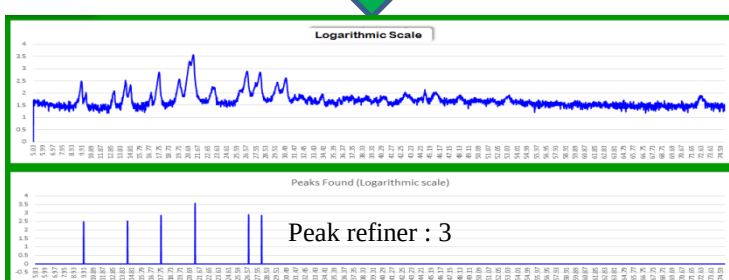
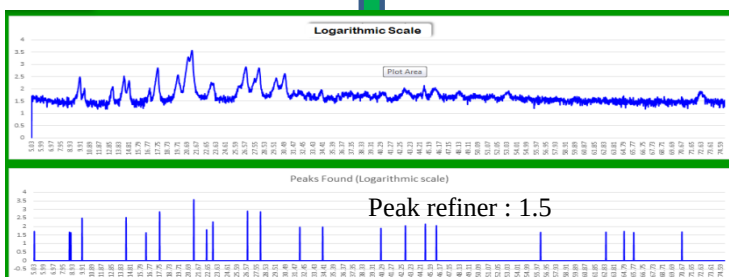
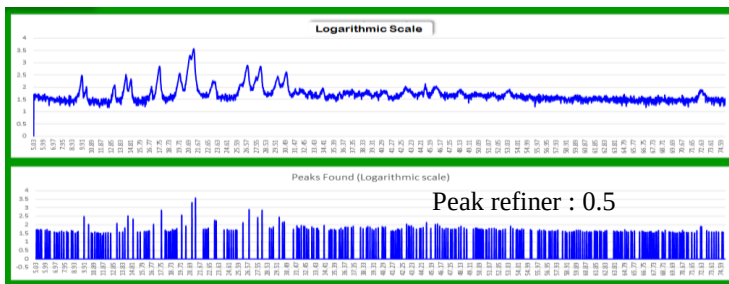


2019

Structure	Mathced results (%)
Cubic	* 8
Tetragonal	* 30
Hexagonal	↓ 38
Rhombohedral	* 4
Orthorhombic	↓ 56
Monoclinic	→ 90
Triclinic	↓ 56

Find XRD Peak & Match with JCPDS

4					56					90				
Rhombodetra					Orthorhombic					Monoclinic				
4 % Matched (Matched Peaks:1)					56 % Matched (Matched Peaks:13)					90 % Matched (Matched Peaks: 18)				
JCPDS Match	XRD (exp)	h	k	l	JCPDS Match	XRD (exp)	h	k	l	JCPDS Match	XRD (exp)	h	k	l
10.0000	9.8900	2	2	12	16.3509	16.3700	1	1	1	16.4502	16.3700	0	1	1
					16.6159	16.3700	1	0	1	16.5341	16.3700	-1	0	1
					22.9195	22.5100	0	0	2	16.8528	16.3700	1	0	1
					22.9195	23.1500	0	0	2	16.8528	16.3700	1	1	0
					23.4844	23.1500	0	2	0	23.1095	23.1500	0	0	2
					26.4725	26.6500	1	2	0	23.5792	23.1500	0	2	0
					33.9948	34.2700	2	2	0	26.3051	26.6500	0	2	1
					42.3079	42.6500	0	2	3	26.5850	26.6500	1	2	0



MANIKANDAN J

2/12/2019

Contents

1.	Paste the XRD data	2
2.	Enter name of the material	3
3.	Paste the JCPDS values of 7 crystal systems of the material to be analysed	4
4.	Refine number of peak (s) using PEAK REFINER VALUE	5
5.	Click SHOW PEAKS then Range	10
6.	Fix range	11
	<i>What is range?</i>	12
7.	Click match.....	13
8.	Detailed Result	14

1. Paste the XRD data

Step 1.

2 Theta	Intensity
5.01	49
5.03	49
5.05	52
5.07	49
5.09	47
5.11	36
5.13	31
5.15	54
5.17	47
5.19	52
5.21	39
5.23	42
5.25	46
5.27	44
5.29	49
5.31	39
5.33	43
5.35	41
5.37	45
5.39	41
5.41	41

Material

Result Graph

Cubic

Paste the JCPDS Peaks and hkl values of 0 for the Cubic structure.

Clear

h	k	l	JCPDS

Tetragonal

Paste the JCPDS Peaks and hkl values of 0 for the Tetragonal structure.

Clear

h	k	l	JCPDS

Hexagonal

Paste the JCPDS Peaks and hkl values of 0 for the Hexagonal structure.

Clear

h	k	l	JCPDS

2. Enter name of the material

Step 2.

	2 Theta	Intensity
1	5.01	49
2	5.03	44
3	5.05	52
4	5.07	49
5	5.09	47
6	5.11	36
7	5.13	31
8	5.15	54
9	5.17	47
10	5.19	52
11	5.21	39
12	5.23	42
13	5.25	46
14	5.27	44
15	5.29	49
16	5.31	39
17	5.33	43
18	5.35	41
19	5.37	45
20	5.39	41
21	5.41	41

Material:

Result **Graph**

Cubic

Paste the JCPDS Peaks and hkl values of wo3 for the Cubic structure.

Clear

h	k	l	JCPDS

Tetragonal

Paste the JCPDS Peaks and hkl values of wo3 for the Tetragonal structure.

Clear

h	k	l	JCPDS

Hexagonal

Paste the JCPDS Peaks and hkl values of wo3 for the Hexagonal structure.

