X-Light quick guide

X-Light is an open-source software, which is written in Python with a Graphical User Interface. X-Light is developed to determine the residual stress by X-ray diffraction. This software can process the 0D, 1D and 2D diffraction data obtained with laboratory diffractometers or synchrotron radiation.

I. 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

II. Supported formats

1D XRD scan: Bruker (raw1.01, raw4.00, uxd), Seifert (nja), Proto (profiles) and text binary with 2 columns (2theta and intensity)

2D XRD image: Bruker (gfrm), Nexus (nxs), Binary (raw), X-Light (xlf) and FabioImage

III. 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

IV. How to import a new XRD format?

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

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

V. 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

VI. 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

VII. The quick guide to the function of all buttons

Home window:

“1D XRD STRESS”: access to 1D XRD stress analysis

“2D XRD STRESS”: access to 2D XRD stress analysis

“2D pyFAI-calib”: access to 2D pyFAI calib GUI

“XEC ANALYSIS”: access to X-ray elastic constant analysis (ongoing development)

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

“Export as image”: export the chosen data as image

“Export as text”: export the chosen data as text

“Export all as image”: export all data as image

“Export all as text”: export all data as text

“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

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

“Import poni parameters”: import the geometrical correction parameters

"RUN CALIBRATION": execute the geometrical correction process

"Definition": basic explanation of the geometrical correction parameters

"Create PONI parameters": access to 2D pyFAI calib GUI

"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

"STRESS PARAMETERS" tab:

"Import template": import the template for peak search and stress determination parameters (*.spt)

"Export template": export the template for peak search and stress determination parameters (*.spt)

"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

"Peak shift correction": import the peak-shift correction coefficients (psc). The psc can be obtained from "OTHER INFO" tab

"Lock": lock the access to modify the X-ray source wavelength

"Unlock": unlock the access to modify the X-ray source wavelength

"Add": add more init-ranges, which mean more peaks

"RUN CALCULATION": execute the peak search and stress determination process

"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.

"STRESS TENSOR" tab:

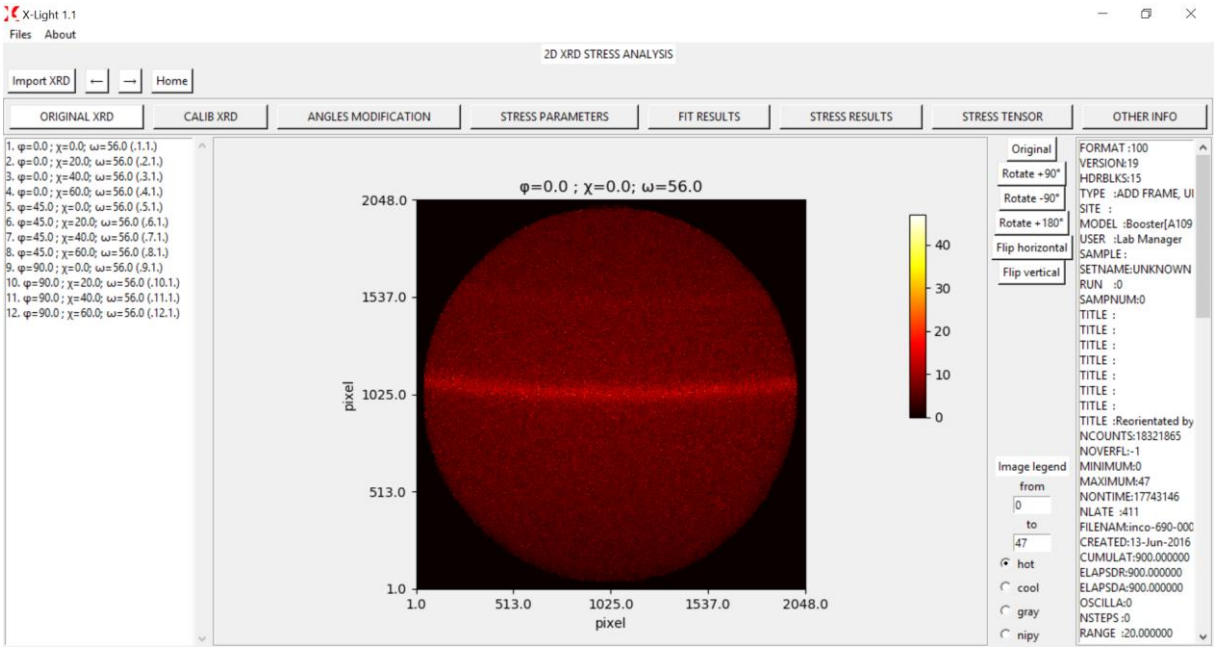
"Show": calculate the stress in user-defined direction ϕ

