X-Light User Guide

for Residual Stress evaluation

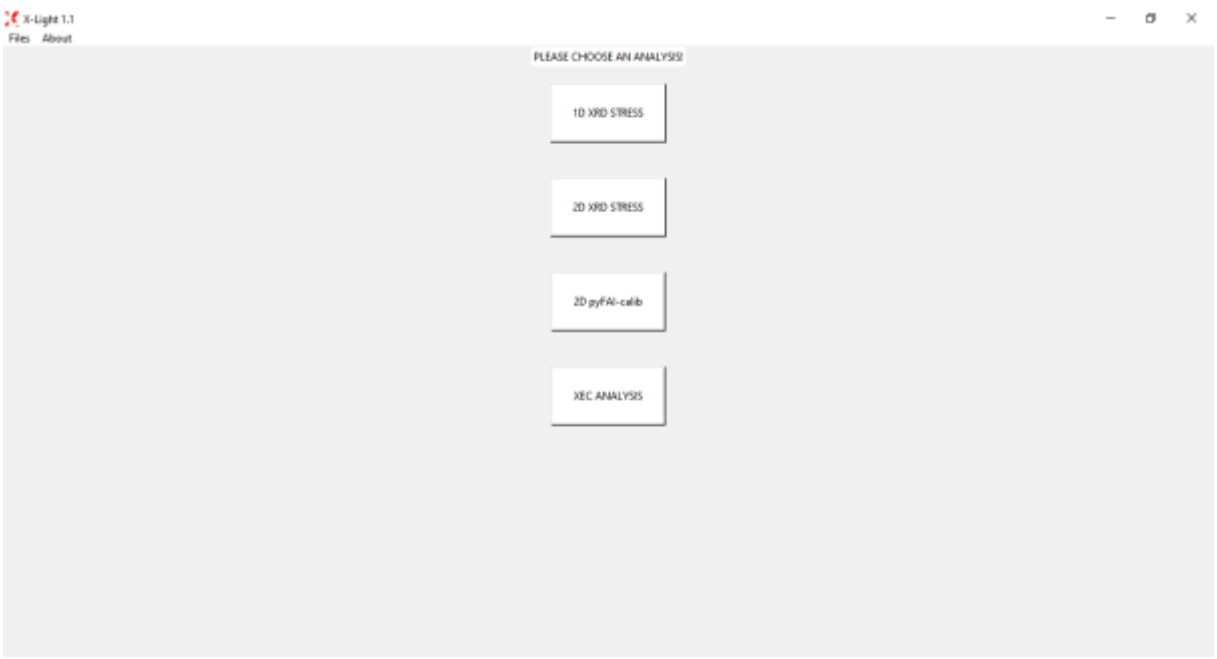
using X-Ray Diffraction data

acquired with a 2D detector

1. INTRODUCTION

X-Light is a software dedicated to the evaluation of residual stresses using X-ray diffraction. The present document gives practical information on the use of X-Light for data acquired with a 2D detector. The calibration of the data is performed using pyFAI module, an open-source python module available on the web.

The evaluation of residual stresses using X-ray diffraction data acquired with a 2D detector requires the calibration of the frames. This step consists in assigning to each pixel of the frame angular values in the (2θ,γ) space, 2θ being the diffraction angle and γ the azimuth angle, corresponding to (ψ,ϕ) values. In the following document, the distinction is made between the calibrant measurement (hereafter named calibrant), and the specimen of interest.

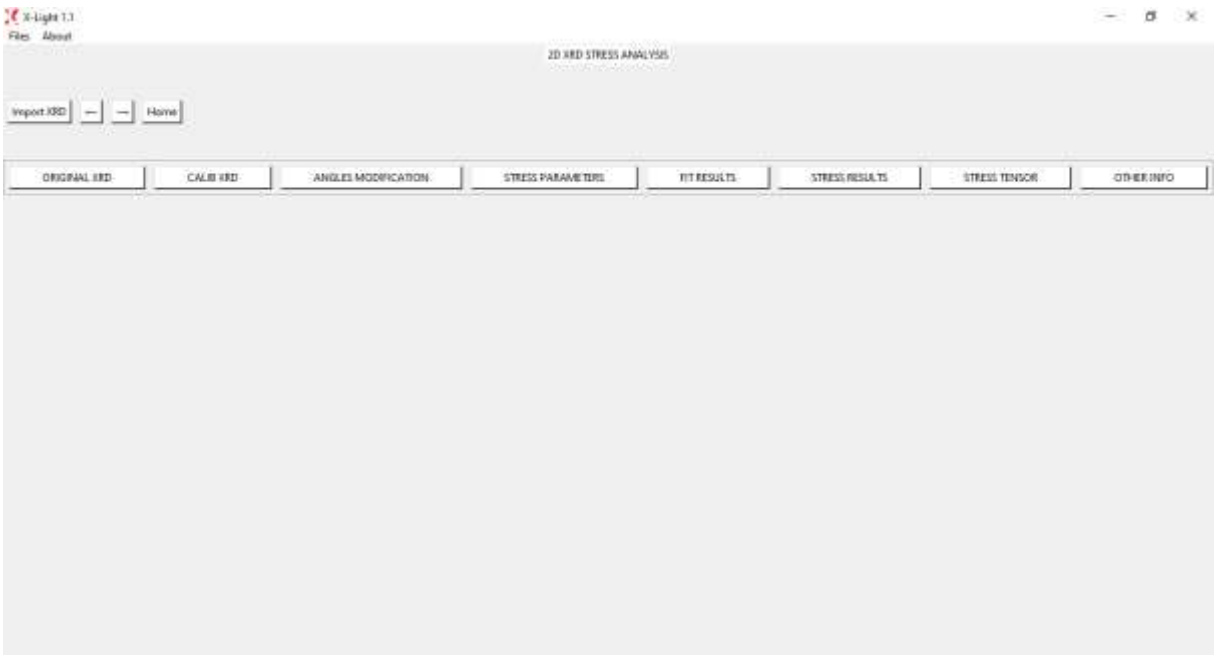


- Project: DECOR 2D
- Language: Python
- License: GPL-v3, open-source
- Link: https://github.com/sangpham171/X-Light
- System: Window, Linux
- Supported formats:
  - 1D: Bruker (raw1.01, raw4.00, uxd), Seifert (nja), Proto (profiles)
  - 2D: Bruker (gfrm), Nexus (nxs), Raw (raw)
    EDF image (edf), TIFF image (tif, tiff),
    NumPy binary (npy), CBF (cbf), MarCCD image (mccd),
    Fit2D mask files (msk)

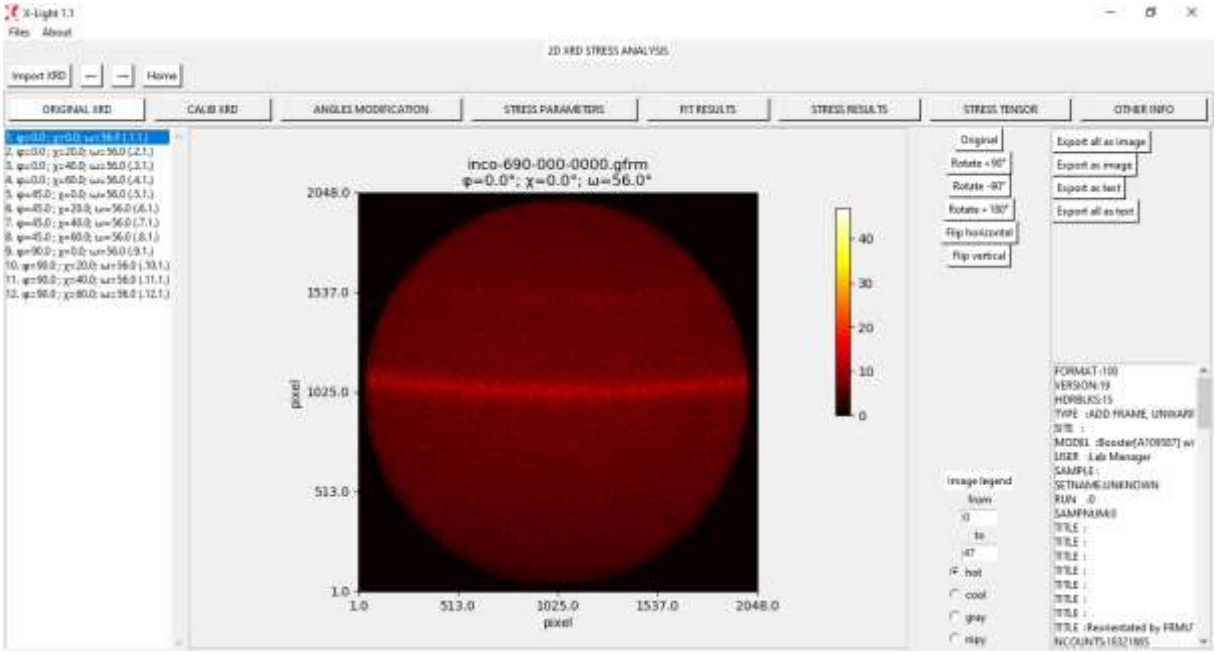
2. 2D XRD STRESS ANALYSIS

File supported: Bruker (gfrm), Nexus (nxs), Raw (raw), EDF image (edf), TIFF image (tif, tiff), NumPy binary (npy), CBF (cbf), MarCCD image (mccd), Fit2D mask files (msk))

Button “Import XRD”: Import the 2D data
Button “Home”: get back to main screen
Button “→”: next panel
Button “←”: previous panel



2.1. “ORIGINAL XRD” panel



The original imported image is presented in the middle with 2 axes in pixel units. The image color can be changed by changing the image legend “from” and “to” and the type of color “hot”, “cool”, “gray”, “nipy”, then click on the list on the left. In order to view the original presentation, delete the entire inserted number, and then click on the list on the left.

The list of files is on the left panel.
The information about each image is showed on the right panel.

Click on the list on the left to show the export buttons. The image can be exported as image or as text. “Export as image” and “Export as text” are used to export the image on screen. “Export all as image” and “Export all as text” are used to export the entire image on the list.

