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**Supporting information for article:**

***PYXIS*: an integrated software package for synchrotron micro/nanodiffraction data analysis**

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**PYXIS v5.0**

**USER MANUAL**

**Jiawei Kou, Kai Chen**

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# Introduction

## 1 Introduction

### 1.1 Before Use



Welcome to PYXIS!

PYXIS is a synchrotron irradiation Laue microbeam diffraction ( $\mu$ XRD) data analysis software developed on Matlab platform. PYXIS contains various functions for analyzing Laue diffraction and energy scan patterns, such as diffraction pattern viewing, diffraction peak searching and analysis, diffraction peak indexation, orientation/strain refinement, energy scan data analysis, and dislocation analysis.

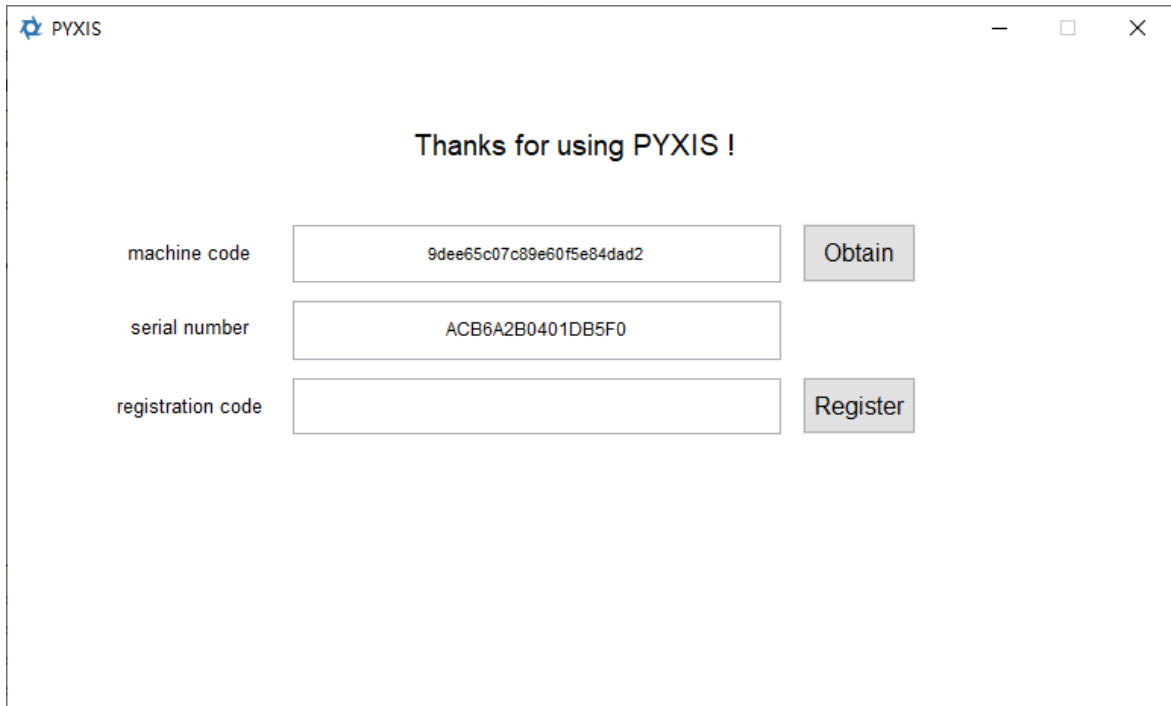
Before using this version of PYXIS, please install Matlab Runtime 9.3 first ([MATLAB Runtime - MATLAB Compiler - MATLAB \(mathworks.cn\)](#)).

This version of PYXIS is registered by the hardware configuration of the computer. The machine code used for registration is encrypted from the serial number of the central processing unit (CPU) and the hard disk on which the operation system installed. If you change the CPU or the hard disk on which the operation system installed, the registration will be invalidated. Therefore, since some of the diffraction pattern analysis performed by PYXIS require a high computing power, you are reminded to choose the computer to install PYXIS carefully.

### 1.2 Installation & Registration

Before installation, please make sure that you have successfully installed the Matlab Runtime on your computer as required in Section 1.1.