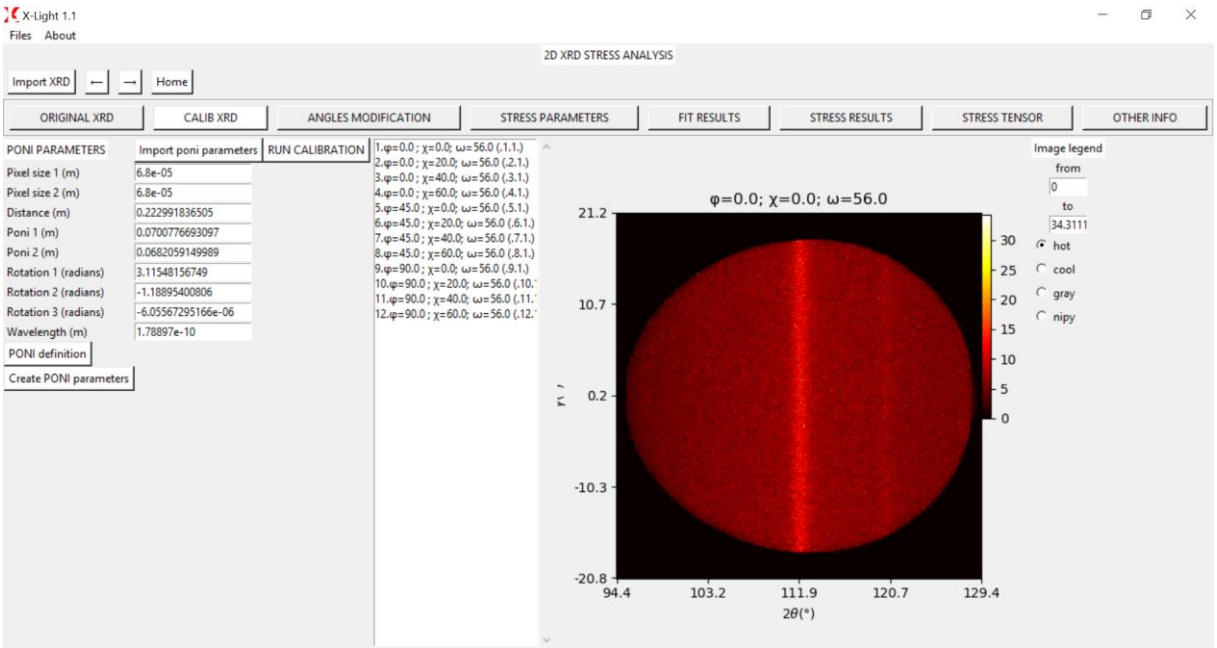
"OTHER INFO" tab:

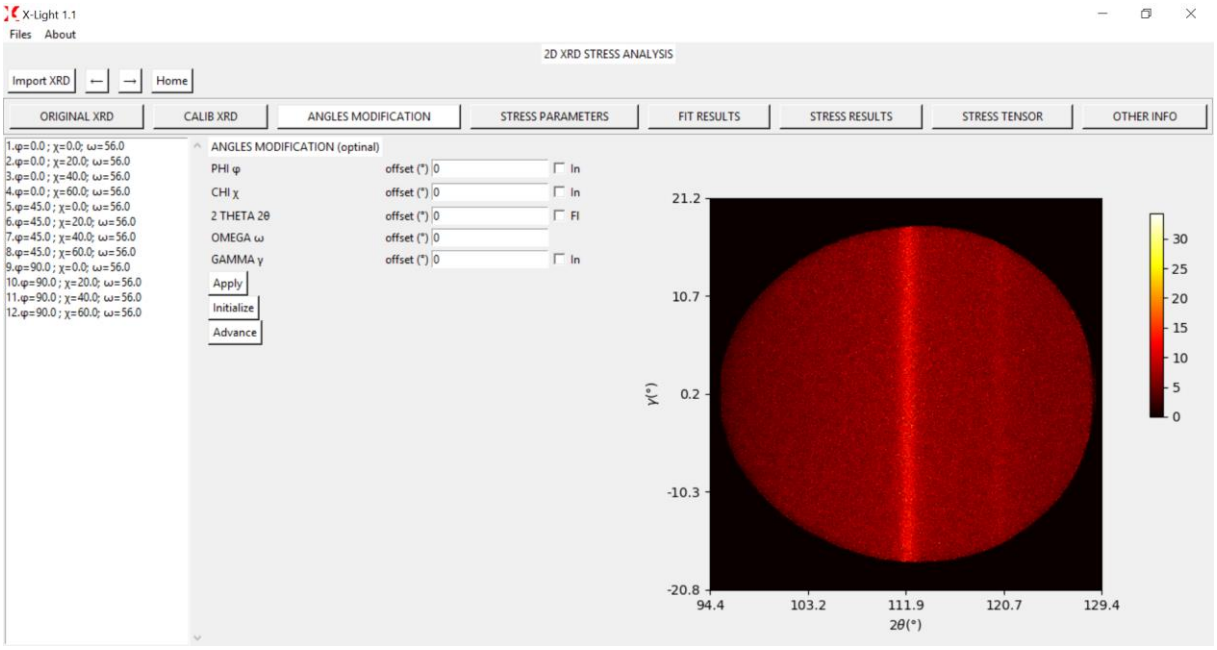
"Fit": polynomial fit of the peak-shifts vs angles χ curve

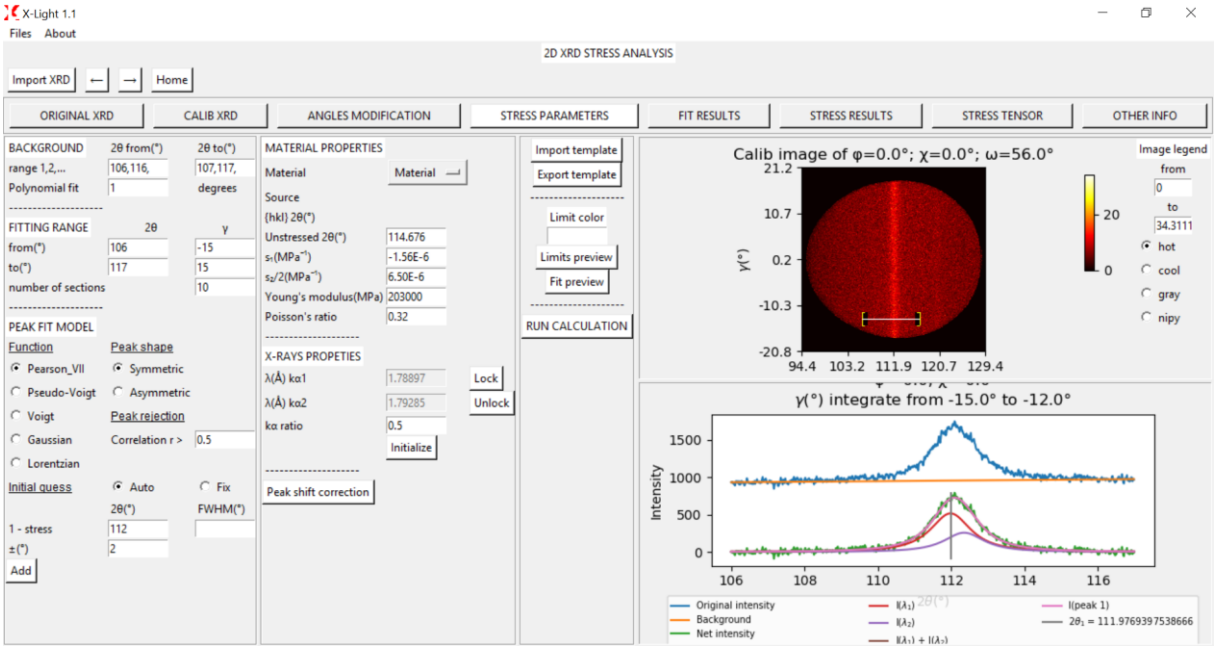
"Export peaks correction": export the peak-shift correction coefficients into text file, then these coefficients can be imported by "peak-shift correction" button in "STRESS PARAMETERS" tab