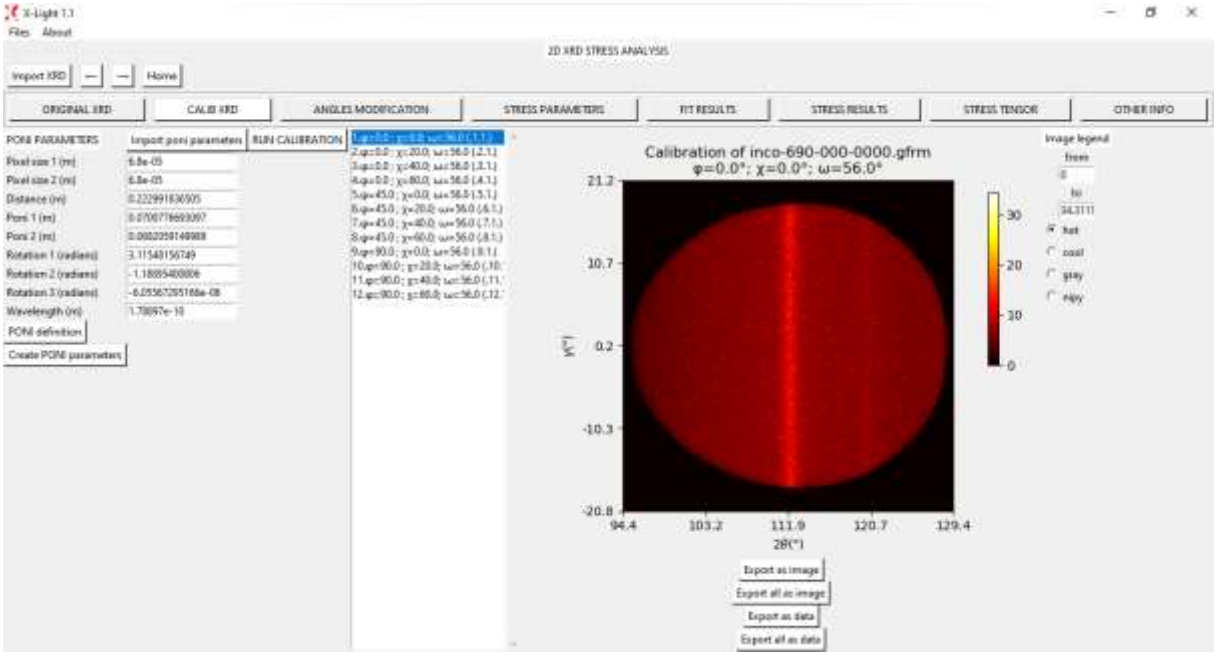
The buttons “original”, “rotate+90”, “rotate-90°”, “rotate+180” are used to rotate the images.
The buttons “flip horizontal”, “flip vertical” are used to flip the images.

2.2. “CALIB XRD” panel

The button “Import poni parameters” is used to import the PONI file. The PONI file contains the calibration parameters after the calibration process with pyFAI module (cf. calibration part). The definition of each parameter will be shown by clicking on “PONI definition”.

The pyFAI graphical user interface can be opened by clicking on “Create PONI parameters”.

After importing the PONI parameters, click “Run calibration” to obtain the calibrated images information.



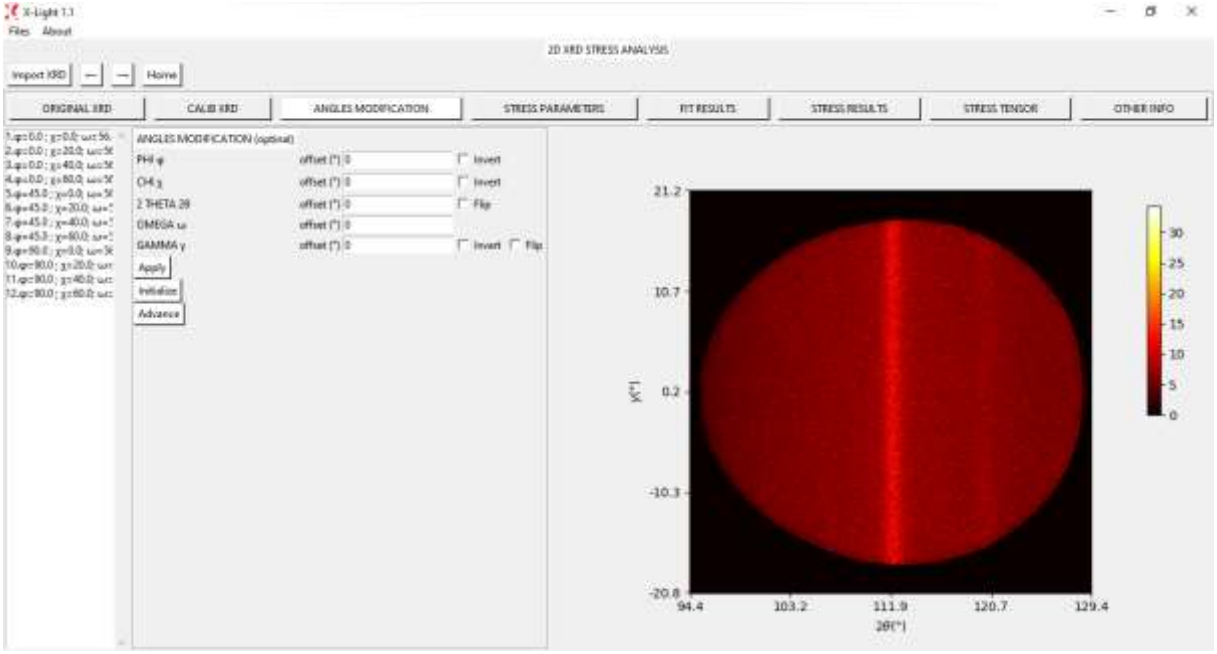
The calibrated image is presented with the angle 2θ(◦) as horizontal axe and γ(◦) as vertical axe. The γ axe is equivalent to the azimuthal axe in pyFAI with a normalized zero in the center. The 2θ axe is equivalent to the 2θ axe obtained by pyFAI.

Note: The images XRD for stress analysis must be in the same goniometer configuration with the calibrant XRD image.

Click on the list of file to show the export buttons. The calibrated images can be exported as image or as text. “Export as image” and “Export as data” are used to export the current image. “Export all as image” and “Export all as data” are used to export the entire image.

The color of image can be changed by changing the image legend and the color type “hot”, “cool”, “gray”, “nippy”.

2.3. “ANGLE MODIFICATION” panel

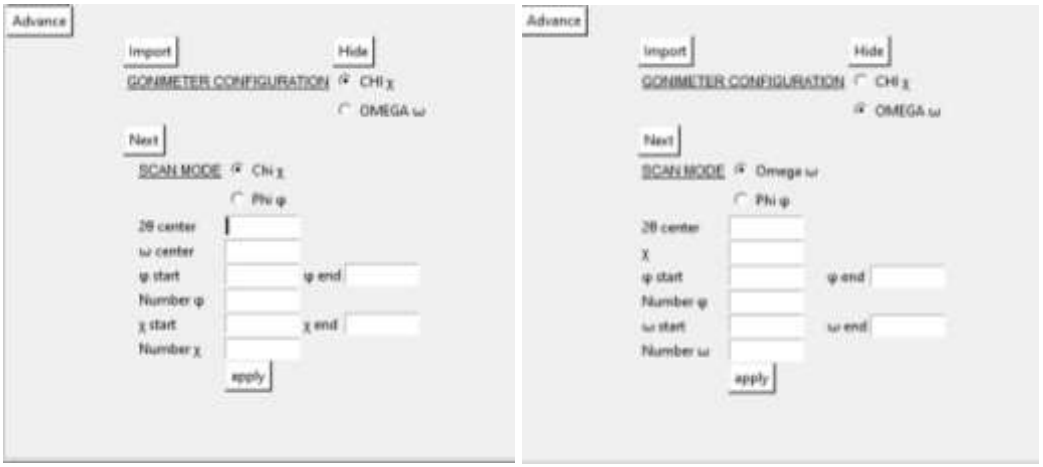


The angle phi, chi, 2theta, omega, gamma can be changed by adjusting an offset or invert or flip the direction by using the button “Apply”.

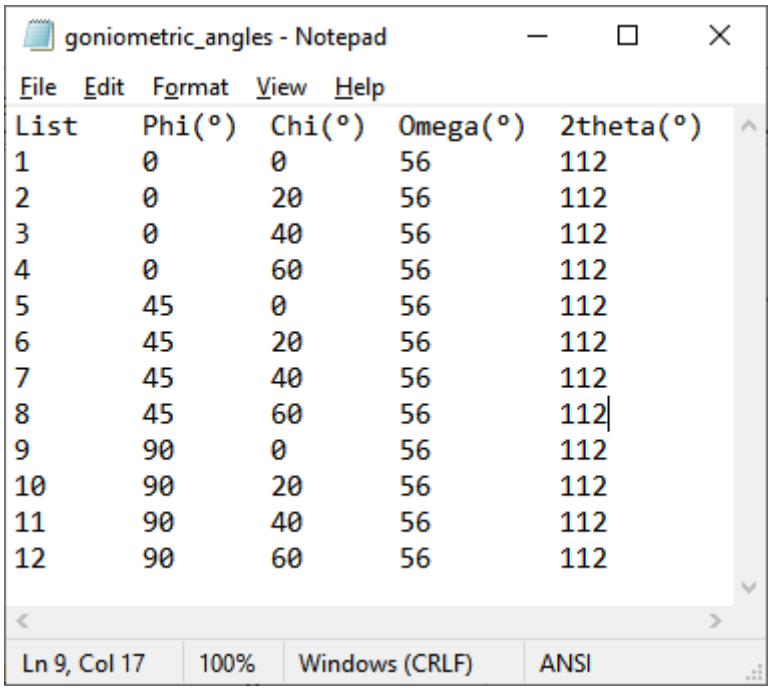
The button “Initialize” is used to reset the original values.

The “Advance” button gives more option to change the value by recreating the goniometer configuration. This option is useful when the images don't contain the angles information. In this case, the user must recreate the entire goniometer angles.