Clear

h	k	l	JCPDS

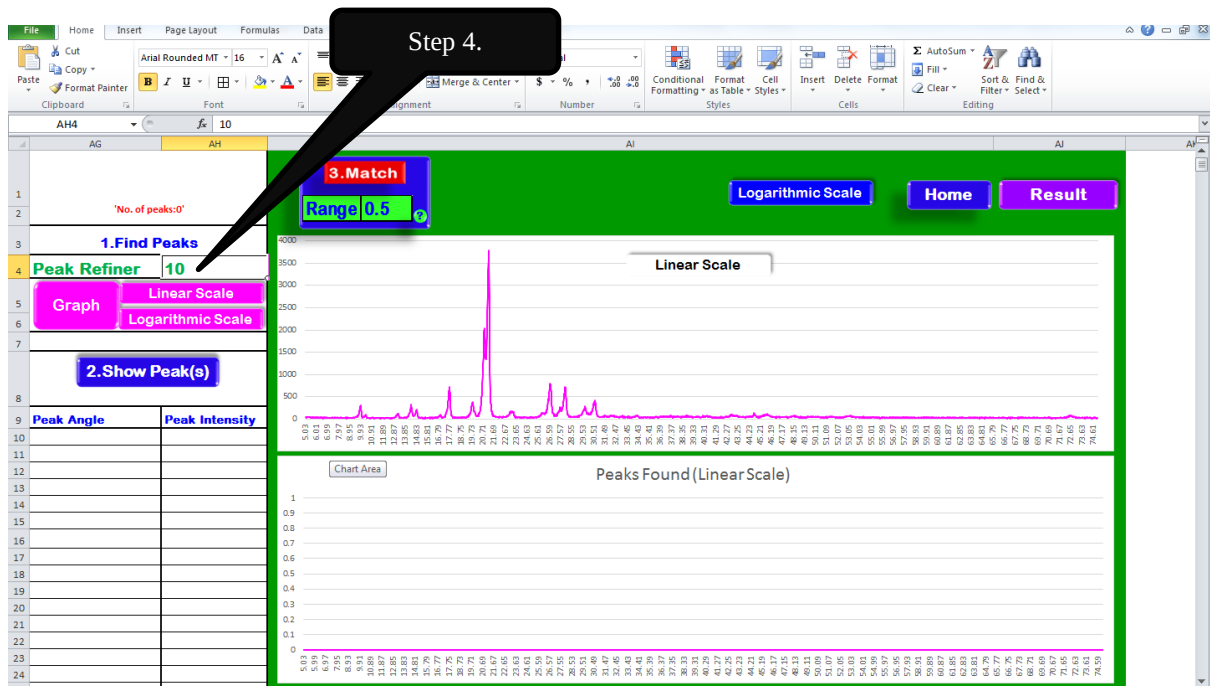
3. Paste the JCPDS values of 7 crystal systems of the material to be analysed

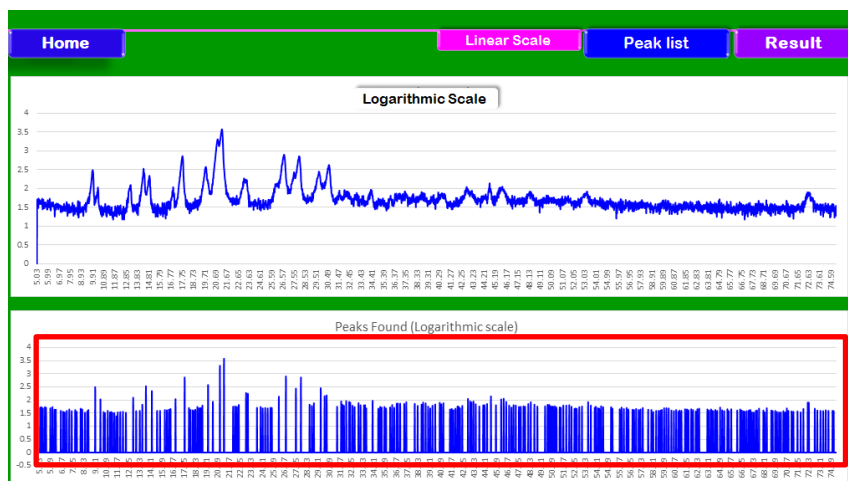
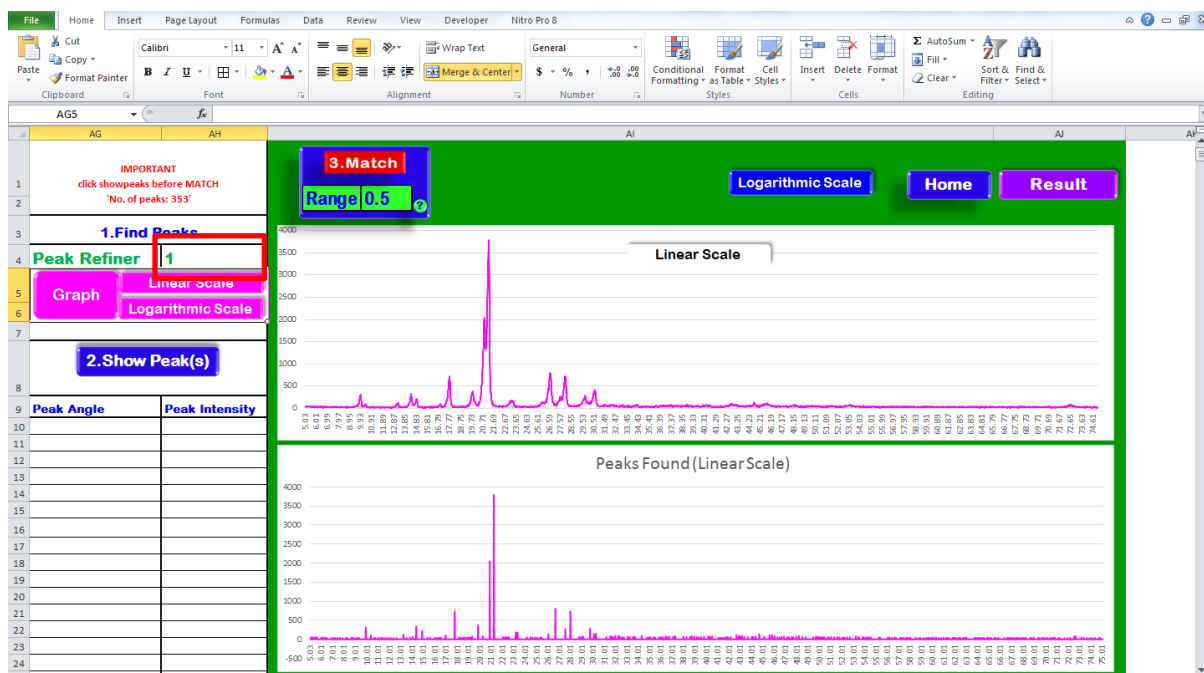
Step 3.

