Date: 01/22/2020 Experiment No. 2 Set: .....

PHY 1701 (Engineering Physics) Lab Manual and Records.

OBJECTIVE OF THE EXPERIMENT:

ENGINEERING APPLICATIONS OF NANOMATERIALS

Tools Required:-

- XRD pattern
- Peak fitting program (fityk, gnuplot or qtiplot)

SLO :-

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

Formula to Use:-

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

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

Here,

- Peak width (β in radians).
- Crystallite size (D)
- Scherrer Constant (K).
- X-ray wavelength (λ).
- Peak-position (θ).

DATA GIVEN:

Instrumental Broadening : 0.01°

Wavelength of X-ray Used : 1.546 Å

Scherrer Constant: 0.94 (assuming the crystallites are spherical in shape).

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Reg.No:- 20BDS0405

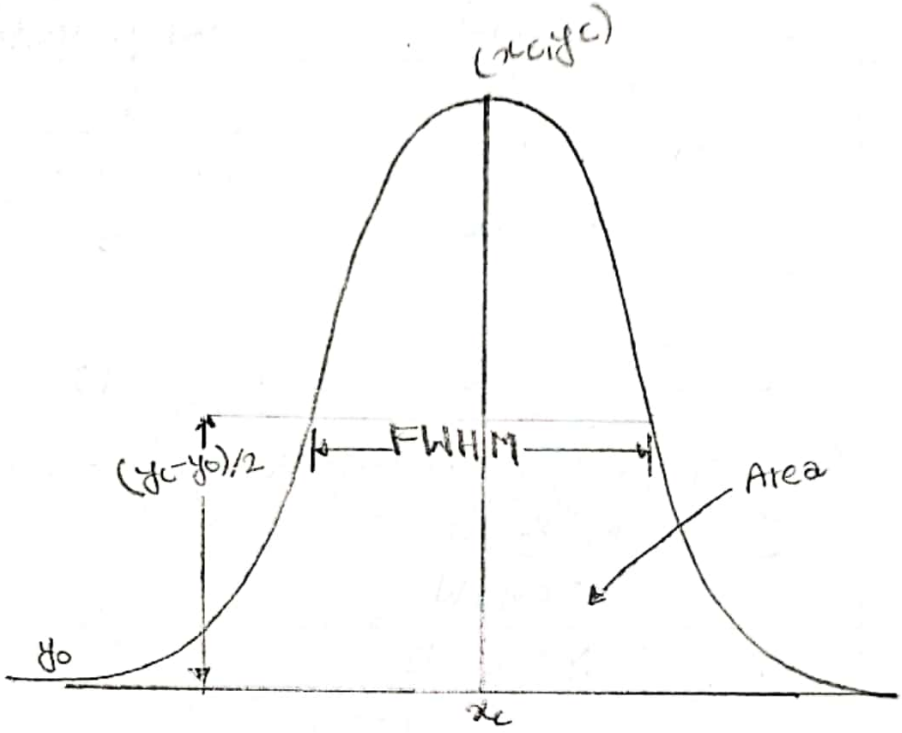

Fig:- Peak Fitting Using Gaussian/Pseudovoigt function.

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Tabulation:-

Peak Center (degree)	FWHM (degree)	FWHM after instrumental broadening correction. (degree)	FWHM (in radian)	Average Crystallite Size (Å)
28.57	0.33	0.320	0.00558	199.5
47.540	0.390	0.380	0.00663	218.4
56.370	0.389	0.379	0.0066	267.45
33.130	0.420	0.410	0.00716	163.04
59.13	0430	0.420	0.00733	259.93