Click on the “Advance” , then “Next” button to show the following panel

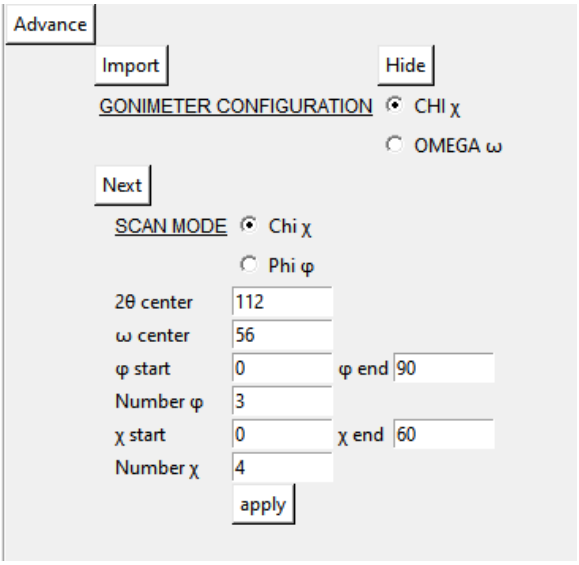


The button “Import” is used to import the goniometer angle in a specific format “.gma” as following. You can find an example of this format in \\example_template\goniometric_angles.gma. The following example file value gives the same angles in the below screen shot images.



Otherwise, user can recreate the angle for goniometer configuration “chi” or “omega”.

- In “chi” mode, the angles “omega” and “2theta” are fixed. Two scan modes are proposed: “chi” or “phi” scan mode. With “chi” scan mode, the values will start changing the “chi” value then “phi” value. And with “phi” scan mode, the values will start changing the “phi” value then “chi” value. For example, the following setup will give the same angles in the below screen shot images.



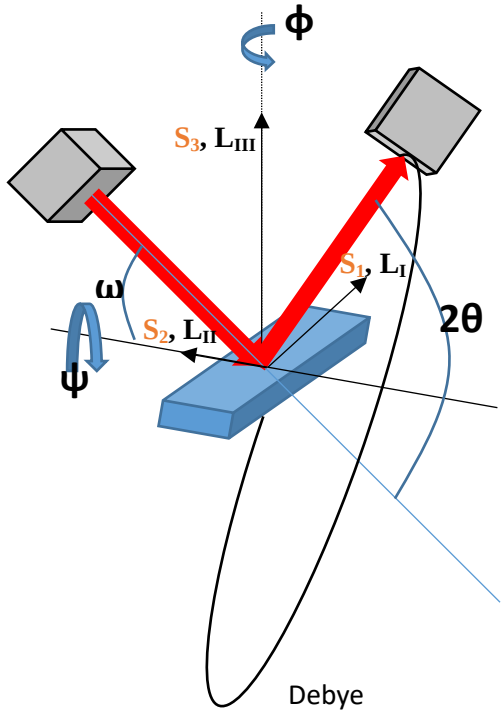
- In “Omega” mode the angles “chi” and “2theta” are fixed. Two scan modes are proposed: “omega” or “phi” scan mode. With “omega” scan mode, the values will start changing the “omega” value then “phi” value. And with “phi” scan mode, the values will start changing the “phi” value then “omega” value.

Click on “apply” to recreate the goniometer angles.

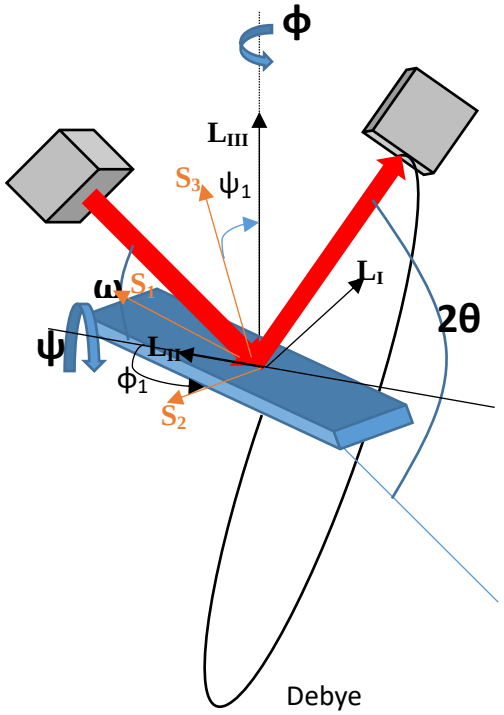
X-Light is designed for a specific reference angle, so please verify if your goniometer configuration is the same as follow.

Note: L is the laboratory system's coordinates; S is the sample's coordinates.

At ϕ=0, ψ=0

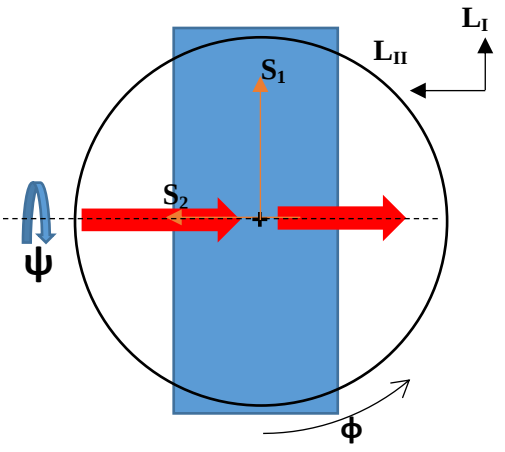


At ϕ=ϕ1, ψ=ψ1

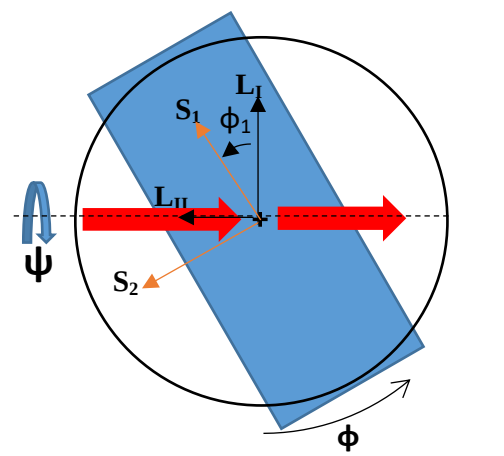


Look from the top:

At ϕ=0, ψ=0

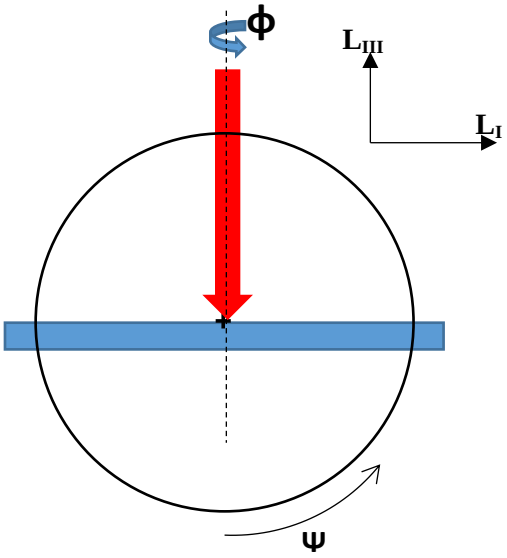


At ϕ=ϕ1, ψ=0

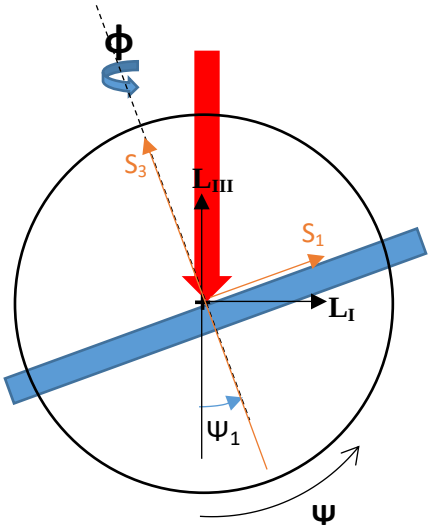


Look from the left:

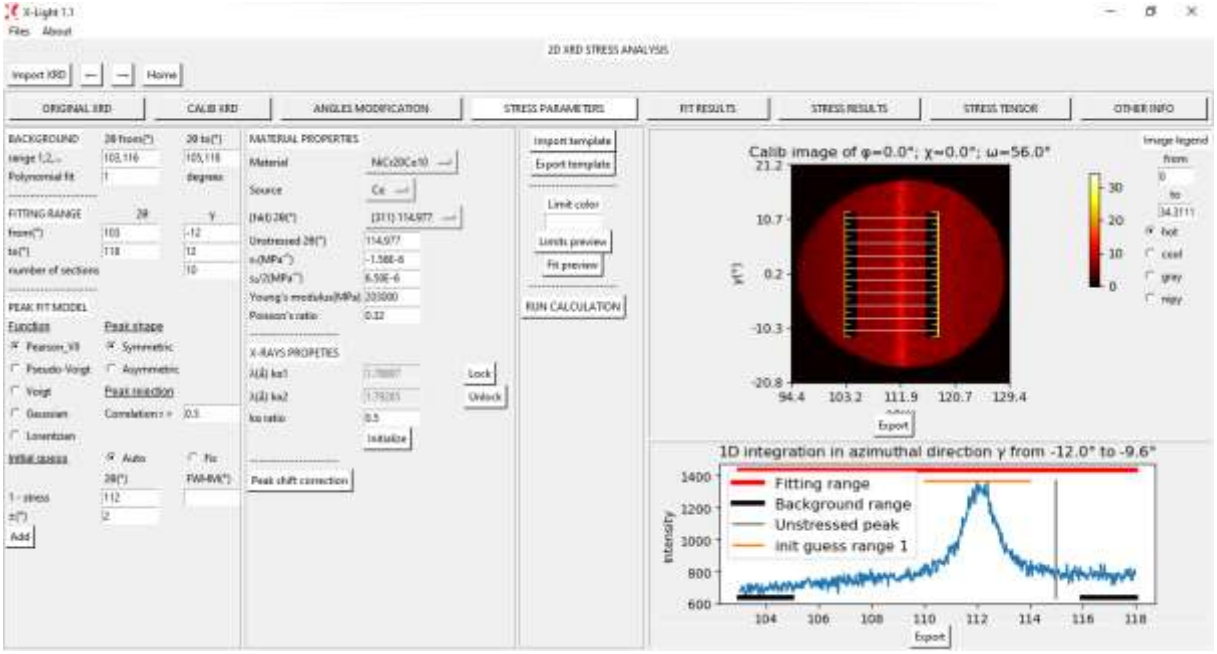
At ϕ=0, ψ=0



At ϕ=0, ψ=ψ1



2.4. “STRESS PARAMETERS” panel



The background can be chosen by multi range. For example, user wants to select the range [a1; b1], [a2; b2]…. The values a1, a2… will be put in the entry “2θ from” and the values b1, b2 … will be put in the entry “2θ to”. All the values must be separated by “,”. In the below example screen shot, the background is limited by [103,105] and [116,118]. The user can also define the degree of the polynomial fit function for the background.