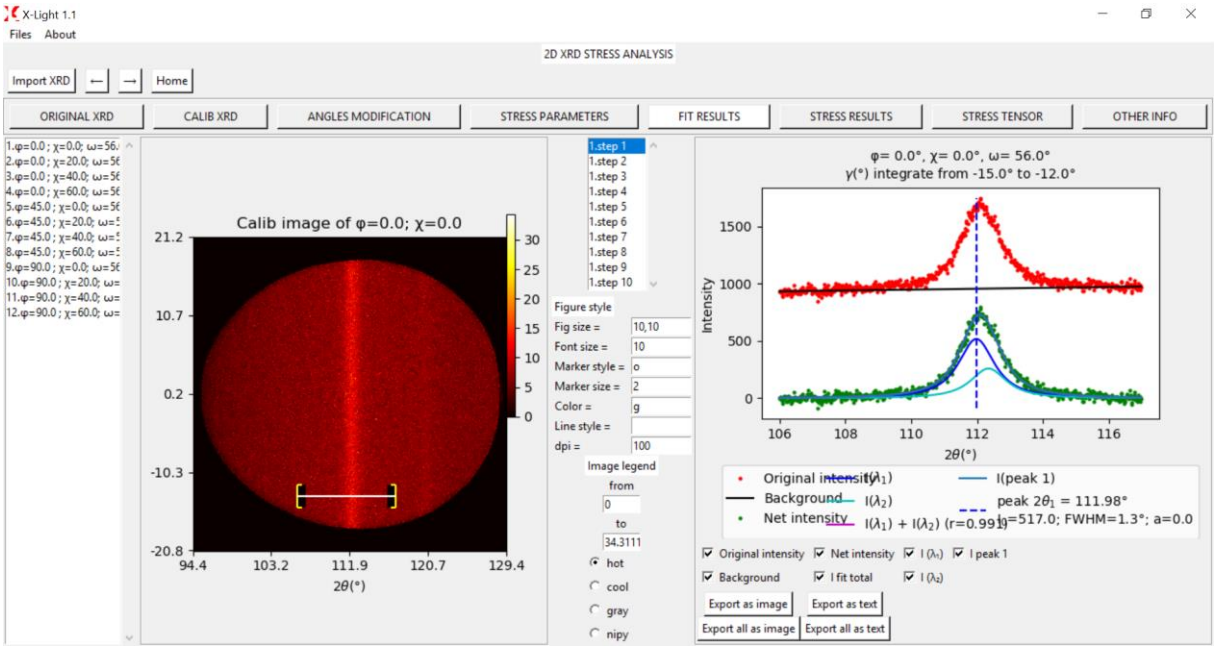
VIII. Example of results






X-Light 1.1
Files About
2D XRD STRESS ANALYSIS
Import XRD
Home
ORIGINAL XRD
CALIB XRD
ANGLES MODIFICATION
STRESS PARAMETERS
FIT RESULTS
STRESS RESULTS
STRESS TENSOR
OTHER INFO
1.φ=0.0 ; χ=0.0; ω=56.0
2.φ=0.0 ; χ=20.0; ω=56.0
3.φ=0.0 ; χ=40.0; ω=56.0
4.φ=0.0 ; χ=60.0; ω=56.0
5.φ=45.0 ; χ=0.0; ω=56.0
6.φ=45.0 ; χ=20.0; ω=56.0
7.φ=45.0 ; χ=40.0; ω=56.0
8.φ=45.0 ; χ=60.0; ω=56.0
9.φ=90.0 ; χ=0.0; ω=56.0
10.φ=90.0 ; χ=20.0; ω=56.0
11.φ=90.0 ; χ=40.0; ω=56.0
12.φ=90.0 ; χ=60.0; ω=56.0
ANGLES MODIFICATION (optinal)
PHI φ
CHI χ
2 THETA 2θ
OMEGA ω
GAMMA γ
offset (°)
In
Apply
Initialize
Advance
21.2
10.7
0.2
-10.3
-20.8
γ(°)
94.4
103.2
111.9
120.7
129.4
2θ(°)
30
25
20
15
10
5
0


