

gaXRD User Manual

Nguyen Duy Sang Updated: July 2024

ndsang@ctu.edu.vn

Summary

What is GaXRD?	2
Compatibility	4
How do I start using it?	5
Clone the repository	6
Run a simple command in the Terminal	7
Make your database file	8
Run GaXRD Example	9
python main.py	9
Errors and warnings when running the program	11

What is gaXRD?

Github repository: [gaXRD](https://github.com/sangduynguyen/gaXRD) (<https://github.com/sangduynguyen/gaXRD>)
Needed: [Python](https://www.python.org/) (<https://www.python.org/>)

GaXRD is an XRD pattern plotting Python program which estimates the peak parameters of the X-ray diffraction (XRD) glow curves by the genetic algorithm (GA) combined with finding the peak by interacting between the computer mouse and the screen. This program executes through the Terminal ('commandline') and the execution is easy and straightforward.

The script, **python main.py**, calculates the XRD patterns and plots them in a figure, where the order of the plots can be easily customized by the user through the Terminal.

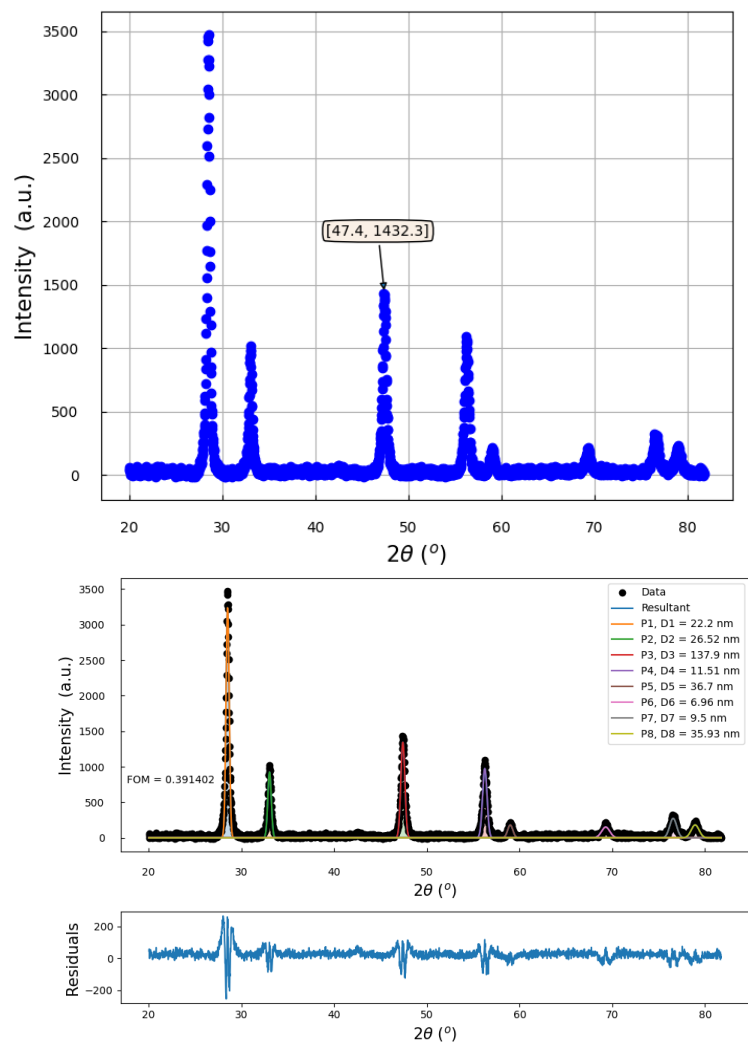


Figure 1: This is the output after running the command: **python main.py** of the XRD1 (file XRD1.csv in Github) spectrum data. Note: This curve is matched to one peak and selected by mouse click.

Compatibility

GaXRD runs on Python, which technically makes it multiplatform. However, I have only tested it in **Windows** operating systems.

How do I start using it?

Taking a pragmatic approach you may find the use of gaXRD to be very straightforward. You're encouraged to watch the instructional video of gaXRD in github (file: **demo.gif**).

Clone the repository

Github repository: [gaXRD](https://github.com/sangduynguyen/gaXRD) (<https://github.com/sangduynguyen/gaXRD>)

Needed: [Git](https://git-scm.com/) (git-scm.com)

Optional: [Github account](https://github.com/) (github.com)

You may need to learn the basics of Git, which aren't complicated to do. Creating a Github account will allow you to fork my repository and share any changes you may make of your forked version(s).