The Fitting range is defined by the angle 2θ and γ. X-Light use caking method to cut the image in different area. Each area will be then transformed to 1D signal by integration method. The number of area will be defined by “number of sections”. The peak fitting will be performed on the 1D intensity signal.

X-Light give 5 peak fitting model Pearson VII, Pseudo-Voigt, Voigt, Gaussian, Lorentzian with 2 types peak shapes “symmetric” and “asymmetric”.

The “peak rejection” is used to eliminate the entire peak fitting which give a correlation coefficient r below a user defined value. By default, the correlation r is set at 0.5. This coefficient can be varying from 0 to 1.

The “initial guess” is an useful option when the signal has two peaks close to each other. By default, the “initial guess” is detected automatically by the algorithm. If the peak fitting with automatic initial guess doesn’t function well enough, user can define the initial guess manually by changing to “fix” mode. User can define the position and the full width at half maximum of the initial guess. A good define of the initial guess will give more precise solution and faster the calculation.

By default, X-Light considers the signal has only one peak. User can also define more than one peak by click on “Add”. In the case of multi peak, the “initial guess” is recommend switch to “fix” mode, then manually predefine the position of each peak. The first peak is used to calculate the residual stress.

The material information can be chosen in the database, or insert manually. 3 values obligated (unstressed peak 2θ, s1, s2/2) or (unstressed peak 2θ, E, v). X-Light use the values that are visible on screen.

The material database and the X-ray source database can be changed by changing the file \\read_file\mat_database.mdb, and x_ray_source.xrs. The file format must be respected.

The X-ray properties can be also modified by clicking on "unlock" button. Three values can be changed is kα1, kα2 and kα ratio. The "Initialize" button is used to reset to the original value

Note: the X-ray source in "Material properties" is defined in "x_ray_source.xrs". This information is only used to calculate the material properties from one source to others. Meanwhile, the X-ray source in "X-ray properties" is used to do the peak fitting.

The "peak shift correction" button is an option which is built to correct the goniometer configuration. Click on "peak shift correction" to import the correction file (cf OTHER INFO panel). The correction file has a specific format that will be explained in OTHER INFO panel.

All the parameters can be exported in a template format by clicking on "Export template". The file format is ".spt'' that user can see an example in \\example_template\ stress_para_template.spt

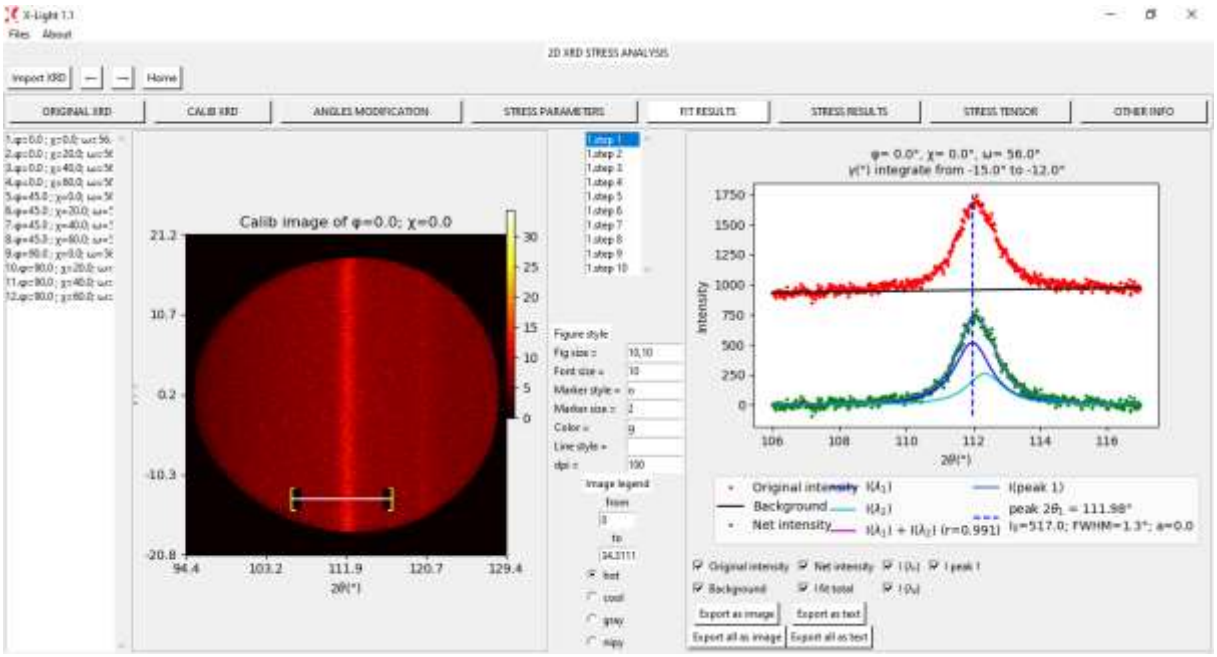
The parameter template can be imported by the button "Import template"

The button "Limits preview" is used to visualize all the parameter on the image. An integration 1D can be also preview

The button "Fit preview" is used to visualize the peak fitting with the user defined parameter. This option is recommend before running the entire process in order to verify the stress parameter.

The "RUN CALCULATION" is used to do the peak fitting and the stress calculation. The results will be show in the next panel.

2.5. “FIT RESULTS” panel



The list of file is showed on the left. The list of section is showed in the middle list “step 1”, “step 2” ….

The image calibrated is showed on the left next to the list of file. By clicking on the list of file, the export buttons will be showed

By clicking on the list of step, the peak fitting result will be showed on the right. The position of the integration area will be showed on the image. The peak fitting result has the following information: original intensity in function of 2θ, background fitting, the net intensity after excluding the background, the intensity with kα1, the intensity with kα2, the peak position, the FWHM, the intensity max and the coefficient a which define the shape of the peak (a=0 means symmetric peak). The correlation coefficient r is used to exclude the peak if r is inferior to the “peak rejection” value.

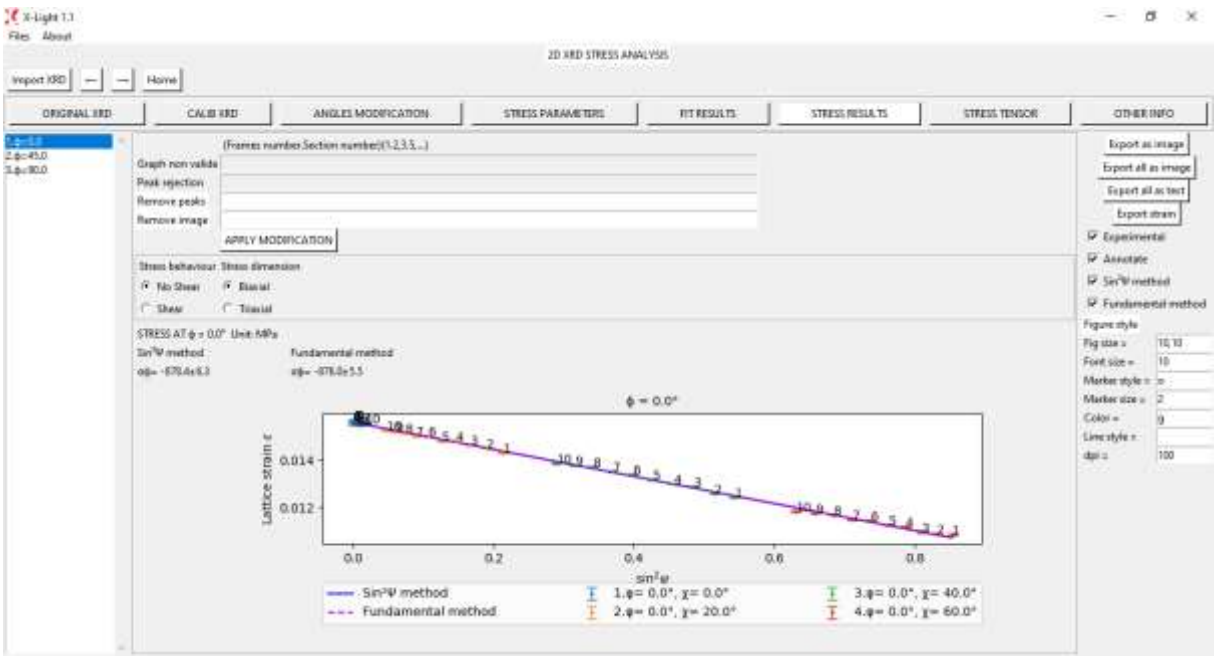
Each figure can be selected to show or hidden by ticking on the case box.

The peak fitting result can be export as image or as text by clicking on buttons “Export as image”, “Export as text”, “Export all as image”, “Export all as text”

The style of peak fitting figure can be modified by different parameters: figure size, font size, marker style, marker size, color, line style, dpi. For the use of these parameters, please refer to matplotlib package document.

The image color can be also modified by changing the image legend and the type of color

2.6. “STRESS RESULTS” panel



X-Light uses the $\sin^2\psi$ method (Müller & Macherauch, 1961) and the fundamental method (*Baoping & Kingsley, 1997)* to determine the residual stress. User can compare the result of these two methods.

Depend on the shape of the curve lattice strain in function of $\sin^2\psi$, user can choose to show the stress behaviour with or without shear. The stress dimension “biaxial” or “triaxial” depend on how many angle “phi”. The “triaxial” is not recommend if there are less than 3 angle phi.

The “graph non valide” show the 1D intensity figures on which the algorithm cannot do the peak fitting. User can review these figures in “Fit results” panel. The reason is usually the figure has a bad original intensity. The residual stress calculation will not use these figures.