Sample Calculation:-

For 1st order maxima, $K = 0.94$, $\lambda = 1.04$ Å

Peak Center (θ) = 28.57°

FWHM (β) = 0.00558°

$$\therefore \text{Crystallite size} = \frac{K\lambda}{\beta \cos\theta} = \frac{0.94 \times 1.04}{0.00558 \times \cos(28.57)^{\circ}} \text{ Å}$$

$$D_1 = 199.488 \text{ Å}$$

$$\approx 199.5 \text{ Å}$$

Similarly, $D_2 = 218.4$ Å, $D_3 = 267.45$ Å, $D_4 = 163.04$ Å, $D_5 = 259.93$ Å

Now, Average of all values is $D = \frac{D_1 + D_2 + D_3 + D_4 + D_5}{5}$

$= 221.6$ Å

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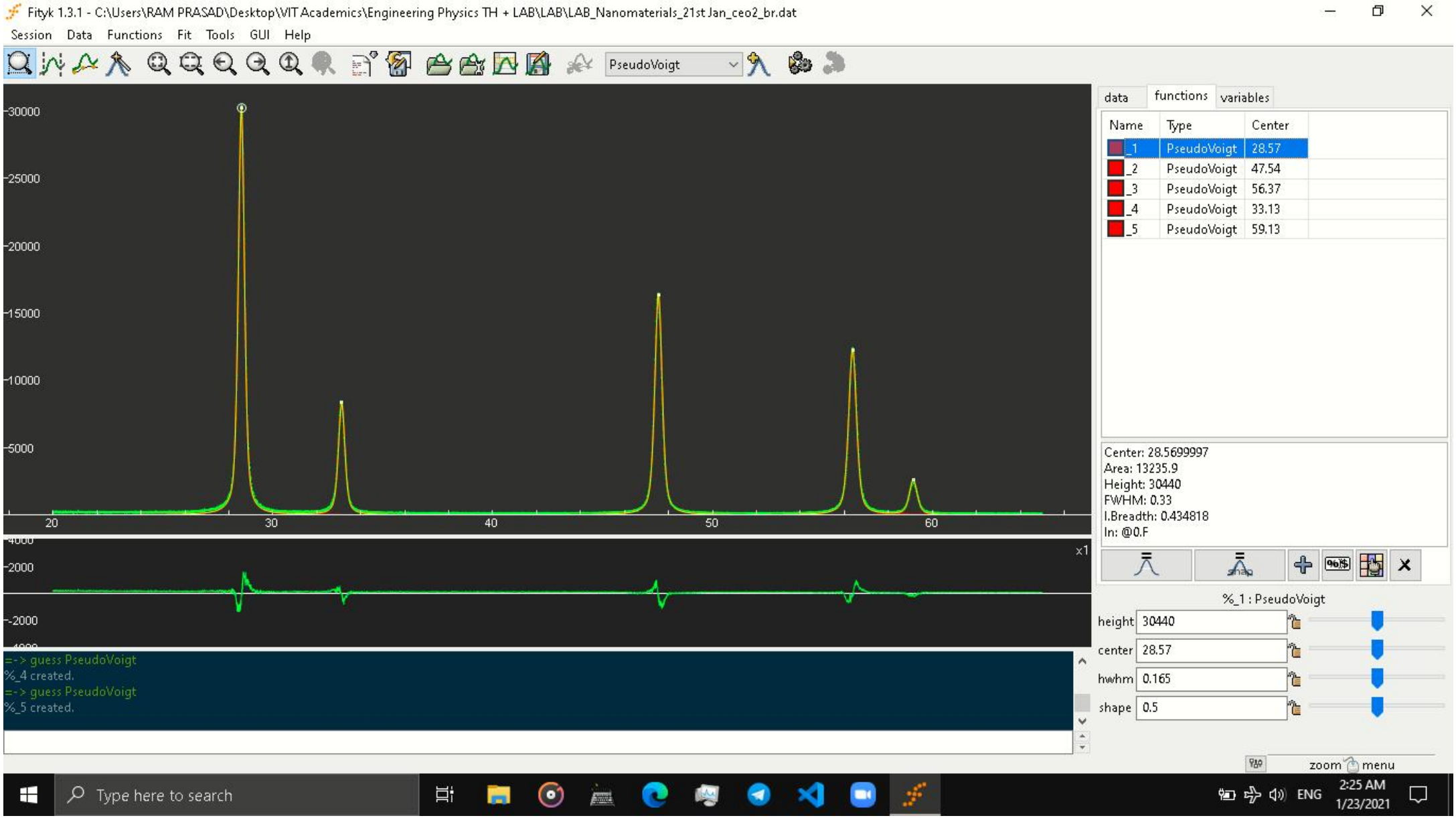
Inference:-