X-Light 1.1
Files About
2D XRD STRESS ANALYSIS
Import XRD
Home
ORIGINAL XRD
CALIB XRD
ANGLES MODIFICATION
STRESS PARAMETERS
FIT RESULTS
STRESS RESULTS
STRESS TENSOR
OTHER INFO
BACKGROUND
2θ from(°)
2θ to(°)
range 1,2,...
106,116,
107,117,
Polynomial fit
1
degrees
FITTING RANGE
2θ
γ
from(°)
106
-15
to(°)
117
15
number of sections
10
PEAK FIT MODEL
Function
Pearson_VII
Pseudo-Voigt
Voigt
Gaussian
Lorentzian
Peak shape
Symmetric
Asymmetric
Peak rejection
Correlation r >
0.5
Initial guess
Auto
Fix
2θ(°)
FWHM(°)
1 - stress
112
±(°)
2
Add
MATERIAL PROPERTIES
Material
Source
(hkl) 2θ(°)
Unstressed 2θ(°)
114.676
Young's modulus(MPa)
203000
Poisson's ratio
0.32
X-RAYS PROPETIES
λ(Å) kα1
1.78897
λ(Å) kα2
1.79285
kα ratio
0.5
Lock
Unlock
Initialize
Peak shift correction
Import template
Export template
Limit color
Limits preview
Fit preview
RUN CALCULATION
Calib image of φ=0.0°; χ=0.0°; ω=56.0°
Image legend
from
0
to
34.3111
hot
cool
gray
nipy
γ(°) integrate from -15.0° to -12.0°
Intensity
Original intensity
Background
Net intensity
I(peak 1)