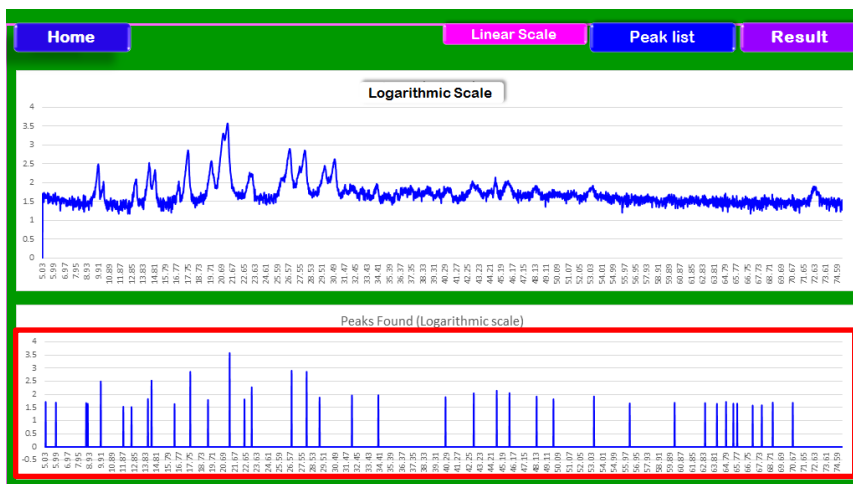
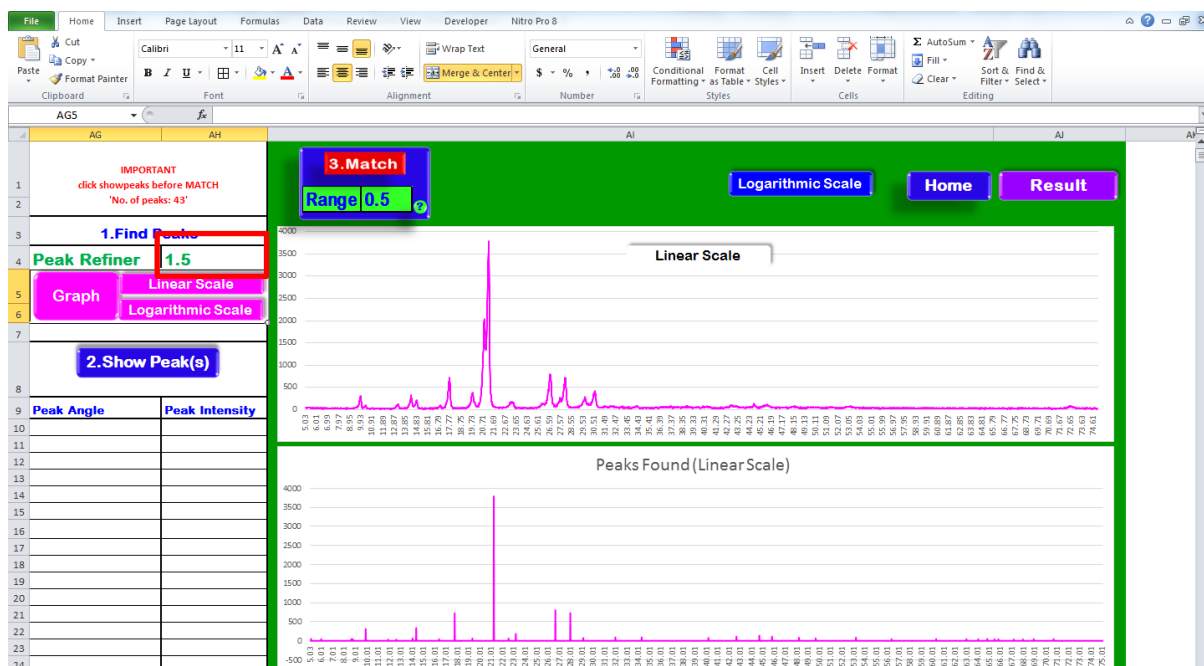
2 Theta	Intensity	Material	wo3
5.01	49		
5.03	44		
5.05	52		
5.07	49		
5.09	47		
5.11	36		
5.13	31		
5.15	54		
5.17	47		
5.19	52		
5.21	39		
5.23	42		
5.25	46		
5.27	44		
5.29	49		
5.31	39		
5.33	43		
5.35	41		
5.37	45		
5.39	41		
5.41	41		