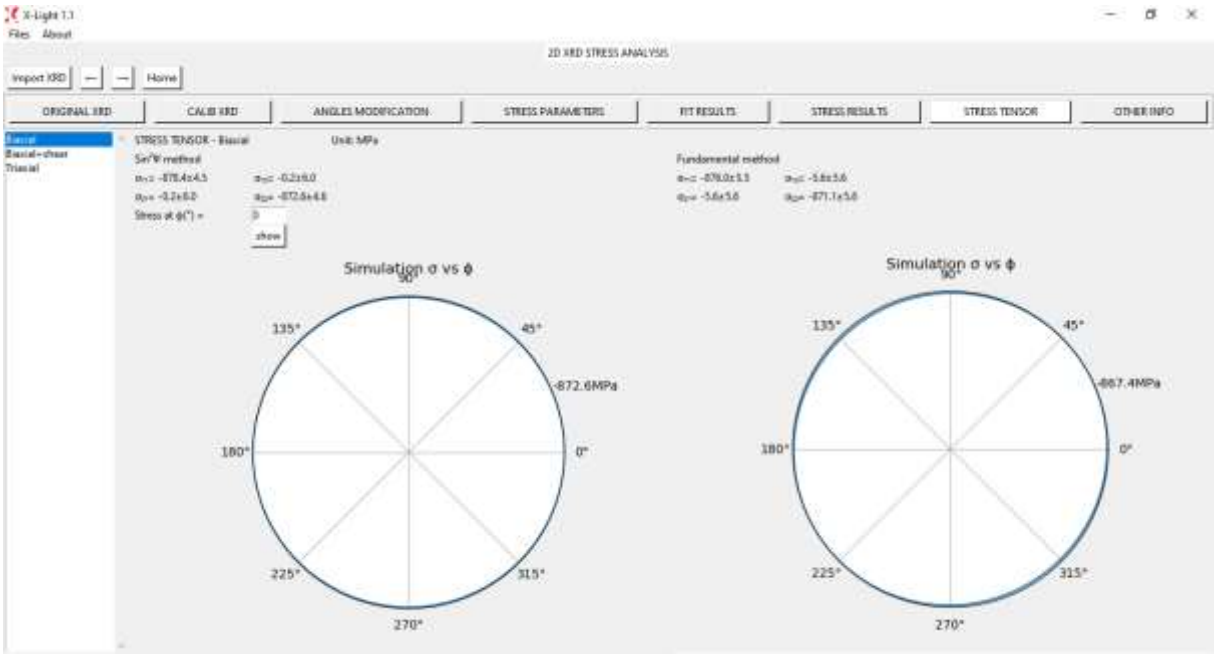
The “peak rejection” show the figures that the correlation coefficient r is inferior the “peak rejection” value in stress parameter. The residual stress calculation will not use these figures.

User can also delete any peak or any image by insert in the entry “Remove peak” and “remove image”. For example, user wants to delete the peak number 2 of image 3 and the peak number 1 of image 4, user will insert in “remove peak” the following text: 3.2, 4.1. Two peak must be separate by “,”. If user wants to remove image 1 and 4, user will insert in “remove image”: 1, 4. Then click on “Apply modification”.

The stress results figure can be exported as image and as text by clicking on export buttons. User can also choose which information will be showed on the figure by ticking on the case box “experimental”, “annotate”, “$\sin^2\psi$ method”, “fundamental method”

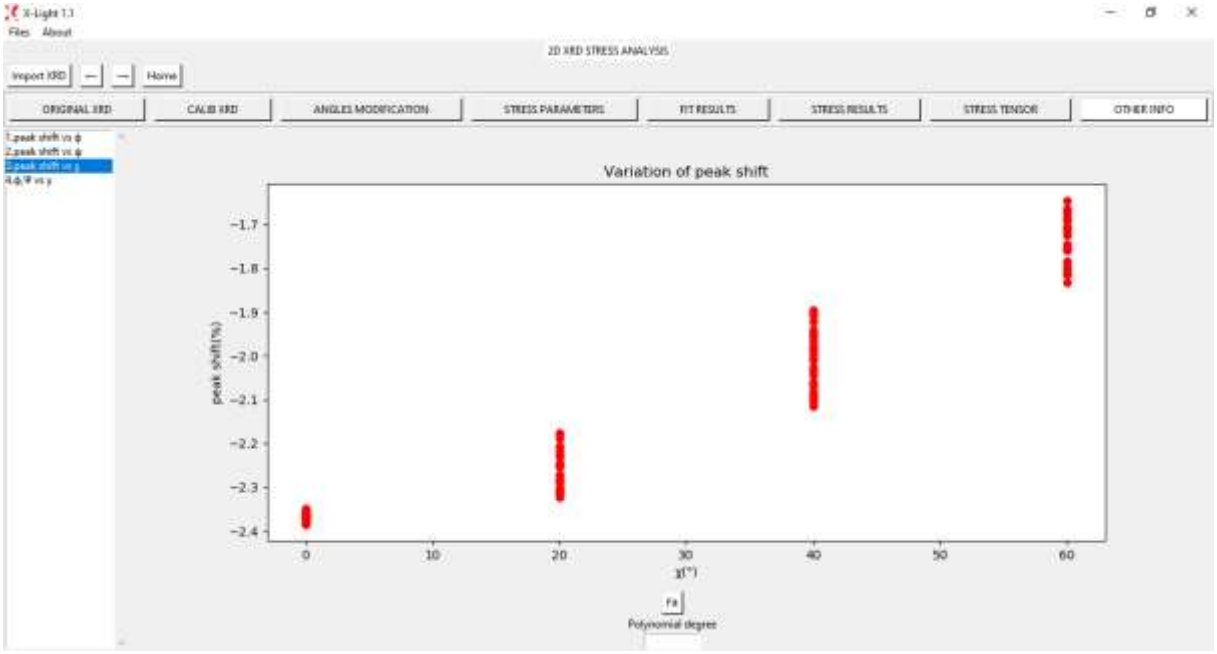
To use the “figure style”, please refer to matplotlib document

2.7. STRESS TENSOR panel



The stress tensor panel will show the component stress σij. The stress value at specific ϕ can be estimated by entering the value of ϕ and click “show”.

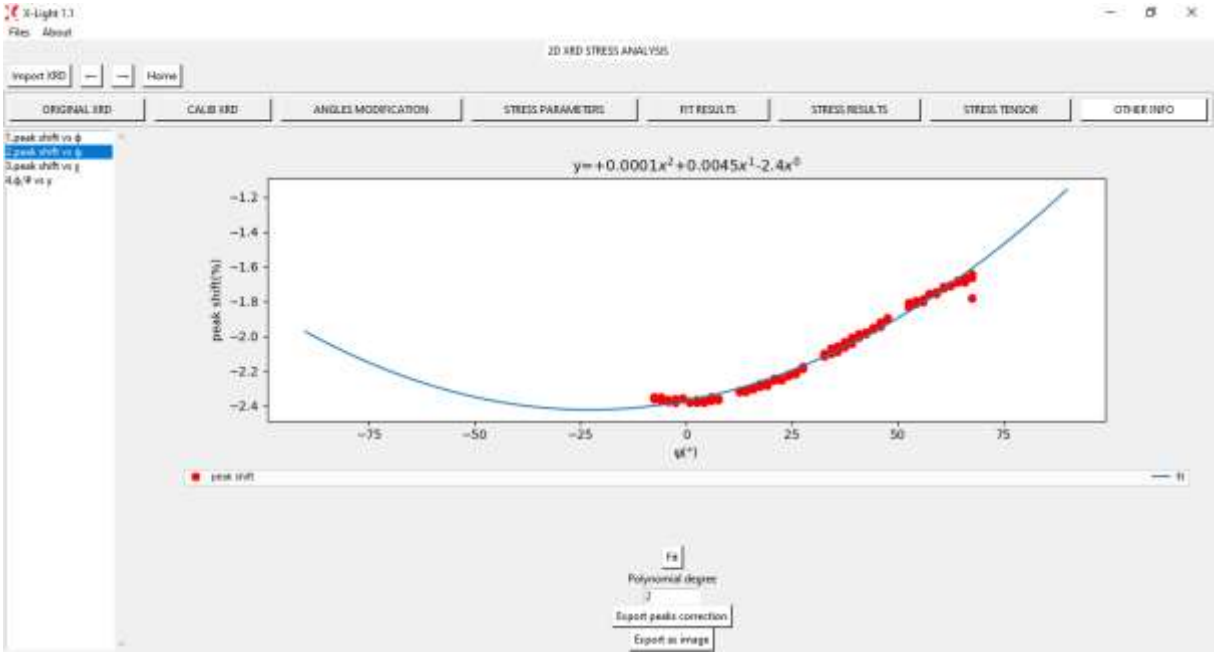
2.8. OTHER INFO panel



This panel shows the peak shift in function of angle phi ϕ, psi χ, chi ψ, and the angle phi ϕ, chi ψ in function of gamma γ.

In order to use the “peak shift correction” in stress parameter, user will define a polynomial function to fit the curve of peak shift in function ψ or χ. Then export the coefficient of the polynomial function in a specific file format (.psc). These coefficients can be then imported in “stress parameter” panel by using the “peak shift correction” button. This correction is recommended being done with a no stress sample. The idea is that the peak-shift variation must be constant with a no stress sample. If it is not the case, the polynomial function can be used to determine the peak-shift correction.

User can find the format of the peak shift correction in \\example_template\ peak_shift_correction.psc



3. 2D XRD CALIBRATION PROCESS

This calibration step is performed through the measurement of a standard stress-free specimen (e.g. LaB6 powder, Si powder, TiC powder…) in the exactly same experimental conditions than those used for the residual stress evaluation in the specimen of interest. The points to be checked should be :

- X-ray wavelength
- X-ray incidence angle
- Detector position

The data corresponding to the calibrant correspond to a single frame acquired at (ψ,ϕ)=(0°,0°). Optionally, correction parameters can be determined by measuring this calibrant for different values of (ψ,ϕ) (same values than those used for the specimen measurements), assuming that the calibrant sample can be tilted. The procedure for the evaluation of correction parameters using X-Light is described in OTHER INFO panel.

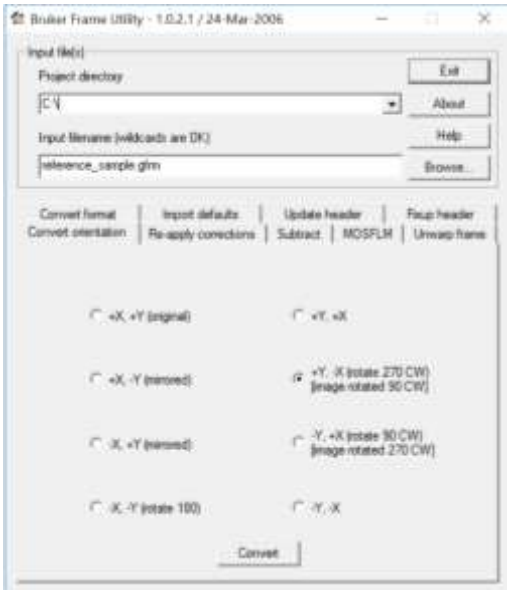
3.1. File format considerations

The calibration is done using the pyFAI module of Python. The pyFAI module only accepts frames with a .tif format. For Bruker detectors, the gfrm file format can be converted to tif using FrmUtility.exe.