X-Light 1.1
Files About
2D XRD STRESS ANALYSIS
Import XRD
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ORIGINAL XRD
CALIB XRD
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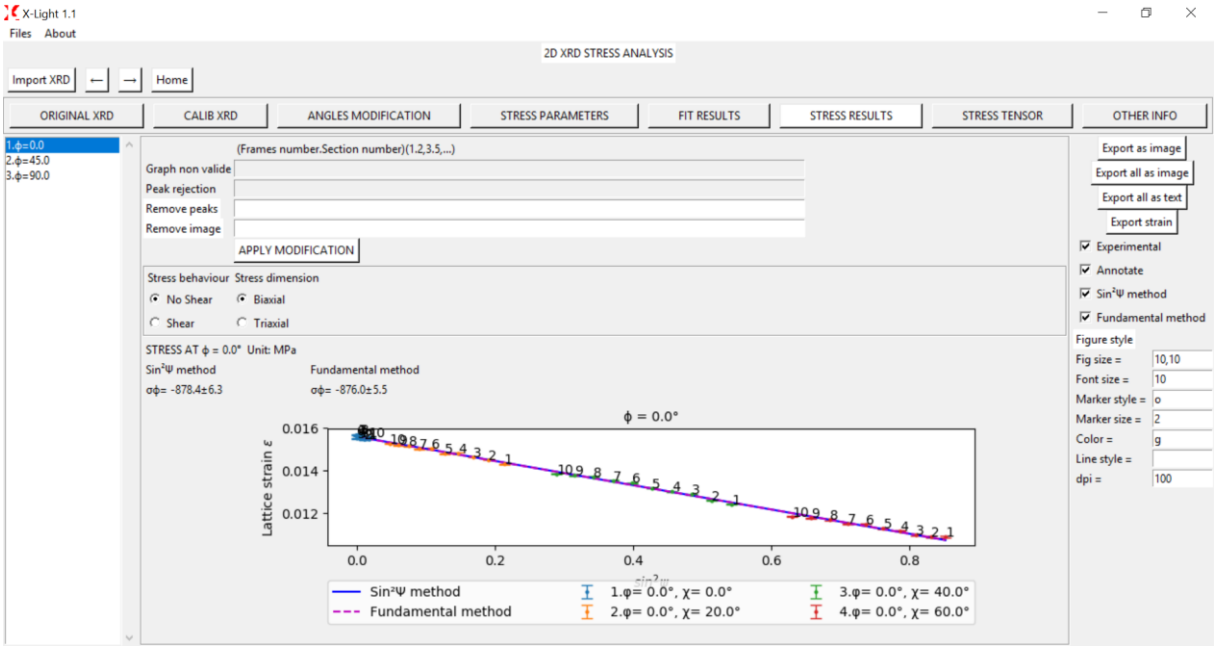
STRESS PARAMETERS
FIT RESULTS
STRESS RESULTS
STRESS TENSOR
OTHER INFO
Calib image of φ=0.0; χ=0.0
2θ(°)
φ= 0.0°, χ= 0.0°, ω= 56.0°
γ(°) integrate from -15.0° to -12.0°
Intensity
Original intensity I(λ1)
Background I(λ2)
Net intensity I(λ1) + I(λ2) (r=0.9919)
I(peak 1)
peak 2θ1 = 111.98°
I=517.0; FWHM=1.3°; a=0.0
Export as image
Export as text
Export all as image
Export all as text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2D XRD STRESS ANALYSIS
Import XRD
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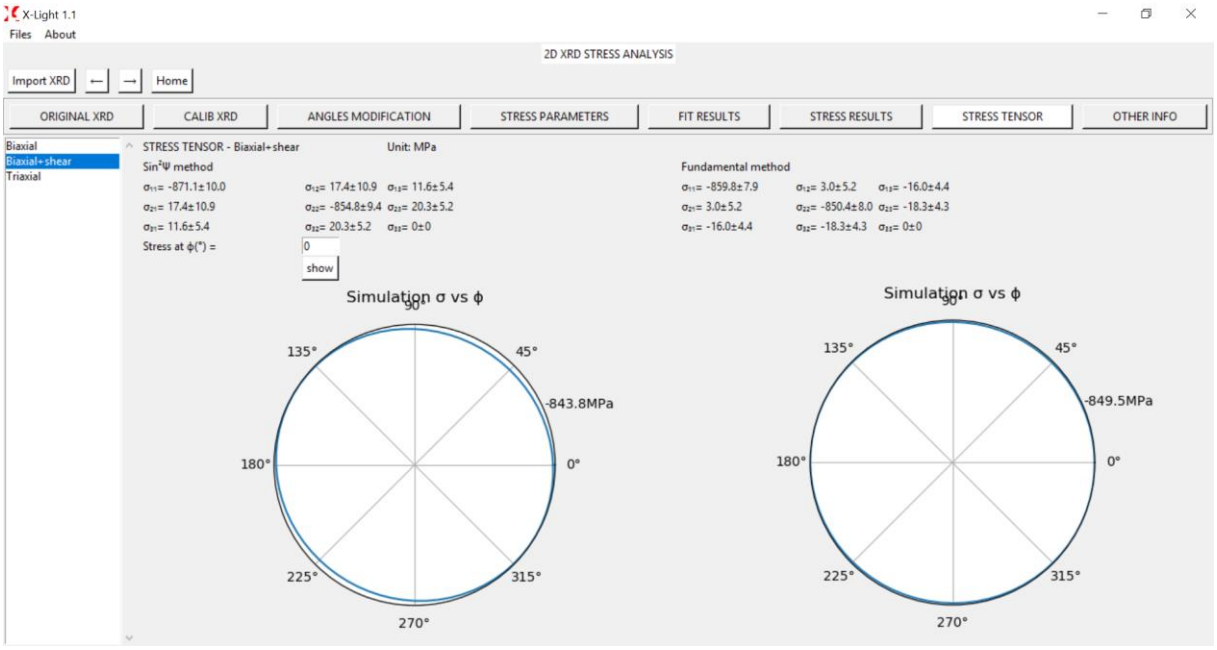
ORIGINAL XRD
CALIB XRD
ANGLES MODIFICATION
STRESS PARAMETERS
FIT RESULTS
STRESS RESULTS
STRESS TENSOR
OTHER INFO
(Frames number.Section number)(1.2,3.5,...)
Graph non valide
Peak rejection
Remove peaks
Remove image
APPLY MODIFICATION
Stress behaviour
No Shear
Shear
Stress dimension
Biaxial
Triaxial
STRESS AT ϕ = 0.0° Unit: MPa