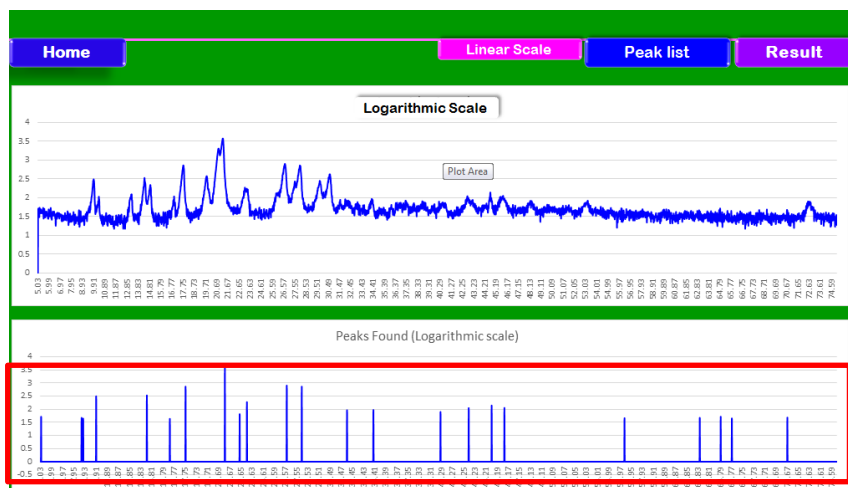
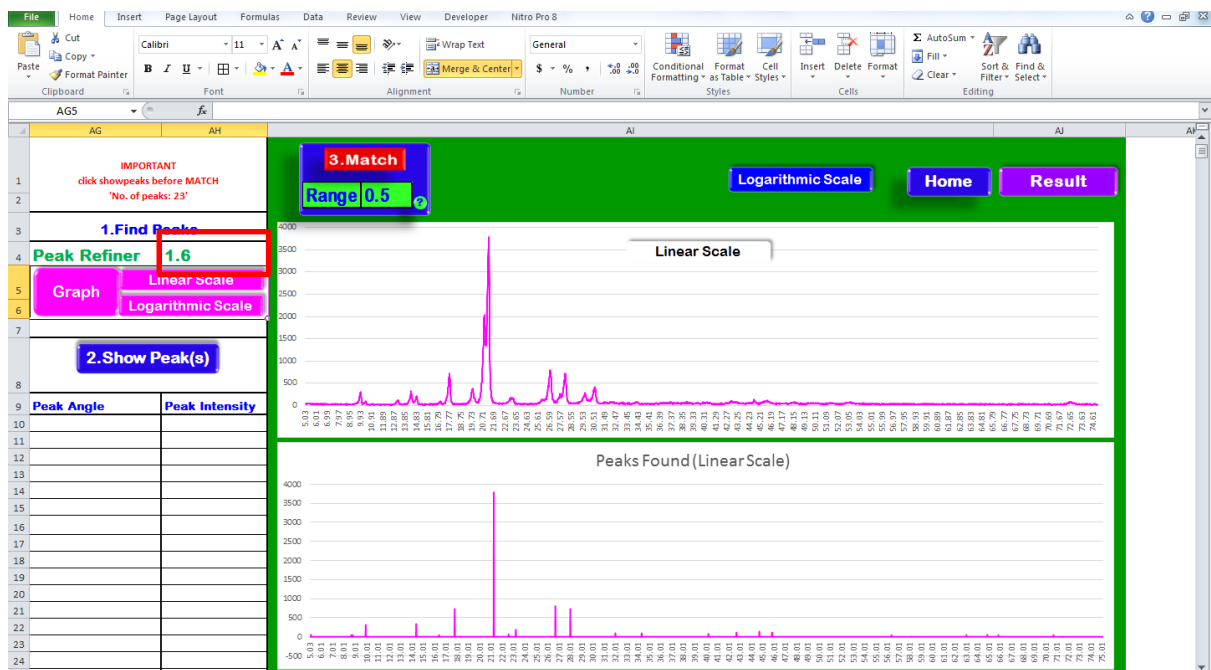
Cubic				Tetragonal				Hexagonal			
h	k	l	JCPDS	h	k	l	JCPDS	h	k	l	JCPDS
1	0	0	22.3	0	0	2	22.6466	1	0	0	14.0006
1	1	0	34.0478	1	1	0	23.831	0	0	1	22.7884
1	1	1	42.111	1	0	2	28.3256	1	1	0	24.3729
2	0	0	49.0413	1	1	2	33.109	1	0	1	26.8446
2	1	0	55.258	2	0	0	33.9554	2	0	0	28.2159
2	1	1	61.0747	2	1	1	39.8643	1	1	1	33.6105
				2	0	2	41.2039	2	0	1	36.5716
				2	1	2	44.7864	2	1	0	37.6224
				0	0	4	46.2439	3	0	0	42.8921
				2	2	0	48.7806	2	1	1	44.4394
				1	0	4	49.5368	0	0	2	46.5465
				2	1	3	52.1673	1	0	2	48.8481