The Crystallite Size was calculated to be 221.6 Å.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Session Data Functions Fit Tools GUI Help
PseudoVoigt
data functions variables
Name Type Center
_1 PseudoVoigt 28.57
_2 PseudoVoigt 47.54
_3 PseudoVoigt 56.37
_4 PseudoVoigt 33.13
_5 PseudoVoigt 59.13
Center: 28.5699997
Area: 13235.9
Height: 30440
FWHM: 0.33
I.Breadth: 0.434818
In: @0.F
%_1 : PseudoVoigt
height 30440
center 28.57
hwhm 0.165
shape 0.5
=-> guess PseudoVoigt
%_4 created.
=-> guess PseudoVoigt
%_5 created.
zoom menu
Type here to search
ENG
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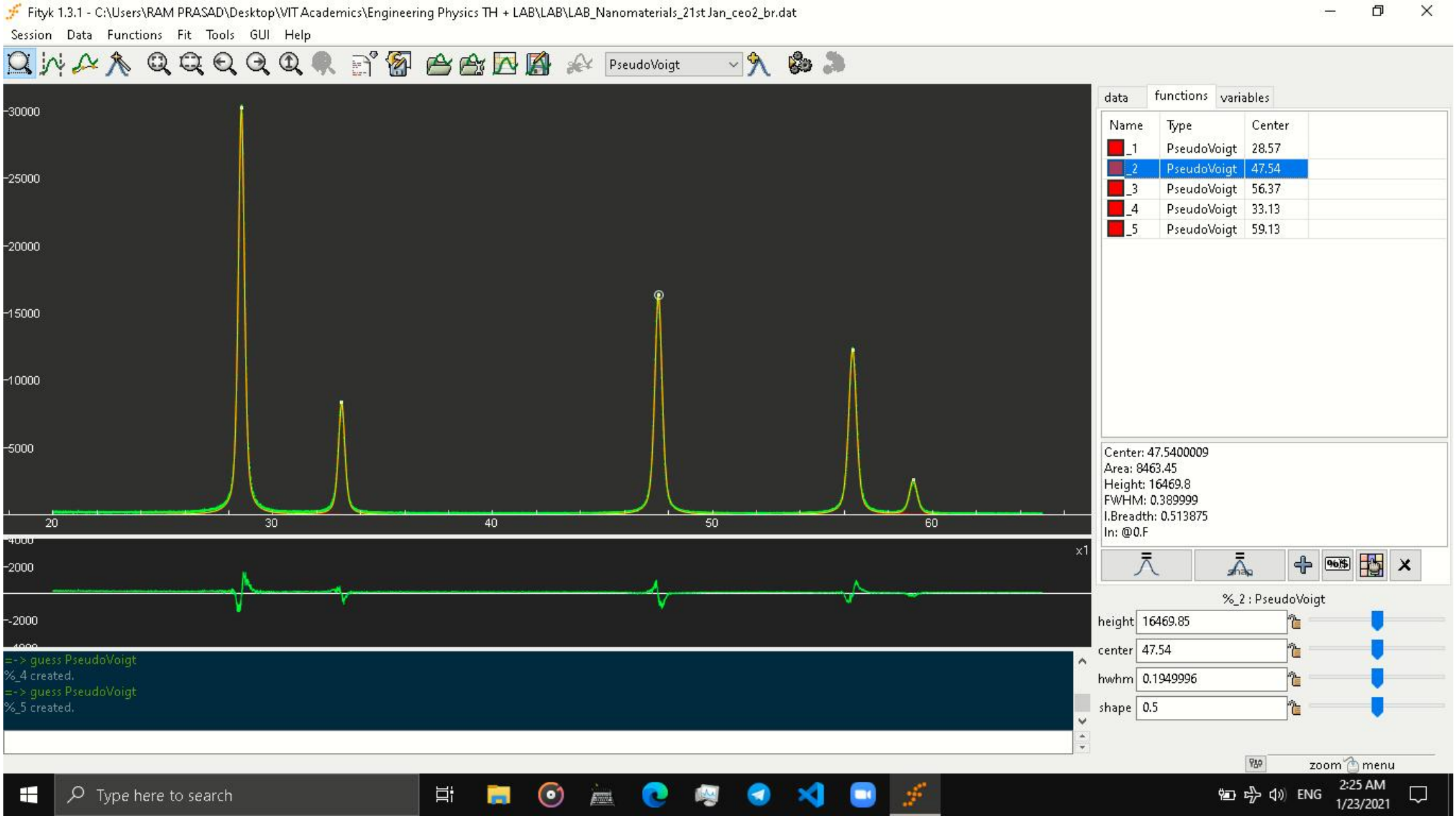