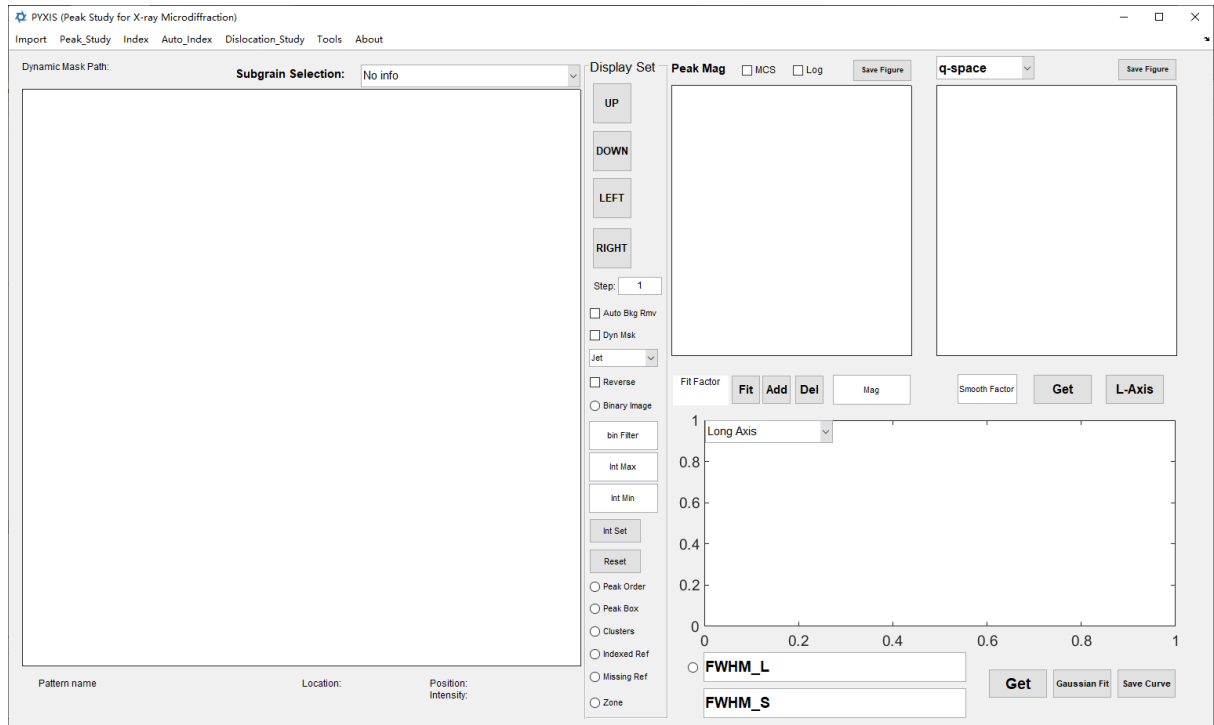
1. Extract the PYXIS software package.
2. Open the executable file PYXIS.exe. If it is the first time you use PYXIS, the following registration interface will be shown.



If the machine code is not generated, click "Obtain" button to refresh the machine code. Provide the machine code and serial code to the software provider, who will provide you with a registration code for the computer.

3. After obtaining the registration code, please input the registration code and click "Register" button. The software will check the machine code, serial code and registration code, and complete the registration.