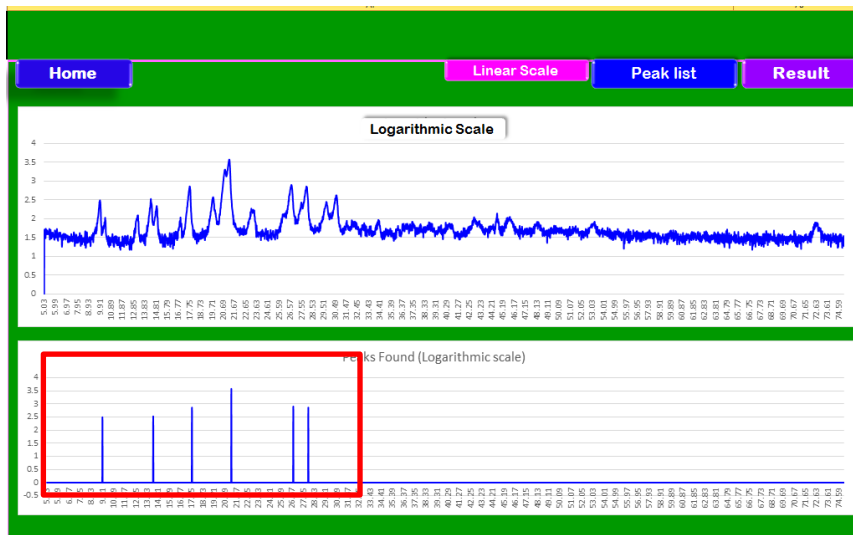
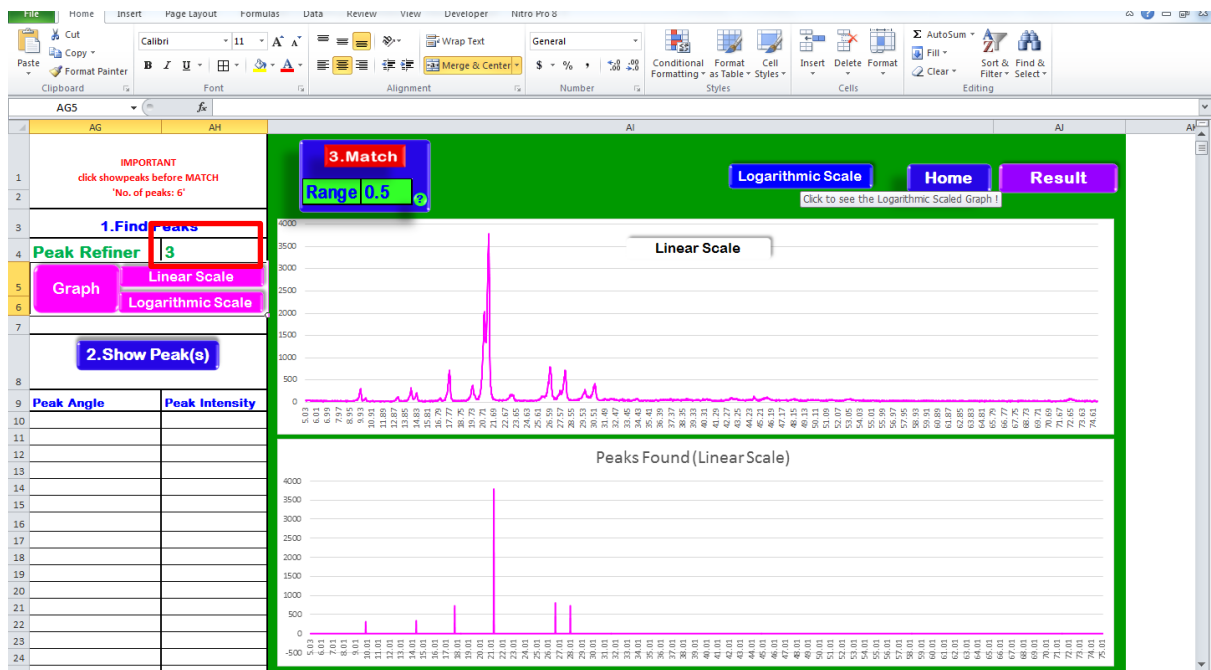
- Refine number of peak (s) using **PEAK REFINER VALUE**
(Number of peaks can be seen in the graphs while change the peak refiner value)