1/23/2021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Session Data Functions Fit Tools GUI Help
PseudoVoigt
30000
25000
20000
15000
10000
5000
20
30
40
50
60
2000
-2000
x1
=-> guess PseudoVoigt
%_4 created.
=-> guess PseudoVoigt
%_5 created.
data
functions
variables
Name Type Center
_1 PseudoVoigt 28.57
_2 PseudoVoigt 47.54
_3 PseudoVoigt 56.37
_4 PseudoVoigt 33.13
_5 PseudoVoigt 59.13
Center: 47.5400009
Area: 8463.45
Height: 16469.8
FWHM: 0.389999
l.Breadth: 0.513875
In: @0.F
%_2 : PseudoVoigt
height 16469.85
center 47.54
hwhm 0.1949996
shape 0.5
zoom menu
Type here to search
ENG
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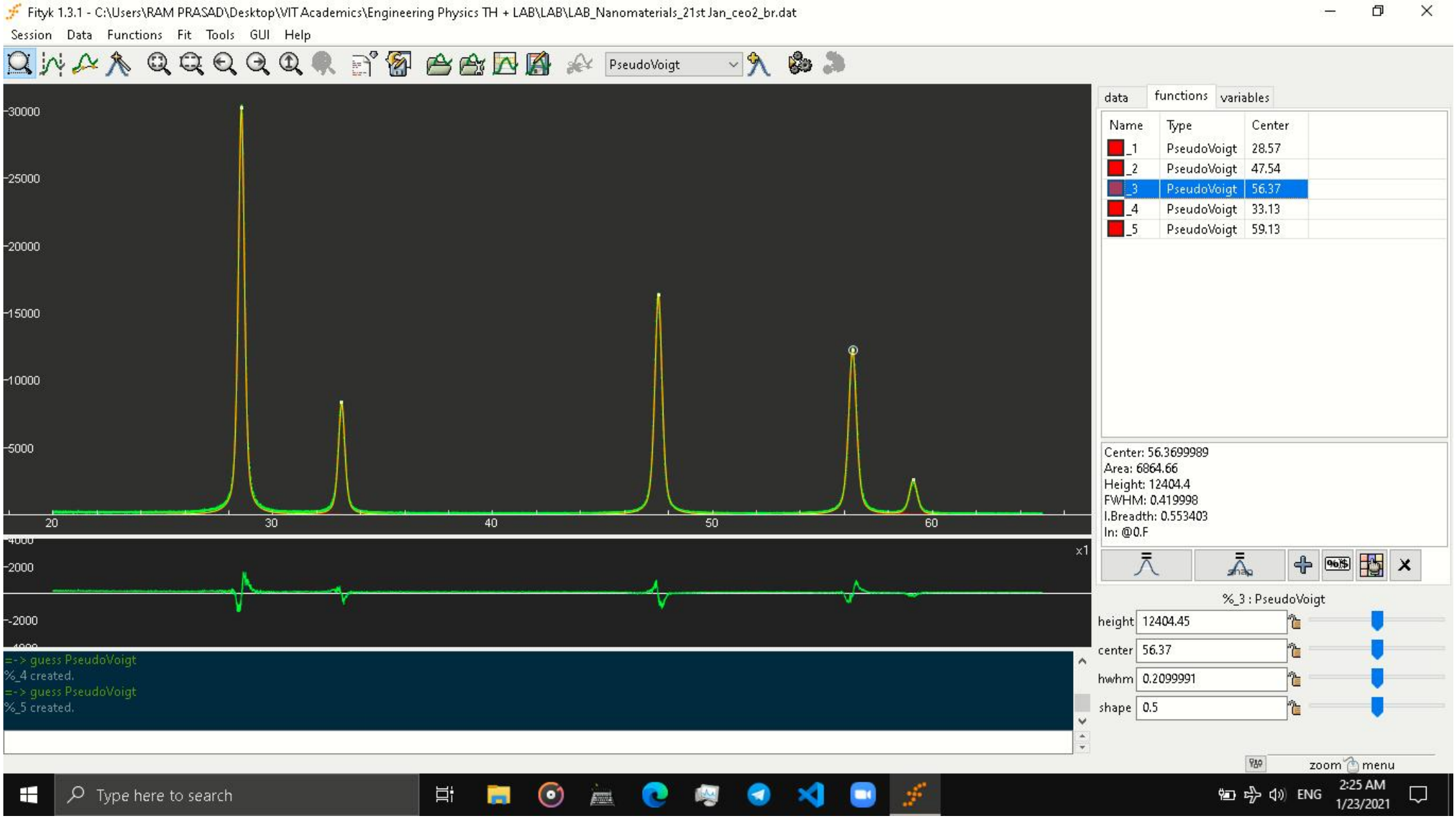