4. After successful registration, restart PYXIS to open the main interface.



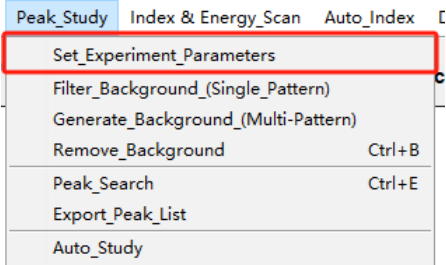


# Basis Parameters Setting

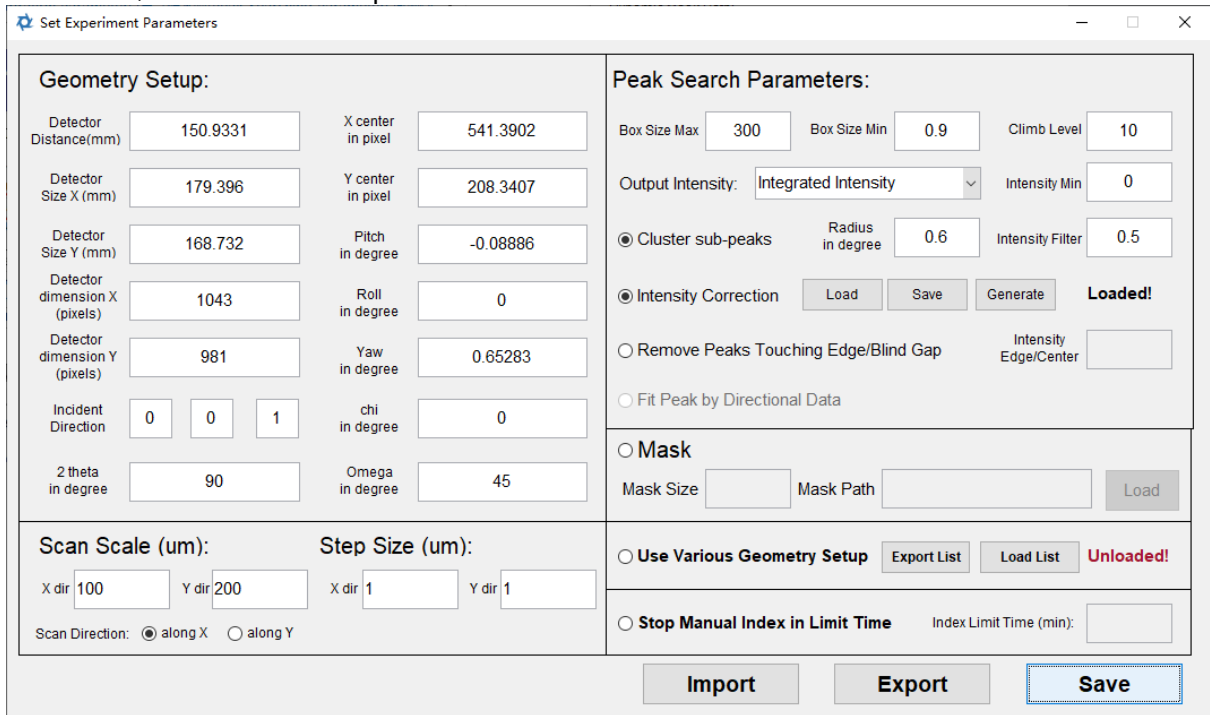
## 2 Basis Parameters Setting

### 2.1 Geometry Setup Parameters & Peak Searching Parameters

Before analyzing the microdiffraction patterns, please set the experiment geometry setup parameters and the peak searching parameters. Following is the details on the setting.



After click, the interface is opened.



The geometry setup parameters are entered in the Geometry setup box in the interface.

Before using any analysis function of PYXIS, please these parameters first. The meaning of the parameters are:

Detector distance (mm): the distance from the beam focal point on the sample to the plane of the detector;

Detector size (mm) X: size of the detector in the X axis in millimeters;

Detector size (mm) Y: size of the detector in the Y axis in millimeters;

Detector dimension (pixel) X: number of pixels in the X axis of the detector;

Detector dimension (pixel) Y: number of pixel in Y axis of the detector;

X center in pixel: X axis coordinate of the projection of the beam focal point on the detector plane;

Y center in pixel: Y axis coordinate of the projection of the beam focal point on the detector plane;

Pitch in degree: spatial tilt angle of the detector;

Roll in degree: spatial tilt angle of the detector, set as 0 for almost all synchrotron irradiation beamlines.

Yaw in degree: spatial tilt angle of the detector;

Incident Direction: direction of incident beam, generally [0 0 1];

2 theta in degree: detector position in 2 theta direction;

chi in degree: detector position in chi direction;

Omega: the tilt angle of the sample.

It is noted that the definitions of the geometry setup parameters are the same as those of XMAS, which developed by Nobumichi Tamura from Beamline 12.3.2 at advanced light source.

In the Scan Scale (um) box, enter the parameters of the scanned area of the experiment, in micrometer. Before using any function of PYXIS, please enter these parameters. The meaning of the parameters are:

Scan Scale (um): the size of the scanned area;

Scan Step (um): the length of the scanning step;

Scan Direction: the direction of the first line of the scan.

Peak searching parameters are entered in the Peak Search Parameter box. Before using the peak search function of PYXIS, please enter these parameters. The meaning of the parameters are:

Box Size Max: the maximum side length of the enclosed rectangle of the diffraction peak, usually set as 100;

Box Size Min: the minimum side length of the enclosed rectangle of the diffraction peak, usually set as 2;

Climb Level: the sensitivity of the subpeak identification. The larger the value, the identification of subpeak more sensitive, usually set as 10. If no subpeak exist, set as 0 to turn off subpeak identification.