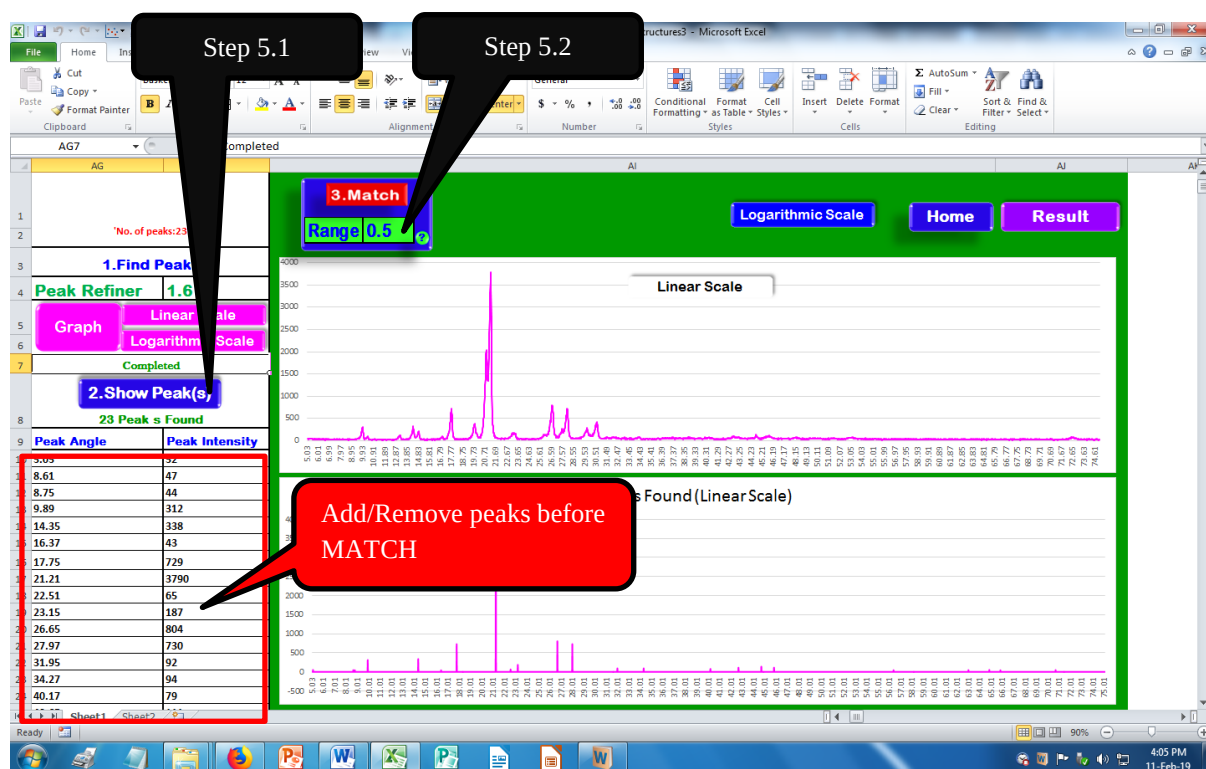






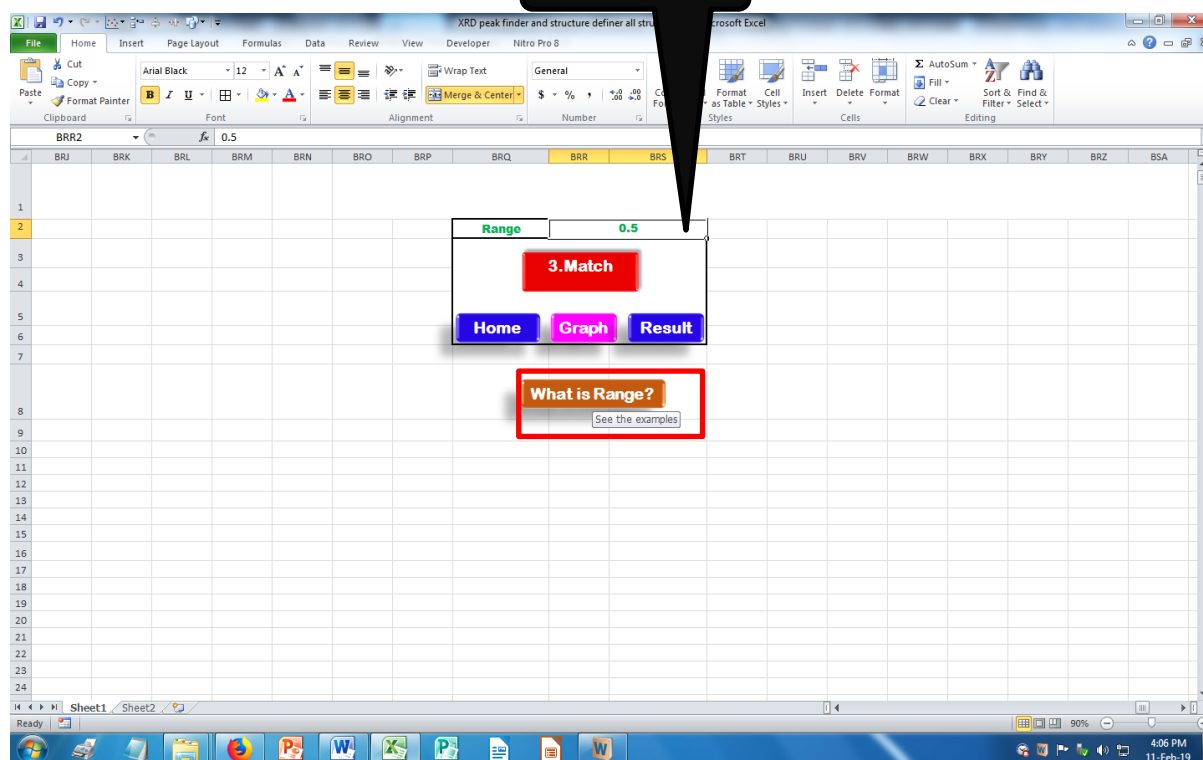


5. Click **SHOW PEAKS** then **Range**



6. Fix range

Step 6.



What is range?

What is range? It is a value used to match the JCPDS peak with EXPERIMENTAL XRD peak. For example, consider a JCPDS peak (23) given in the table below. The tables on the right explain how the matched result will become. The same way all JCPDS peaks will be compared with all XRD peaks.

Experimental XRD	JCPDS
24.3	23
24.2	23.5
24.1	24
24	24.5
23.9	25
23.8	25.5
23.7	26
23.6	26.5
23.5	27
23.4	27.5
23.3	28
23.2	28.5
23.1	29
23	29.5
22.9	30
22.8	30.5
22.7	31
22.6	31.5
22.5	32
22.4	32.5
22.3	33
22.2	33.5
22.1	34
22	34.5

Consider this JCPDS peak

If Range = 0.5

Example 1: If Range = 0.5, Result will be

Experimental XRD	JCPDS	Result
24.3	23	not matched
24.2	23	not matched
24.1	23	not matched
24	23	not matched
23.9	23	not matched
23.8	23	not matched
23.7	23	not matched
23.6	23	not matched
23.5	23	matched
23.4	23	matched
23.3	23	matched
23.2	23	matched
23.1	23	matched
23	23	matched
22.9	23	matched
22.8	23	matched
22.7	23	matched
22.6	23	matched
22.5	23	matched
22.4	23	not matched
22.3	23	not matched
22.2	23	not matched
22.1	23	not matched
22	23	not matched

JCPDS

Range

$$23 + 0.5 = 23.5$$

Range

$$23 - 0.5 = 22.5$$

If the XRD peak is between these two JCPDS values 22.5 and 23.5 then the XRD peak will be matched.