The frame orientation might also be an issue. As an example, the 2D frames obtained using a VANTEC-500 detector show vertical diffraction lines. The direct use of this frame in pyFAI leads to improper calibration of the frame. Here again, the orientation of the frame can be modified using FrmUtility.exe. In the case of VANTEC-500, the rotation to be performed is 90° clockwise (-Y, +X). The only way to check that the calibrant frame orientation is fine is to go through the calibration procedure in pyFAI.

Main steps to perform:

Use "FrmUtility" to change the orientation of the reference sample image. Make a copy of the image, because "FrmUtility" will erase the original image.



- Then convert the new ".gfrm" file in ".tif" format

At this point, it is important to keep in mind that in X-Light, the frames corresponding to the measurement of the specimen must have the same orientation as the frame of the calibrant. If a rotation of the frame was performed to the calibrant, it should be applied to the frames from the specimen of interest. FrmUtility accepts wildcards. For example: The name of the file is "poudreTiC-311-000-0000". By putting "poudreTiC-311-00*-000*", the program will apply the action for all other images which have the same name format. There is no need to convert the specimen data in tif format, as X-Light handles .gfrm format.

Summary:

- Calibrant data must be in tif format and in the correct orientation

- Specimen data must have the same orientation as calibrant data. Gfrm format is fine

- You can use FrmUtility.exe to convert X-ray frames

3.2. pyFAI module installation (Windows environment)

The following steps must be performed with administrator rights. Make sure that no other Python distribution is present on your computer. If it is the case, uninstall all Python versions.

1. Install Python 3.7 using Anaconda distribution corresponding to your computer (https://www.anaconda.com/distribution/)

2. During setup, check « Add ANACONDA to my PATH environment variable » and « Register ANACONDA as my default Python3.7 »

3. After setup, run « Anaconda prompt » (admin rights)

4. Install pyFAI typing the following command

   pip install numpy scipy matplotlib fabio silx h5py PyQt5 pyFAI --upgrade

You can check that the installation is correct by typing in Anaconda Prompt : pyFAI-calib –h

3.3. Calibration with pyFAI module

Calibration with pyFAI module (and more particularly pyFAI-calib) produces a .poni file. PONI stands for Point Of Normal Incidence. This poni file is used as in input in X-Light to calibrate all the data from the specimen of interest.

The calibration procedure is based on the manual indexation of the diffraction rings of the calibrant. The user must provide the following informations to the program:

- Calibration frame (experimental data)
- Wavelength of the X-rays (in angströms)
- The pixel size of the detector (in µm)
- A text file (with extension .d) containing the interplanar distances of the calibrant, in decreasing order). As an example, here is the .d file for LaB6 calibrant

For the calibration to proceed correctly, it is mandatory to have identified most of the diffraction rings visible on the calibrant frame, i.e. to have assigned to each ring a d value.

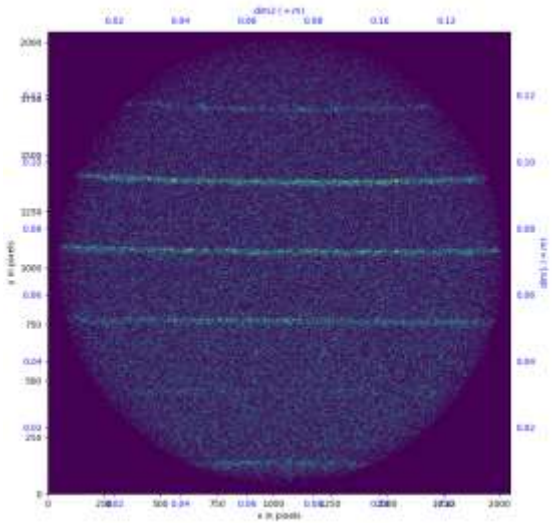
The following procedure shows how to get the poni file.

Step 1: Open anaconda prompt (admin rights)

Step 2: Type the following command

pyFAI-calib –w 1.78897 –c C:\reference_D_spacing.D -p 68 C:\reference_sample.tif

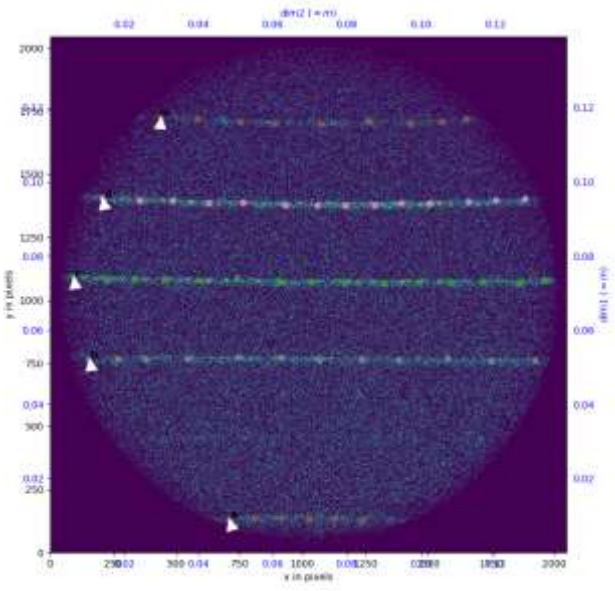
-w : wavelength of X-ray beam in angstrom (In this example, the wavelength is Cobalt -> 1.78897 angstrom)
-p: pixel size in micron (In this example, the size of detector pixel is 68µm)
-c : location of the file containing d-spacing corresponds to the Debye rings of the reference sample



Step 3 : Identify all the rings on the reference sample image. At least 5 points for each ring.

* Right-click (click+n): try an auto find for a ring
* Right-click + Ctrl (click+b): create new group with one point
* Right-click + Shift (click+v): add one point to current group
* Right-click + m (click+m): find more points for current group
* Center-click or (click+d): erase current group
* Center-click + 1 or (click+1): erase closest point from current group

For example: In this image, there are actually 6 rings, but one is very difficult to identify. You can ignore this ring.
Once all the ring are identified. Press Enter



Step 4 : identify the number of the ring, which corresponds to your reference_D_spacing.D. In the file reference_D_spacing.D, the first D_spacing is the ring number 0.

How can identify the number of the ring?

For example: This is the list of all the rings of the calibrant sample (LaB6)

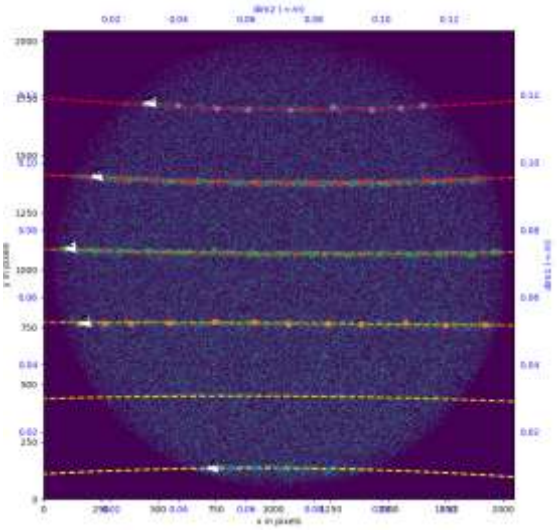
No.	h	k	l	d [A]	2Theta[deg]	I [%]
0	1	0	0	4,15000	24,894	60,0
1	1	1	0	2,94000	35,426	100,0
2	1	1	1	2,39600	43,842	50,0
3	2	0	0	2,07800	50,993	20,0
4	2	1	0	1,86000	57,489	45,0
5	2	1	1	1,69600	63,661	25,0
6	2	2	0	1,47000	74,961	10,0
7	3	0	0	1,38500	80,457	20,0
8	3	1	0	1,31300	85,883	16,0
9	3	1	1	1,25200	91,195	10,0
10	2	2	2	1,19800	96,602	4,0
11	3	2	0	1,15300	101,753	8,0
12	3	2	1	1,10900	107,524	12,0
13	4	0	0	1,03800	119,025	4,0
14	4	1	0	1,00700	125,313	12,0
15	3	3	0	0,97900	132,036	12,0
16	3	3	1	0,95300	139,635	6,0
17	4	2	0	0,92900	148,666	8,0
18	4	2	1	0,90600	161,711	14,0

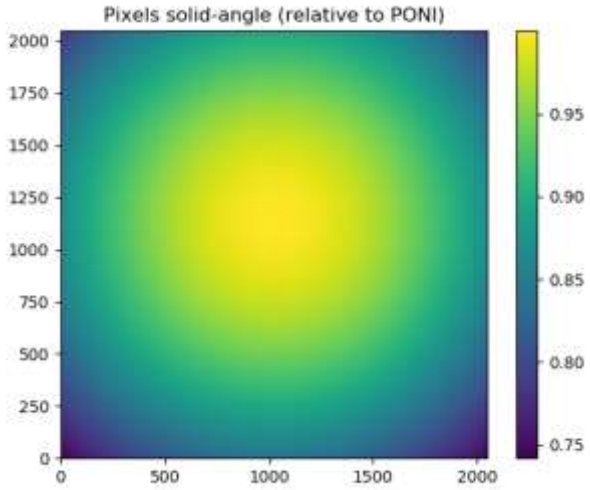
In this case, the middle of the sample is 87°, so the peak number 8 will be in the middle (group c)

On the left of the ring number 8, there are 3 rings and one rings has a very small intensity. If we look at the list, the ring with small intensity must be the ring number 10. With the knowledge of 2 rings in one image, we can identify the number of others ring.

