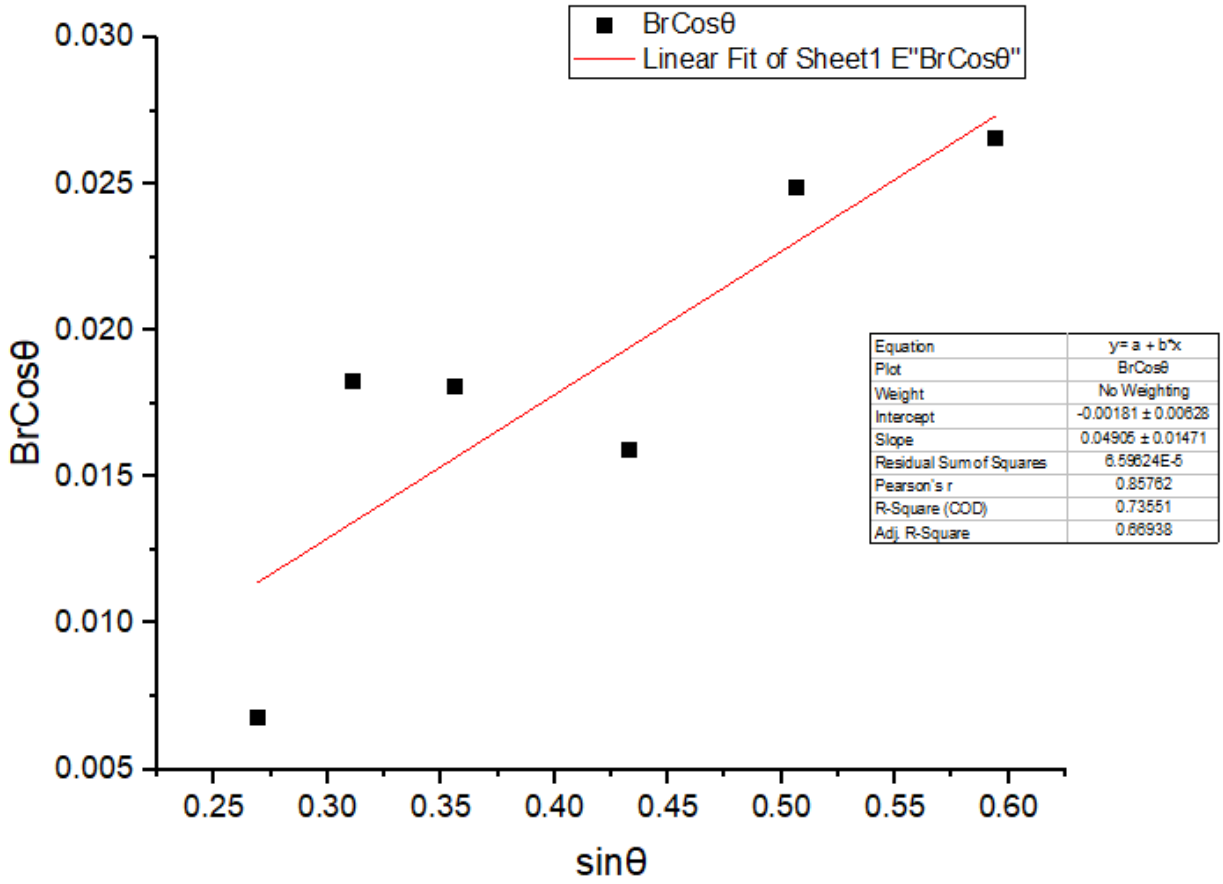
Comparing the above equation with $y = bx + a$ Where, $b = \text{Slope} = \eta$

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



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	$B_r\cos\theta$	sinθ
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*x
Plot	BrCosθ
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

$$\mathrm{b} = \mathrm{Slope} = \eta$$
$$\mathbf{a} = \mathrm{Intercept} = \frac{\mathbf{k}\lambda}{\mathbf{L}}$$
$$\mathrm{Therefore}, \eta = 0.04905$$
$$\frac{\mathbf{k}\boldsymbol{\lambda}}{\mathbf{L}} = 0.00447$$
$$\mathbf{L} = \frac{\mathbf{k}\lambda}{0.00447}$$
$$\mathbf{L} = \frac{0.94 \times 0.154}{0.00447}$$
$$\mathbf{L} = 32.3847 \text{ nm}$$

Result

$\eta = S$train in the material=0.04905
L= Crystallite Size $= 32.3847$ nm