Home Graph Result

If Range = 0.2

Example 1: If Range = 0.2, Result will be

Experimental XRD	JCPDS	Result
24.3	23	not matched
24.2	23	not matched
24.1	23	not matched
24	23	not matched
23.9	23	not matched
23.8	23	not matched
23.7	23	not matched
23.6	23	not matched
23.5	23	not matched
23.4	23	not matched
23.3	23	not matched
23.2	23	matched
23.1	23	matched
23	23	matched
22.9	23	matched
22.8	23	matched
22.7	23	not matched
22.6	23	not matched
22.5	23	not matched
22.4	23	not matched
22.3	23	not matched
22.2	23	not matched
22.1	23	not matched
22	23	not matched

Home Graph Result

JCPDS

Range

$$23 + 0.2 = 23.2$$

$$23 - 0.2 = 22.8$$

Range

If the XRD peak is between these two JCPDS values then the xrd peak will be matched.

Home Graph Result

If Range = 0

Example 1: If Range = 0, Result will be

Experimental XRD	JCPDS	Result
24.3	23	not matched
24.2	23	not matched
24.1	23	not matched
24	23	not matched
23.9	23	not matched
23.8	23	not matched
23.7	23	not matched
23.6	23	not matched
23.5	23	not matched
23.4	23	not matched
23.3	23	not matched
23.2	23	not matched
23.1	23	not matched
23	23	matched
22.9	23	not matched
22.8	23	not matched
22.7	23	not matched
22.6	23	not matched
22.5	23	not matched
22.4	23	not matched
22.3	23	not matched
22.2	23	not matched
22.1	23	not matched
22	23	not matched

Home Graph Result

Change Range

JCPDS

Range

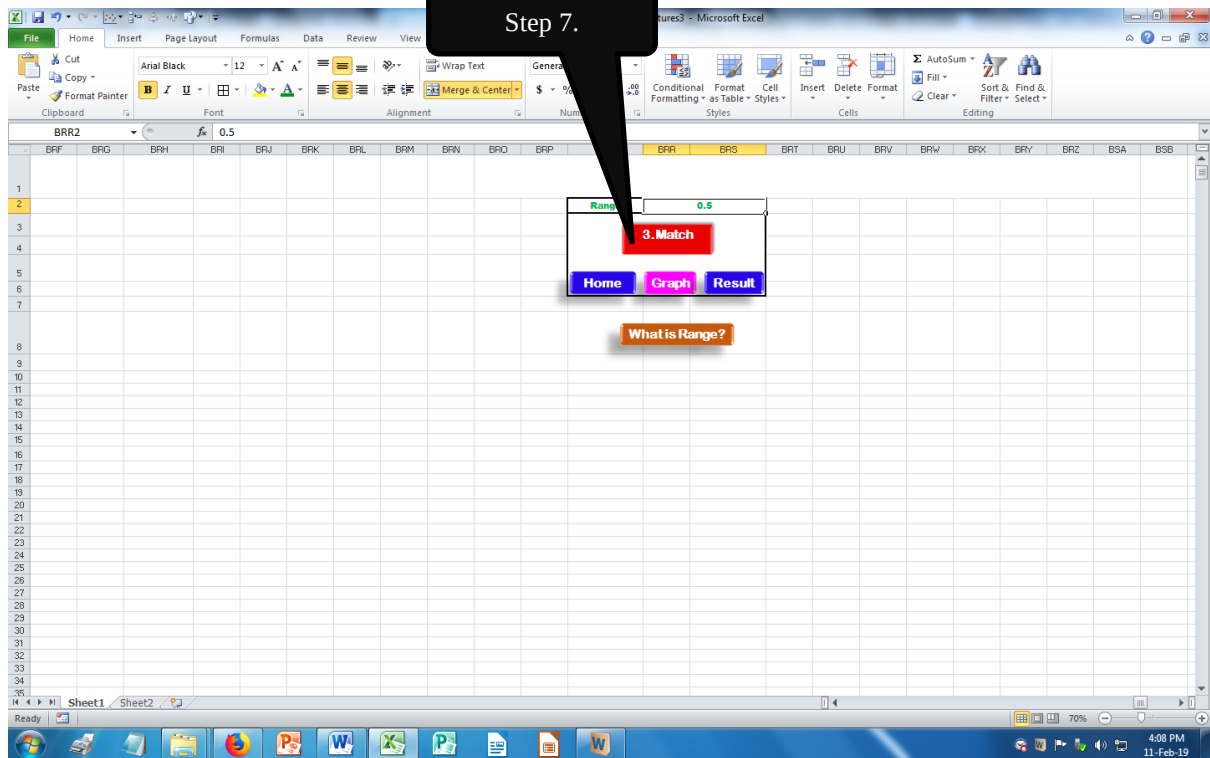
$$23 + 0 = 23$$

$$23 - 0 = 23$$

Range

If the XRD peak is between these two JCPDS values then the xrd peak will be matched.