Group a will be peak number 6, group b – peak 7, group d- peak 9 and group e- will be peak 11

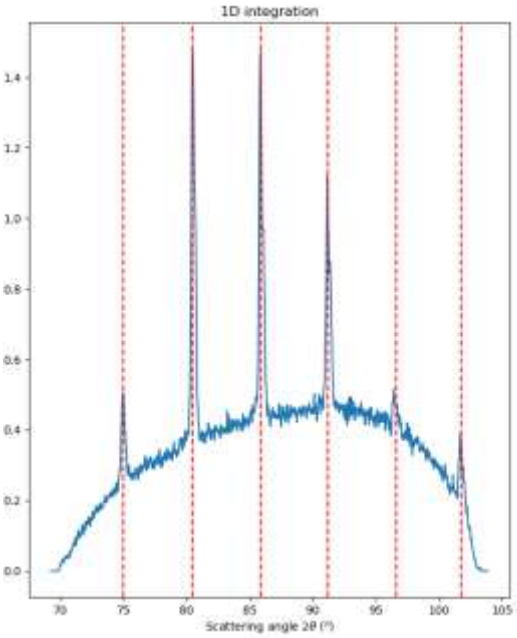
Each image is different. You can always identify the ring in the middle, which correspond the 2θ angle if the detector is well centered. Then you can try in two direction of the ring order. The following step will show you how to be sure that you have a good identification. « Pixels solid-angle" figure presents the solid angle of each pixel with the view from the origin of the sample. It depends on the orientation of the detector surface. The maximum value of the angle solid is 1 at the pixel where the normal of the detector surface cross the origin of the sample. If the detector surface is well centered, you will have the maximum angle solid in the center, showing that the calibration went fine.

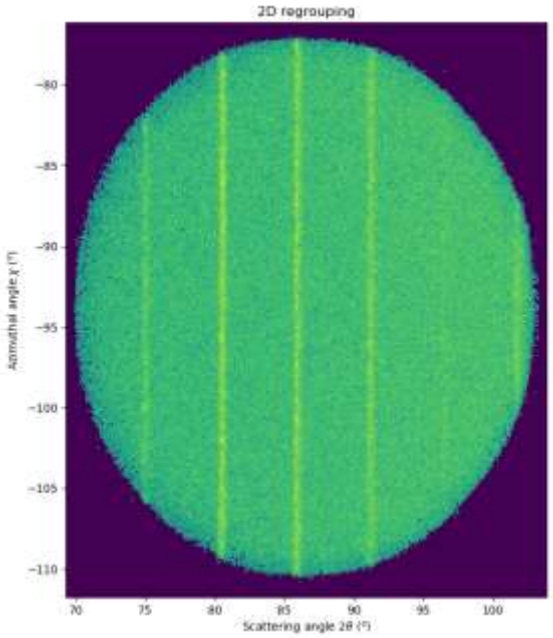




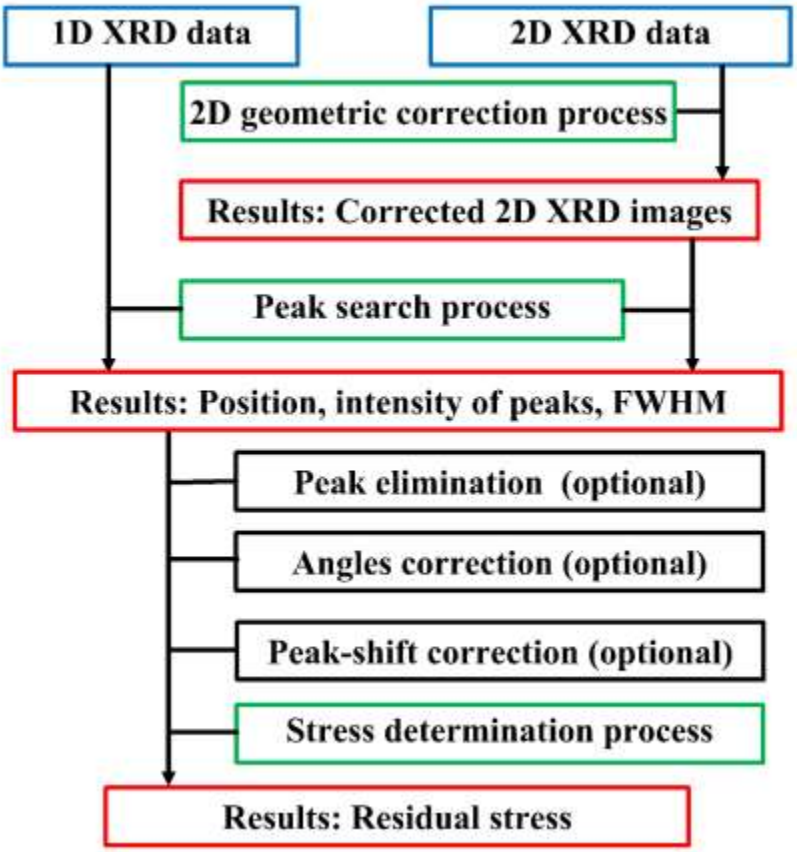
Step 5 : Type done

The “2D regrouping” figure presents the typical 2D images obtained after the calibration process. Axe x presents the angle 2θ, axe y presents the angle azimuth. If the interval of the angle azimuth is 360°, the calibration is not correct. In order to have a continuously calibrated image, the orientation of the frame from your calibrant sample must be modified using FrmUtility.exe





4. ALGORITHM AND MATHEMATICAL FUNCTIONS



4.1. Reading data

The Python code is in folder:
\\read_file\image_2D
\\read_file\scan_1D

The output information:

- Intensity vs 2θ scans in 1D XRD scan
- Intensity map according to the dimensions of the detector in 2D XRD images
- Goniometric angles (φ, χ, ω, 2θ)
- Wavelengths of X-ray source

4.2. Peak search

$$I_e(2\theta) = I_b(2\theta) + I_n(2\theta)$$

- **Background fit function**: $I_b(2\theta) = \sum_0^n a_i \times (2\theta)^i$

- **Net intensity fit function**: $I_n(2\theta) = f(2\theta - 2\theta_1) + k_{\alpha\, ratio} \times f(2\theta - 2\theta_2)\Big)$
  Where *f* is one of 5 spectral profiles: Pearson VII, Pseudo-Voigt, Voigt, Gaussian, Lorentzian.
  The python code of these functions is in folder \\fit_function\

  - $k_{\alpha\, ratio}$: $K\alpha_2/K\alpha_1$ doublet with $\theta_2 = arcsin\left(\frac{\lambda_2}{\lambda_1} * sin(\theta_1)\right)\Big)$

  The asymmetric peak shape is presented by the coefficient "*a*" where:
  $w(x) = \frac{2w}{1+exp(ax)}$ (*Stancik & Brauns, 2008*)

- **Least squares optimization method**: Levenberg-Marquardt (*More 1977*)
  Trust-region reflective (Branch 1999)
  Trust-region framework (Voglis 2004)

- **The output information:**
  Position of peaks ($2\theta_1$),
  Intensity of peaks (I_0),
  FWHM (w),
  Uncertainties "r" (standard deviations according to a Gaussian curve)

$$r = \frac{\sum[I_n(2\theta) - \bar{I_n}] \times [I_m(2\theta) - \overline{I_m}]}{\sqrt{\sum[I_n(2\theta) - \bar{I_n}]^2 \times \sum[I_m(2\theta) - \overline{I_m}]^2}}$$

4.3. Stress determination

The sin²ψ method (Müller & Macherauch, 1961):

$\varepsilon_{\phi\psi} = f(\sigma_{ij}, \phi, \psi, S_1^{hkl},\ S_2^{hkl}/2)$ with ϕ, ψ in **sample coordinates**

- Linear behaviour: $\varepsilon_{\phi\psi} = a * sin^2\psi + c$ => $\sigma_\phi = \frac{a}{S_2^{hkl}/2}$
- Elliptical behaviour: $\varepsilon_{\phi\psi} = a * sin^2\psi + b * sin2\psi + c$

  => $\sigma_\phi = \frac{a}{S_2^{hkl}/2}$; $\tau_\phi = \frac{|b|}{S_2^{hkl}/2}$

Angles conversion from goniometric coordinates ($\varphi,\ \chi,\ \theta,\ \omega,\ \gamma$) to sample coordinates ($\phi,\ \psi$) (François, 2008):

- 2D XRD

$$cos\ \psi = cos\ \gamma\ cos\ \theta_1\ cos\ \chi\ cos\ \omega + sin\ \gamma\ cos\ \theta_1\ sin\ \psi + sin\ \theta_1\ cos\ \chi\ sin\ \omega$$

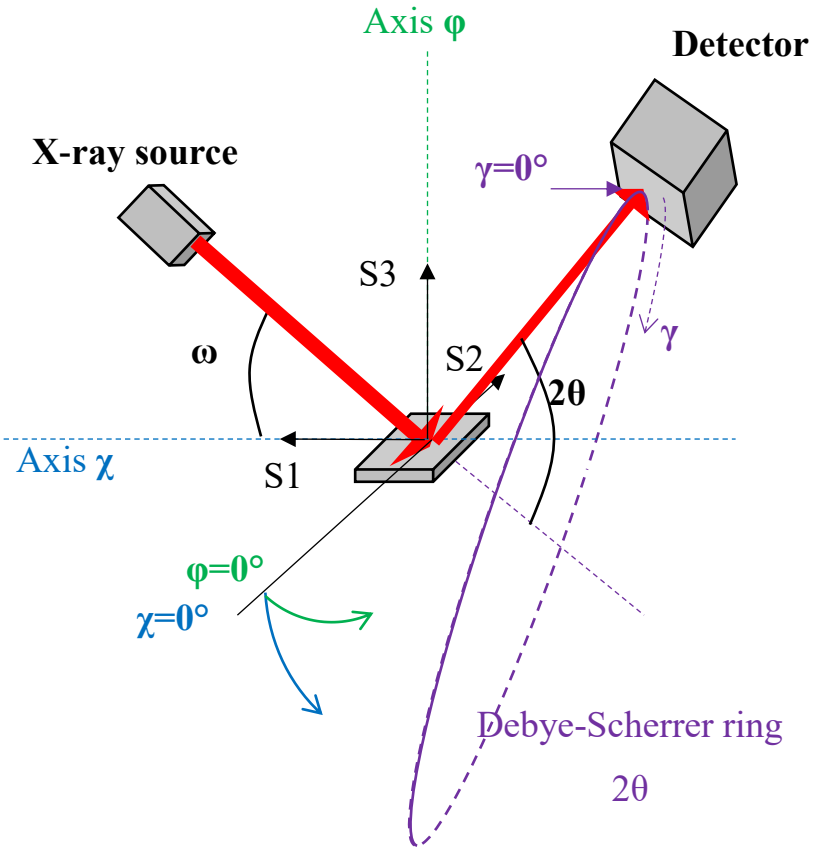
$$\phi = \varphi + \Delta\varphi$$

$$tan(\Delta\varphi) = \left|\frac{-sin\ \gamma\ cos\ \theta_1\ cos\ \chi\ +\ cos\ \gamma\ cos\ \theta_1\ sin\ \chi\ cos\ \omega\ +\ sin\ \theta_1\ sin\ \chi\ sin\ \omega}{cos\ \gamma\ cos\ \theta_1\ sin\ \omega\ -\ sin\ \theta_1\ cos\ \omega}\right|$$