Output Intensity: Here you can choose in which type the intensity of the peak is output. There are integrated intensity, the highest intensity or the average intensity. After that, you can enter the minimum intensity of the valid diffraction peaks in "Intensity Min". The peak weaker than that will be ignored.

Cluster Subpeaks: Select whether to cluster subpeaks split from the same Laue peak. If on, the subpeaks will be regarded as one Laue peak after clustering when identifying the zone axis and indexing the Laue peaks.

Radius (in degree): the maximum value of the angle between the scatter vectors of the subpeaks split from the same Laue peak.

Intensity Filter: In order to avoid detector noise or a small number of weak peaks affecting the clustering, the peaks with intensity less than the "Intensity Filter" times of the brightest subpeak among the cluster will not participate in the clustering processing. Usually set as 0.25;

Intensity Correction: When this function is turned on, the software will calculate the actual spatial angle covered by each pixel, and normalize them. After opening this function, the software will prompt "Unload". If you use it for the first in the current geometry setup parameters, you can click "Generate" button to calculate the spatial angle of each pixel. After the calculation is completed, the software will display "Loaded". Since the calculation may take several minutes, the spatial angles can be saved as .icp file by clicking "Save" button. And it can be used by loading it with "Load" button.

Remove Peak Touching Edge/Blind Gap: Select whether or not to remove the peak in contact with the detector edge or blind gaps, which exist for all PILATUS detectors. The locations of the gaps in PILATUS 1M, PILATUS 2M, and PILATUS 6M are available. If data from other detectors, please provide the detector's gap position to the software provider for an update. "Intensity Edge/Center" is the ratio of the intensities from the peak center and the edge. It is used as the threshold to judge how close the peak is touching the gap. If the ratio of a peak is larger than that, it is removed. Otherwise, it is kept.

Fit Peak By Directional Data: This feature is not yet available.

The mask parameters are entered in the Mask box in the interface. If you need to use the mask function, you need to click the "Mask" button. The meaning of the specific parameters are:

Mask Size: the size of each mask area. The area is square and Mask Size is the side length of the square with unit as pixel.

Mask: Click the "Load" button to load the file stored the locations of the mask areas. All files with peak coordinates can be loaded, including .pkl, .idx, and .stn files. After loading, the recorded peak coordinates are used as the center of the mask areas, and PYXIS will remind you to save a .msk file to store the coordinates. The .msk file can be loaded directly for subsequent use.

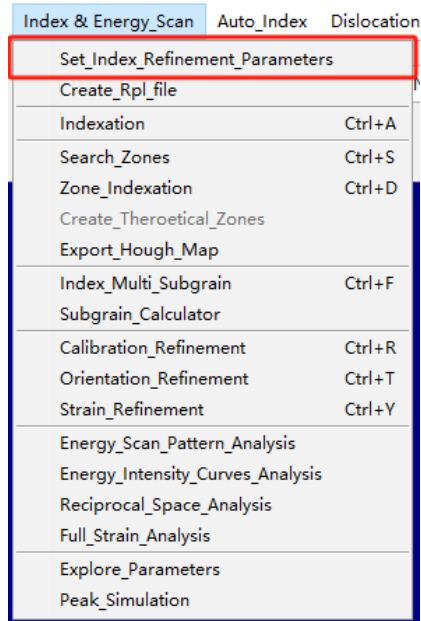
Use Various Geometry Setup: When the surface of the sample is uneven, the geometry setup for each point is different. Click the "Export List" button to export an empty list containing the coordinates of the scanned positions. Fill in the geometry setup of each point in the list and click "Load List" to import the list. When this feature is turned on, the automatic analysis will use the parameters in this list. However, manual analysis will still use the parameters entered in this interface.

Stop Manual Index in Limit Time: When this feature is turned on, you can enter the maximum time for manual indexation in the input box afterward. The software will force to stop the indexation processing when it exceeds this time.

After all parameters are set, click "Export" button to export and store all parameters as .gms file. The file is ASCII encoded text file and can be edited. Click "Import" button, you can load a .gms file. If you close the window directly, PYXIS will save the parameters automatically. But it is encouraged to click "Save" button to save the parameters in case the error on the data transfer between interfaces.

