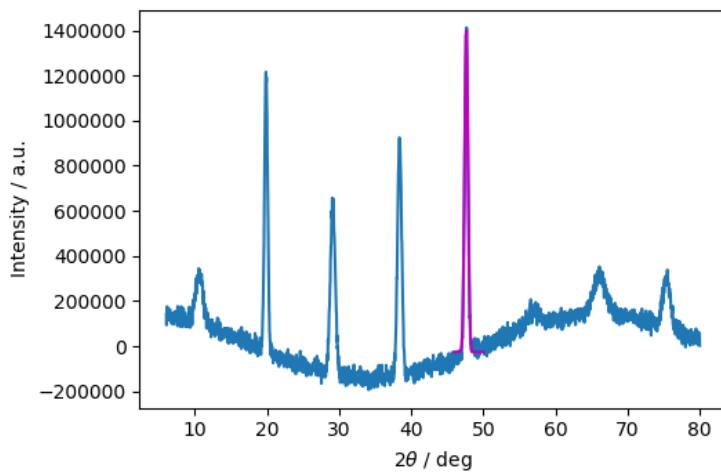


# XRDpy

A module for X-Ray Diffraction (XRD) pattern analysis



– CRYSTALLITE SIZE CALCULATION -  
SCHERRER WIDTH--

...  
...  
...

$FWHM == \sigma * 2 * \sqrt{2 * \ln(2)}$ :

0.40012203511351285 degrees

K (shape factor): 0.9

K-alpha: 0.154 nm

max 2-theta: 19.91162984576907 degrees

Scherrer Width ==  $K\lambda / (FWHM * \cos(\theta))$

**SCHERRER WIDTH: 20.15036943566489 nm**

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## **What is XRDpy**

XRDpy is in layman terms, an XRD pattern plotting program which calculates crystallite size in an easy way. It is currently divided into 2 main scripts, XRDsingle.py and XRD.py, which plot and calculate the Scherrer width for a single XRD and multiple XRD patterns at a time, respectively.

## XRD.py script

### Optional arguments

#### **-h, --help**

Typing `python XRD.py -h` in your command prompt terminal will give you the complete list of arguments you can run to process your XRD pattern [all the ones you see here below] .

#### **-p, --path\_database\_file**

`python XRD.py -p drive\folder\...\folder/database.xlsx`

This specifies the address and file name of your excel database of XRD patterns, where the second column displays the file names of your XRD patterns (which should be changed to .csv extensions) and the first column can be a short name you use to easily call the .csv file [see database\_template.xlsx].

For easy execution, please update the default address to your address with your excel file on the Python script and save it (line 23 XRD.py)

#### **-p2, --path\_files\_folder**

`python XRD.py -p2 drive\folder\...\folder\_with\_XRD\_files/`

This specifies the path of your folder housing all your XRD patterns which should be mentioned in your Excel database.

For easy execution, please update the default address to your address with your excel file on the Python script and save it (line 27 XRD.py)

#### **-d --see\_database**

`python XRD.py -d True`

Boolean which, when set to True, displays every common name of the XRD patterns written in your Excel database. It is defaulted to False; if you ever want to look at the contents of your database before running the plotting script, type the above underlined command.

#### **-ka, --K\_alpha\_wavelength**

#### **-b, --background\_sub**

**-o, --overlaid**

**-x, --overlaid\_split**

**-s, --single**

**-u, --units**

**-r, --Scherrer\_range**

**-K, --shape\_factor\_K**

## How to Run

```

Command Prompt - python XRD.py -o e1 e3 e5 e4 -x 4 -s e1 e2 e5 -r 36.41 -b false
[-1.11565375e-02 -4.02174767e-02 3.12650200e-05 -3.12649047e-08]
[ 9.43826148e+00 4.74638613e+01 -3.12649047e-08 5.85796480e-05]]

FWHM == sigma*2*sqrt(2*ln(2)): -1.6194673674426716 degrees
K (shape factor): 0.9
K-alpha: 0.154 nm
max 2-theta: 38.31428928616077 degrees
Scherrer Width == K*lambda / (FWHM*cos(theta))

SCHERRER WIDTH: -5.19105422144936 nm

e5
---CRYSTALLITE SIZE CALCULATION - SCHERRER WIDTH---
-Gaussian fit results-
y-shift 103011.45014805837
amplitude 233510.1645641375
mean 38.37441789645877
sigma 0.09205306637961484
covariance matrix
[[ 1.01839688e+06 -4.98484696e+05 1.44454157e-10 -1.31006608e-01]
 [-4.98484696e+05 2.49485389e+06 3.09171850e-09 6.55671766e-01]
 [ 1.44454157e-10 3.09171850e-09 4.66392585e-07 -1.44725638e-12]
 [-1.31006608e-01 6.55671766e-01 -1.44725638e-12 4.83245283e-07]]

FWHM == sigma*2*sqrt(2*ln(2)): 0.21676840591728158 degrees
K (shape factor): 0.9
K-alpha: 0.154 nm
max 2-theta: 38.38829853731716 degrees
Scherrer Width == K*lambda / (FWHM*cos(theta))

SCHERRER WIDTH: 38.790852667028425 nm

```