- 1D XRD

$$cos\ \psi = cos\ \chi\ \cos(\theta_1 - \omega)$$

$$\phi = \varphi + \Delta\varphi \text{ ; with: } tan(\Delta\varphi) = \left|\frac{sin\ \chi}{tan(\theta_1 - \omega)}\right|$$



The fundamental method (*Baoping & Kingsley, 1997*)

$\varepsilon_{\phi\psi} = g(\sigma_{ij}, \varphi, \chi, \omega, \theta, \gamma, S_1^{hkl},\ S_2^{hkl}/2)$ with $\varphi, \chi, \omega, \theta, \gamma$ in **goniometer coordinates**

- Multi equations solutions => σ_{ij}

4.4. The quick guide to the function of all buttons

- Home window:

"1D XRD STRESS": access to 1D XRD stress analysis
(\\GUI\GUI_1D_stress.py)

"2D XRD STRESS": access to 2D XRD stress analysis
(\\GUI\GUI_2D_stress.py)

"2D pyFAI-calib": access to 2D pyFAI calib GUI
"XEC ANALYSIS": access to X-ray elastic constant analysis (ongoing development)
(\\GUI\GUI_XEC.py)

- Analysis tabs:

"ORIGINAL XRD": display the input experimental XRD scans
"CALIB XRD": where the user defines the geometrical correction parameters, executes the geometrical correction process and displays the 2D XRD after correction. This window is only available for 2D XRD STRESS analysis
"ANGLES MODIFICATION": where the user can modify the goniometric angles
"STRESS PARAMETERS": where the user defines the peak search parameters, the X-ray and material's properties and executes the peak search and stress calculation process
"FIT RESULTS": display the peak search results
"STRESS RESULTS": display the stress results in direction ϕ with lattice strain vs $\sin^2\psi$ curves
"STRESS TENSOR": display the stress tensor σ with a stress simulation tool. This window is only available with at least two angles ϕ.
"OTHER INFO": display the variation of the peak positions vs other angles
All the parameters can be entered or displayed by Entry widget of Tkinter package.

- Import, export buttons:

"Import XRD": import the original experimental XRD scans
(\\residual_stress_1D\import_XRD_1D.py)
(\\residual_stress_2D\import_XRD_2D.py)

"Export as image": export the chosen data as image
"Export all as image": export all data as image
(\\tools\export_graph_1D.py)
(\\tools\export_image_2D.py)

"Export as text": export the chosen data as text
"Export all as text": export all data as text
(\\tools\export_data_1D.py)
(\\tools\export_data_2D.py)

- "ORIGINAL XRD" tab:

"Rotate +90°": rotate the 2D XRD image 90° clockwise
"Rotate -90°": rotate the 2D XRD image 90° Counterclockwise
"Rotate 180°": rotate the 2D XRD image 180° clockwise
"Flip horizontal": flip the 2D XRD image with the vertical axis of symmetry

“Flip vertical”: flip the 2D XRD image with the horizontal axis of symmetry
“Original”: get back to the original 2D XRD image
(\\residual_stress_2D\animation_original_frame_2D.py)

- “CALIB XRD” tab: (only available for 2D XRD STRESS analysis)

“Import poni parameters”: import the geometrical correction parameters
(\\tools\import_poni_parameters_2D.py)

“RUN CALIBRATION”: execute the geometrical correction process
(\\residual_stress_2D\calib_XRD_2D.py)

“Definition”: basic explanation of the geometrical correction parameters
(\\visualisation\definition_poni.py)

“Create PONI parameters”: access to 2D pyFAI calib GUI
(\\tools\create_poni_parameters.py)

- “ANGLES MODIFICATION” tab:

“Apply”: apply the modification of goniometric angles
“Initialize”: restore the goniometers angles to the initial values
“Advance”: advanced option to modify the goniometric angles
(\\residual_stress_1D\angles_modification_1D.py)
(\\residual_stress_2D\angles_modification_2D.py)

- “STRESS PARAMETERS” tab:

“Import template”: import the template for peak search and stress determination parameters (*.spt)
(\\tools\calcul_parameters.py)

“Export template”: export the template for peak search and stress determination parameters (*.spt)
(\\tools\calcul_parameters.py)

“Limits preview”: an overall view of limits ranges (background, fitting range, gamma sections, init-range, and unstressed peak position)
“Fit preview”: a preview of the peak search result
(\\visualisation\preview_1D.py)
(\\visualisation\preview_2D.py)

“Peak shift correction”: import the peak-shift correction coefficients (psc). The psc can be obtained from “OTHER INFO” tab
(\\tools\peak_shift_correction.py)

“Lock”: lock the access to modify the X-ray source wavelength
“Unlock”: unlock the access to modify the X-ray source wavelength
(\\residual_stress_1D\import_XRD_1D.py)
(\\residual_stress_2D\calib_XRD_2D.py)

“Add”: add more init-ranges, which mean more peaks
(\\tools\add_peak.py)

“RUN CALCULATION”: execute the peak search and stress determination process

(\\residual_stress_1D\main_calcul_1D.py)
(\\residual_stress_2D\main_calcul_2D.py)

- "STRESS RESULTS" tab:

"APPLY MODIFICATION": re-execute the stress determination process. This option uses the previous results of peak search process. The modifications of goniometric angles, XEC values, peak elimination and peak-shift correction coefficients will be taken into account. The modification of the peak fitting parameters will not be taken into account.
(\\residual_stress_1D\main_calcul_1D.py)
(\\residual_stress_2D\main_calcul_2D.py)

- "STRESS TENSOR" tab:

"Show": calculate the stress in user-defined direction ϕ
(\\visualisation\show_XRD_1D.py)
(\\visualisation\show_XRD_2D.py)

- "OTHER INFO" tab:

"Fit": polynomial fit of the peak-shifts vs angles χ curve
"Export peaks correction": export the peak-shift correction coefficients into text file, then these coefficients can be imported by "peak-shift correction" button in "STRESS PARAMETERS" tab
(\\tools\peak_shift_correction.py)

5. TIPS AND TRICKS

5.1. How to use X-Light?

- Run module __main__.py through IDLE python
- Or open X-Light_win_64.exe on Windows 64bit
- Import XRD 0D, 1D scan or 2D image
- Calibrate the 2D image
- Modify all the goniometric angles if they are not correct
- Define all the stress parameters
- Run the calculation
- Delete all peaks on which the fit is not correct
- Apply the modification

5.2. Python module

List of python modules required for running X-Light:
- tkinter
- numpy
- scipy
- matplotlib
- fabio
- h5py
- silx
- pyopencl
- pyqt5
- pyfai
- nexusformat

Install through cmd window: pip install numpy

5.3. How to import a new XRD format?

5.3.1. 1D data

- (1) Go to “read_file\scan_1D” folder
- (2) If the file is in format ".txt", open “read_text_scan.py”
- (3) modify the line #from read_file.scan_1D.scan_txt_new import read_txt_new
replace 'new' by the name that you want to name your scan, delete '#"
- (4) modify the line #elif 'text' in text: #read_txt_new(f,self)
replace 'text' by a part of the first line in your text scan
replace 'read_txt_new' by the new module
- (5) go to python; create a new file named "scan_txt_new.py”
define a new module named "read_txt_new"
- (6) open the file “scan_1D_template.py” and follow the guide
- (2) If the file is not in format ".txt", open “read_scan_1D.py”
- (3) modify the line #from read_file.scan_1D.scan_new_xxx import read_new_xxx
replace 'new_xxx' by your scan format, delete '#"
- (4) modify the line #elif f_ext in ("new","NEW"): #read_new_xxx(f,self)
replace 'new' by the new format and “read_new_xxx” by the new module
- (5) go to python, create a new file named "scan_new_xxx.py'
define a new module named "read_new_xxx"
- (6) open the file “scan_1D_template.py” and follow the guide
- (7) open “residual_stress_1D\import_XRD_1D.py” and add your new extension format in “format_” variable

5.3.2. 2D data

- (1) Go to “read_file\image_2D” folder
- (2) open “read_image_2D.py”
- (3) modify the line #from read_file.image_2D.image_new import read_header_new, read_data_new
replace 'new' by the name that you want to name your scan, delete '#"
- (4) modify the line #elif f_ext in ("new" or "NEW"): #read_header_new(f,import_XRD)
#elif f_ext in ("new" or "NEW"): #data=read_data_new(f)
replace 'new' by the new format and new module in (3)
- (5) go to python, create a new file named "image_new.py'
define two new modules named "read_header_new" and "read_data_new"
- (6) open the file “image_2D_template.py” and follow the guide
- The module “read_data_2D_template_1” is an example when the format doesn’t have the image dimensions, a new window will appears to define the image dimensions. This module “read_data_2D_template_1” is not obligated
- (7) If the image needs some corrections: open file “image_correction.py”
- (8) modify #from read_file.image_2D.image_correction_new import image_correction_new
replace “new” by the new detector
- (9) modify the line #elif "xxxx" in header[i] and "yyyy" in header[j]: #use header to identify your format #data=image_correction_new(data)
replace “xxxx” and “yyyy” by a part of the header[i] and [j] of the image
- (10) create a new python file “image_correction_new.py” and a module named “image_correction_new”
- (11) open “image_correction_template.py” to follow the guide
- (12) open “residual_stress_2D\import_XRD_2D.py” and add your new extension format in “format_” variable

5.4. How to add a new material and x-ray source?

- open “read_file\mat_database.mdb” and modify
- open “read_file\x_ray_source.xrs” and modify
- These files are in text format

5.5. How to read the format *.xlf (X-Light image format) by fabio and pyFAI

XLF image format can be obtained from “Export as text” from X-Light
- copy 3 files:
  - « X-Light-v1.1\third party\fabio\openimage.py »
  - « X-Light-v1.1\third party\fabio\xlightimage.py »
  - « X-Light-v1.1\third party\fabio\fabioformats.py »

and paste to «Python\Lib\site-packages\fabio » => fabio will read *.xlf
- copy « X-Light-v1.1\third party\pyFAI\ExperimentTask.py »

and paste to “Python\Lib\site-packages\pyFAI\gui\calibration” => pyFAI will read *.xlf