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Session Data Functions Fit Tools GUI Help
PseudoVoigt
30000
25000
20000
15000
10000
5000
20
30
40
50
60
2000
-2000
x1
=-> guess PseudoVoigt
%_4 created.
=-> guess PseudoVoigt
%_5 created.
data
functions
variables
Name Type Center
_1 PseudoVoigt 28.57
_2 PseudoVoigt 47.54
_3 PseudoVoigt 56.37
_4 PseudoVoigt 33.13
_5 PseudoVoigt 59.13
Center: 56.3699989
Area: 6864.66
Height: 12404.4
FWHM: 0.419998
l.Breadth: 0.553403
In: @0.F
%_3 : PseudoVoigt
height 12404.45
center 56.37
hwhm 0.2099991
shape 0.5
zoom menu
Type here to search
ENG
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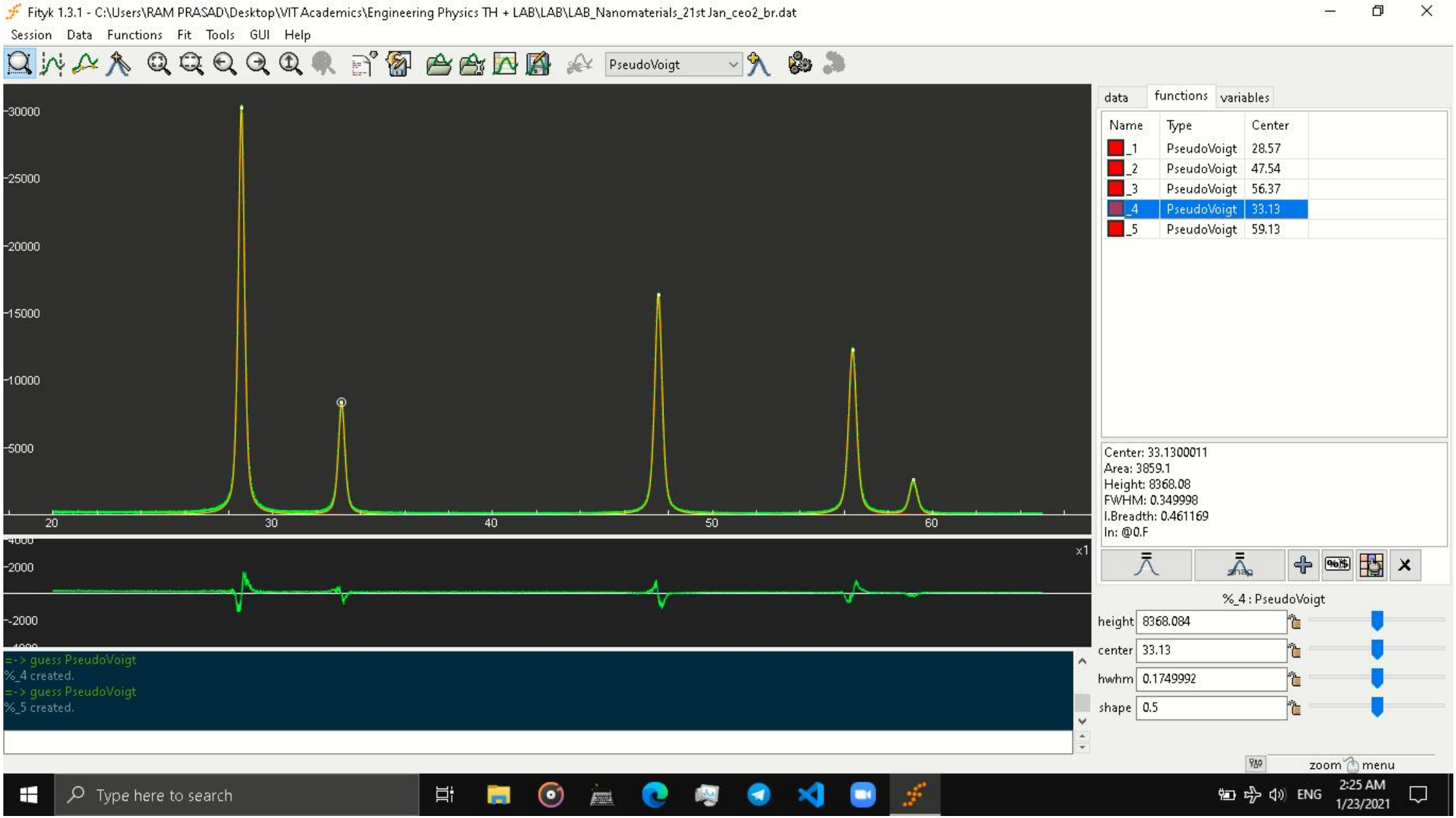
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Session Data Functions Fit Tools GUI Help
PseudoVoigt
data functions variables
Name Type Center
_1 PseudoVoigt 28.57
_2 PseudoVoigt 47.54
_3 PseudoVoigt 56.37
_4 PseudoVoigt 33.13
_5 PseudoVoigt 59.13
Center: 33.1300011
Area: 3859.1
Height: 8368.08
FWHM: 0.349998
I.Breadth: 0.461169
In: @0.F
%_4 : PseudoVoigt
height 8368.084
center 33.13
hwhm 0.1749992
shape 0.5
=-> guess PseudoVoigt
%_4 created.
=-> guess PseudoVoigt
%_5 created.
zoom menu
Type here to search
ENG
2:25 AM
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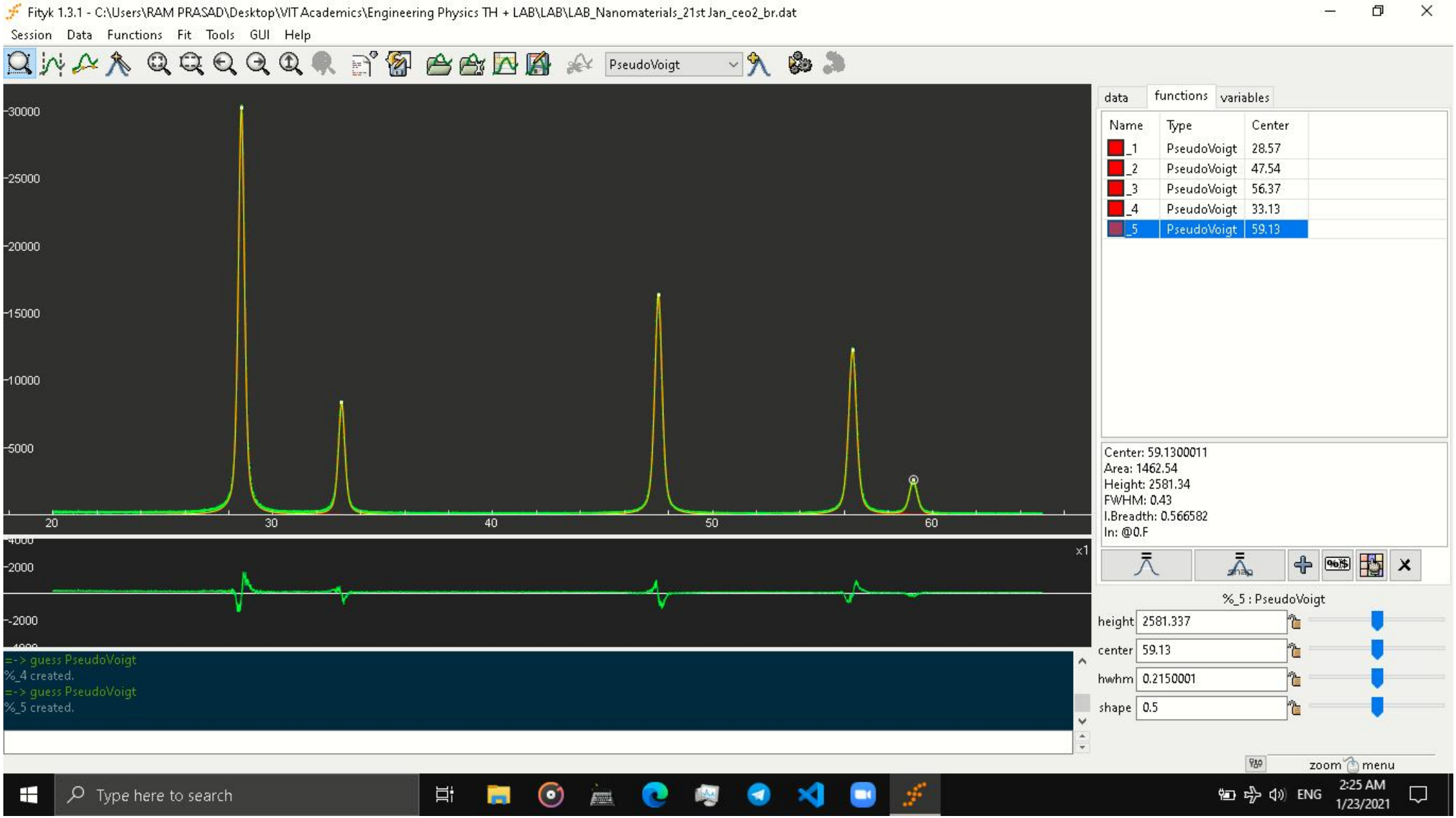
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Session Data Functions Fit Tools GUI Help
PseudoVoigt
30000
25000
20000
15000
10000
5000
20
30
40
50
60
2000
-2000
x1
=-> guess PseudoVoigt
%_4 created.
=-> guess PseudoVoigt
%_5 created.
data functions variables
Name Type Center
_1 PseudoVoigt 28.57
_2 PseudoVoigt 47.54
_3 PseudoVoigt 56.37
_4 PseudoVoigt 33.13
_5 PseudoVoigt 59.13
Center: 59.1300011
Area: 1462.54
Height: 2581.34
FWHM: 0.43
I.Breadth: 0.566582
In: @0.F
%_5 : PseudoVoigt
height 2581.337
center 59.13
hwhm 0.2150001
shape 0.5
zoom menu
Type here to search
ENG
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