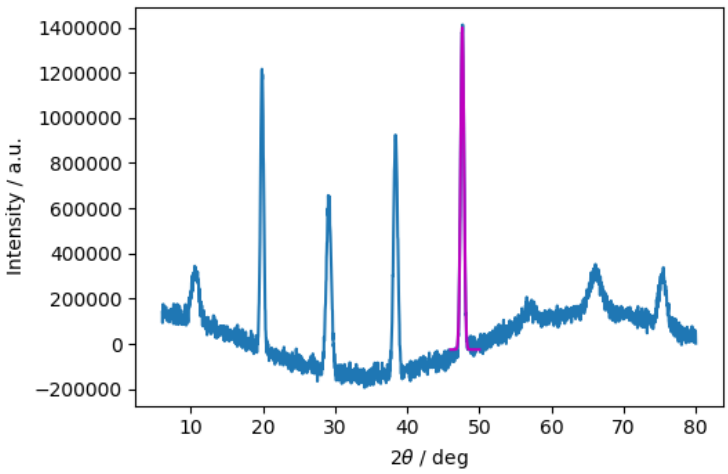
Last Update: Feb 2020

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 == Kƛ / (FWHM*cos(θ))

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 pattterns 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