In the main GaXRD Github repository, there should be a button called "Code" or clone. Click on it and copy the HTTP address

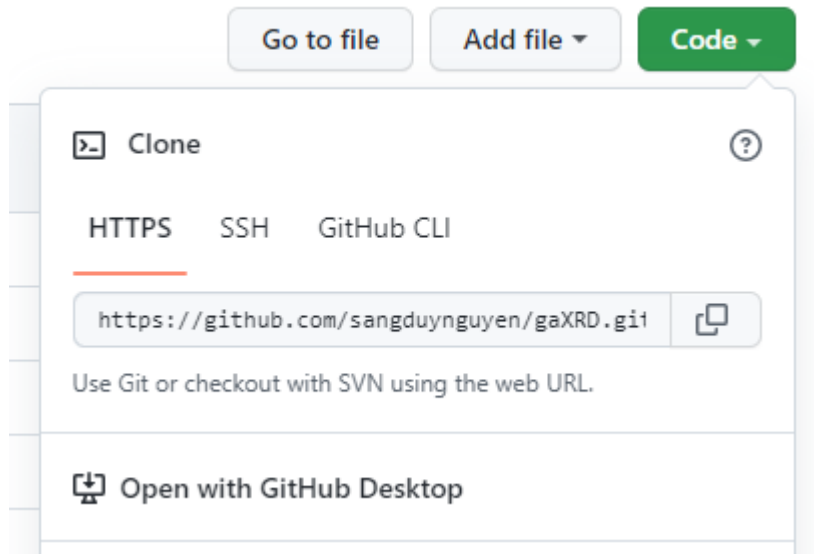


Figure 2: It looks like this

Open your Terminal and select the folder or path where you want to place the gaXRD program (i.e. use `cd` command).

In the Terminal, type: **`git clone [pasted HTTP address]`**

Run a simple command in the Terminal

Open your Terminal (or command line, or shell, whatever you call it)

Change to the folder containing your cloned version of gaXRD (Use the `cd` command to get there)

While in that folder, type: **python main.py**. This should bring up the lists of all the arguments available to customize and make your plot(s).

```
PS C:\Users\Admin\plot\pyGA> python main.py
```

Make your database file

Your database file should contain the names of all your files with their .csv extension (they should be converted or be in csv format).

-

Run GaXRD Example

Type the following commands in your terminal (with the Terminal path set to the GaXRD folder):

python main.py

This will display your database in the Terminal; You will choose the model (i.e. use the numbers 1 2 3 in this example)

```
(base) PS C:\Users\Admin> cd C:\Users\Admin\gaXRD  
(base) PS C:\Users\Admin\gaXRD> python main.py  
Choose task (Baseline:1, XRD:2):
```

Figure 3: This is what you see.

The above command will give you this figure:

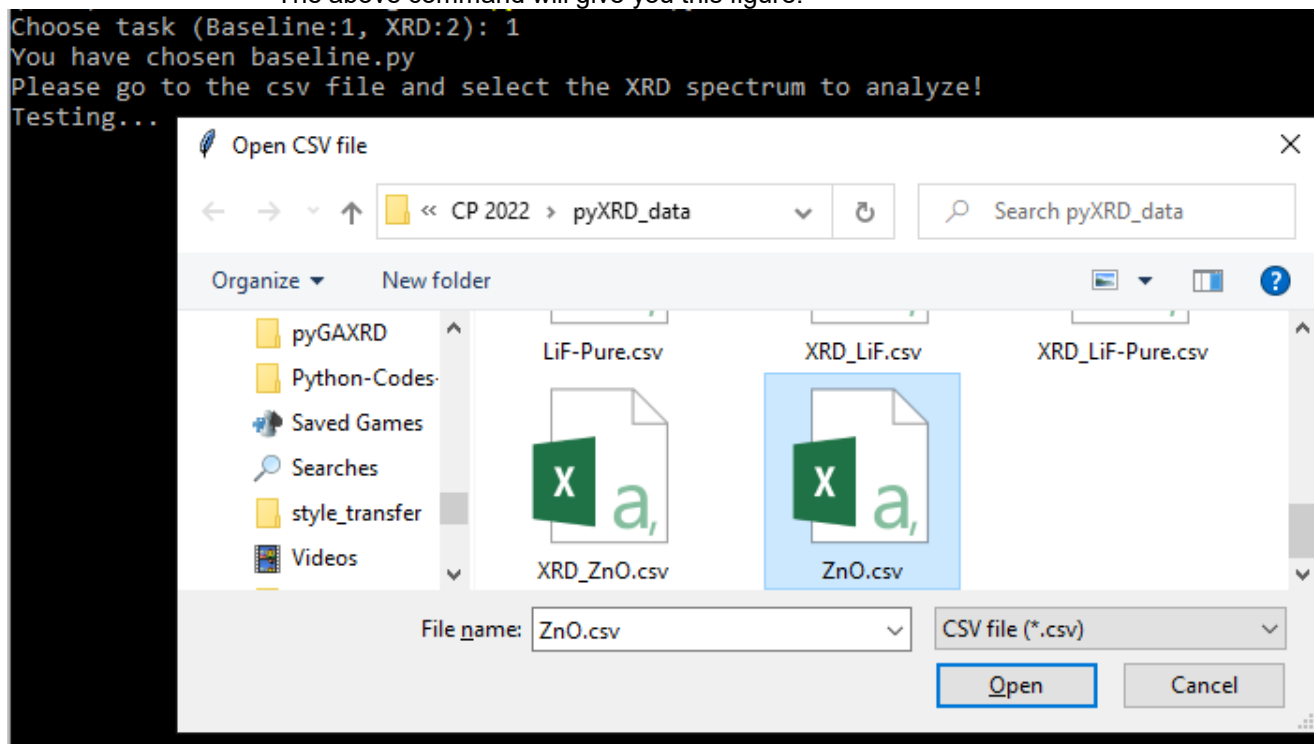


Figure 4: gaXRD Example, Window will open to select csv

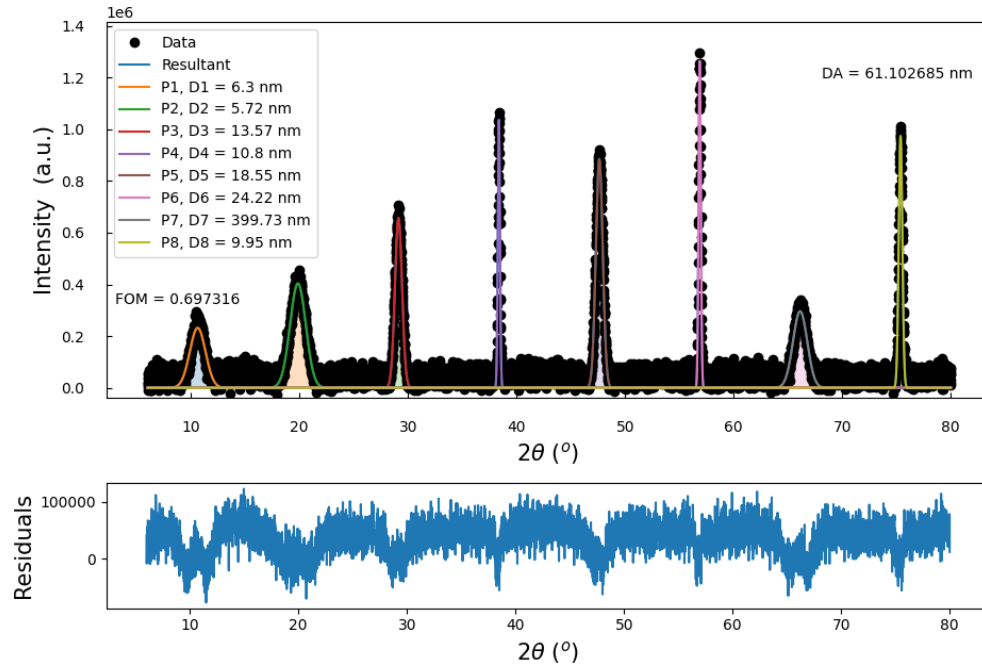


Figure 5: This is the output after running the command: **python main.py** of the XRD (file XRD4.csv in github) XRD data. Note: This curve is matched to 8 peaks and selected by mouse click.

Errors and warnings when running the program

While running the program there may be some warnings in cmd due to the division by zero error. However, if the values are still calculated and the result executes well (small FOM) then the result is acceptable.

If the program does not execute, the user needs to check the steps of this tutorial or review the Demo.gif video.