Sin²Ψ method
σϕ= -878.4±6.3
Fundamental method
σϕ= -876.0±5.5
ϕ = 0.0°
Lattice strain ε
Sin²Ψ method
Fundamental method
1.φ= 0.0°, χ= 0.0°
2.φ= 0.0°, χ= 20.0°
3.φ= 0.0°, χ= 40.0°
4.φ= 0.0°, χ= 60.0°
Export as image
Export all as image
Export all as text
Export strain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2D XRD STRESS ANALYSIS
Import XRD
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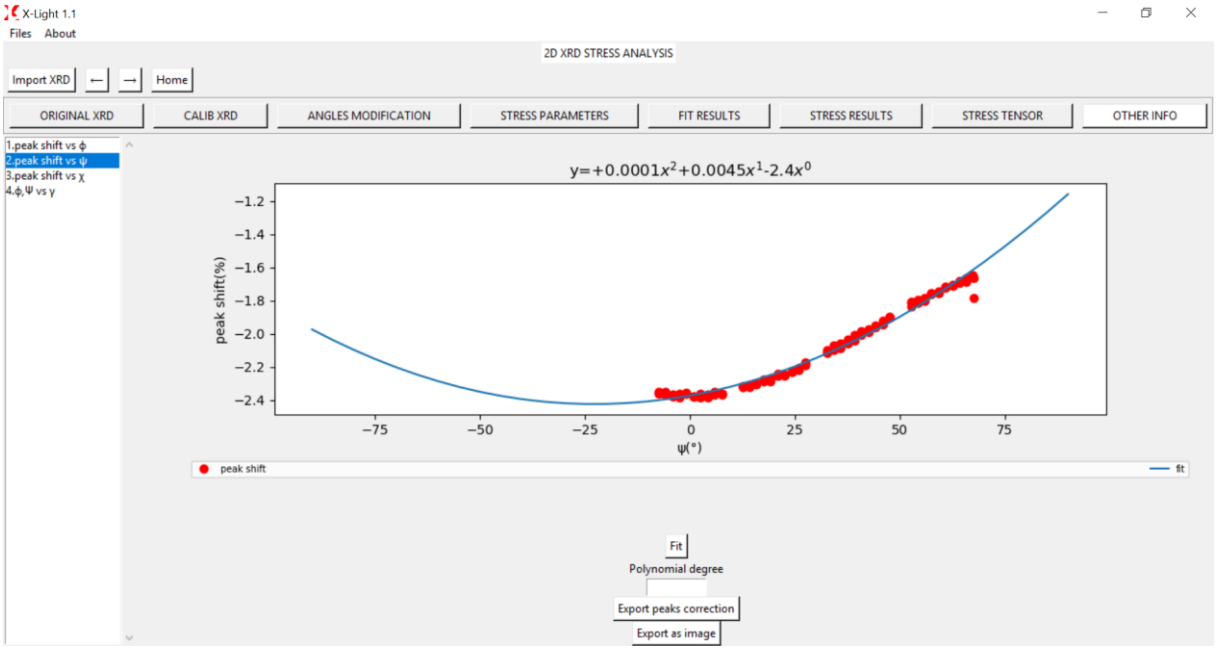
ORIGINAL XRD
CALIB XRD
ANGLES MODIFICATION
STRESS PARAMETERS
FIT RESULTS
STRESS RESULTS
STRESS TENSOR
OTHER INFO
Biaxial
Biaxial+shear
Triaxial
STRESS TENSOR - Biaxial+shear
Unit: MPa
Sin²Ψ method
Fundamental method
Stress at ϕ(°) =
show
Simulation σ vs ϕ
90°
135°
45°
180°
0°
225°
315°
270°
-843.8MPa
-849.5MPa


X-Light 1.1
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ORIGINAL XRD
CALIB XRD
ANGLES MODIFICATION
STRESS PARAMETERS
FIT RESULTS
STRESS RESULTS
STRESS TENSOR
OTHER INFO
1.peak shift vs ϕ
2.peak shift vs ψ
3.peak shift vs χ
4.ϕ,Ψ vs γ
y=+0.0001x²+0.0045x¹-2.4x⁰
peak shift(%)
ψ(°)
peak shift
fit
Fit
Polynomial degree
Export peaks correction
Export as image