7. Click match



8. Detailed Result

Detailed Result !																									Home		Graph																																																																																																
3		Name of the material																							WOS																																																																																																		
4				Match status		Matching Process Completed																																																																																																																					
7		Peaks Found		Cubic						8 % Matched (Matched Peaks:2)						Tetragonal						30 % Matched (Matched Peaks:7)						Hexagonal						38 % Matched (Matched Peaks:9)						Rhombohedral						4 % Matched (Matched Peaks:1)																																																																													
8				JCPDS Match						XRD (exp)						h						k						l						JCPDS Match						XRD (exp)						h						k						l						JCPDS Match						XRD (exp)						h						k						l						JCPDS Match						XRD (exp)						h						k						l					
10		Peak Angle		Peak Intensity		5.05		52		22.3000		22.5100		1		0		0		22.6466		22.5100		0		0		2		14.0006		14.3500		1		0		0		10.0000		9.8900		2		2		12																																																																											
11		8.61		47		34.0478		34.2700		1		1		0		28.3256		27.9700		1		0		2		22.7884		22.5100		0		0		1																																																																																									
12		8.75		44												33.9554		34.2700		2		0		0		22.7884		23.1500		0		0		1																																																																																									
13		9.89		312												39.8643		40.1700		2		1		1		26.8446		26.6500		1		0		1																																																																																									
14		14.35		338												44.7864		44.6700		2		1		2		28.2159		27.9700		2		0		0																																																																																									
15		16.37		43												46.2439		45.7900		0		0		4		42.8921		42.6500		3		0		0																																																																																									
16		17.75		729												64.7537		64.8100		3		2		1		44.4394		44.6700		2		1		1																																																																																									
17		21.21		3790																						65.1400		64.8100		3		0		2																																																																																									
18		22.51		65																						70.6532		70.6700		2		2		2																																																																																									
19		23.15		187																																																																																																																							
20		26.65		804																																																																																																																							
21		27.97		730																																																																																																																							
22		31.95		92																																																																																																																							
23		34.27		94																																																																																																																							
24		40.17		79																																																																																																																							
25		42.65		111																																																																																																																							
26		44.67		139																																																																																																																							
27		45.79		113																																																																																																																							
28		56.35		46																																																																																																																							
29		62.97		47																																																																																																																							
30		64.81		52																																																																																																																							
31		65.79		45																																																																																																																							
32		70.67		48																																																																																																																							
33																																																																																																																											

Rhombohedral					Orthorhombic					Monoclinic					Triclinic				
4 % Matched (Matched Peaks:1)					56 % Matched (Matched Peaks:13)					90 % Matched (Matched Peaks: 18)					56 % Matched (Matched Peaks:13)				
JCPDS Match	XRD (exp)	h	k	l	JCPDS Match	XRD (exp)	h	k	l	JCPDS Match	XRD (exp)	h	k	l	JCPDS Match	XRD (exp)	h	k	l
10.0000	9.8900	2	2	12	16.3509	16.3700	1	1	1	16.4502	16.3700	0	1	1	16.3188	16.3700	0	1	1
					16.6159	16.3700	1	0	1	16.5341	16.3700	-1	0	1	16.6594	16.3700	0	-1	1
					22.9195	22.5100	0	0	2	16.8528	16.3700	1	0	1	16.6594	16.3700	-1	0	1
					22.9195	23.1500	0	0	2	16.8528	16.3700	1	1	0	16.7692	16.3700	-1	1	0
					23.4844	23.1500	0	2	0	23.1095	23.1500	0	0	2	16.8697	16.3700	1	0	1
					26.4725	26.6500	1	2	0	23.5792	23.1500	0	2	0	23.1574	23.1500	0	0	2
					33.9948	34.2700	2	2	0	26.3051	26.6500	0	2	1	23.6447	23.1500	0	2	0
					42.3079	42.6500	0	2	3	26.5850	26.6500	1	2	0	26.2655	26.6500	0	-1	2
					42.7197	42.6500	0	3	2	34.1510	34.2700	2	0	2	26.4659	26.6500	-1	2	0
					44.5482	44.6700	1	3	2	34.1510	34.2700	2	2	0	26.8170	26.6500	1	2	0
					44.5482	44.6700	2	1	3	39.7183	40.1700	1	3	1	26.8170	26.6500	-2	0	1
					45.3990	45.7900	3	1	2	40.4579	40.1700	-3	1	1	28.3673	27.9700	-1	1	2
					56.7684	56.3500	2	3	3	42.6117	42.6500	0	2	3	33.9116	34.2700	-2	2	0
					56.7684	56.3500	4	1	2	42.9541	42.6500	0	3	2	34.1197	34.2700	2	0	2
					63.2077	62.9700	3	4	1	44.2438	44.6700	3	2	0	34.4719	34.2700	2	2	0
					63.2985	62.9700	4	1	3	44.2438	44.6700	-1	2	3	39.7761	40.1700	1	3	1
					64.5473	64.8100	5	0	1	44.4774	44.6700	-2	1	3	39.8601	40.1700	1	-3	1
					64.9285	64.8100	0	2	5	44.6867	44.6700	1	2	3	42.6419	42.6500	0	3	2
					65.8103	65.7900	2	3	4	44.6867	44.6700	-1	3	2	43.1386	42.6500	0	-2	3
					65.8103	65.7900	5	1	1	44.8981	44.6700	1	3	2	44.2115	44.6700	-1	3	2
					66.2215	65.7900	2	4	3	45.3599	45.7900	2	3	1	44.2115	44.6700	-2	1	3
					66.2215	65.7900	3	2	4	45.3599	45.7900	-3	1	2	44.6097	44.6700	3	2	0

Structure	Mathced results (%)
Cubic	✖ 8
Tetragonal	✖ 30
Hexagonal	⬇ 38
Rhombohedral	✖ 4
Orthorhombic	⬇ 56
Monoclinic	⬇ 90
Triclinic	⬇ 56