## 2.2 Indexation Parameters

Before indexing the microdiffraction patterns, the indexation parameters are required to be entered. The interface and the way are shown below:



After clicking, the interface is opened.

The screenshot shows the 'Set Index Parameters' dialog box with the following settings:

- Energy Max: 24
- Energy Min: 5
- Crystal: ni.rpl
- Peak Based Index:
  - Angular Tolerance: 0.2
  - Threshold Num: 8
  - Structure Factor Limit: 0.3
  - Start Set: 6
  - Ref for Index: 100
- Zone Based Index:
  - Box size in phi: 10
  - Box size in psi: 10
  - least intsecLine: 5
  - Peak involved: all
  - Largest Index: 3
  - Zone for Index: 30
  - Zone angularTol: 2
  - Zone Threshold: 4
  - Peak angularTol: 1
  - Peak Threshold: 20
  - Including angularTol: 0.2
  - Zone start set: 4
- Calibration Refinement:
  - dd (selected)
  - pitch
  - xcent
  - yaw
  - ycent
- Theoretical Reflection Cluster:
  - ni.mat
  - Load
  - Calculate
- De-Clustering:
  - Check all Peak Series (selected)
  - Weight Ratio: 0
  - Refine Factor: 1
  - Intensity Ratio: 1
- Bottom options:
  - Judge Dauphine twin (unchecked)
  - Show Missing Reflections (checked)
  - Import
  - Export
  - Save

The meaning of the parameters are:

Energy Max: the maximum energy of the incident X-ray, in the unit of keV;

Energy Min: the minimum energy of the incident X-ray, in the unit of keV;

Crystal: Crystal structure of the sample. You load an available .rpl file by clicking the "Load" button. If the desired crystal structure is not available, the method to generate the .rpl file is described in Section 2.3.

Peak Based Index: The parameter entered in this box are used in the conventional indexation method based on diffraction peaks.

Angular Tolerance: The allowed maximum deviation in indexation between the enclosed angles of the pair of searched peaks and the pair of the corresponded theoretical ones.

Threshold Num: The minimum number of the indexed peaks for a successful indexation.

Structure Factor Limit: We normalize the model of the structure factors for all theoretical Laue peaks by the largest one. The theoretical Laue peak whose normalized structure factor is less than "Structure Factor Limit" will be ignored in indexation processing.

Start Set: The number of the theoretical Laue peaks used for the first step of the indexation.

Usually set as 6. In the case that peaks from several grains emerge on the pattern, the parameter should be larger.

Ref for index: the number of the theoretical Laue peaks used to index the experimental ones. Click "REC" on the right side, PYXIS will calculate the minimum value of "Ref for index" in the current geometry setup and the sample crystal structure. Practically, it should be set larger than the minimum value.

Zone Based Index: The parameters entered in this box are used in the zone axis assisted indexation (ZAAI).

Box size in phi/psi: These parameters define how accurate to identify the zone axes in Hough map. It is set as 5 and 8 in most cases. But they should be enlarged in the case that the peaks are smeared;

Least intsec Line: the least number of the peaks included in a valid zone axis;

Peak involved: The fraction of peaks used for the zone axis identification. It should set from 0 to 1. If all peaks are involved, you can input "all".

Largest Index: The largest number in the possible zone axis indices. It is usually set as 4. For the material with relative small unit cell, such as metal, it should be set larger.

Zone for index: The number of the possible zone axes to be used for indexing the identified zone axes. Click "REC" button on the right side, PYXIS will calculate the theoretical minimum value of "Zone for index" under the current geometry setup and sample crystal structure. Practically, it should be set larger than the minimum value.

Zone angular Tol: The maximum acceptable deviation between the theoretical zone axis and the identified one.

Peak angular Tol: The maximum acceptable deviation between the theoretical Laue peak and the experimental one.

Including angular Tol: It is one more step to filter the possible incorrect indexed Laue peak. It should be set as same as Peak angular Tol as most cases. However, if the peaks are smeared, it should be set a bit less than Peak angular Tol.

Zone start set: The same as Start Set in Peak based index, but used for zone axes. Set as 4 in most cases.

Zone Threshold: This threshold has three operating modes:

- Minimum number of indexed zone axes required for a successful indexation. Input a single value.
- Minimum ratio of indexed zone axes to recognized zone axes, separated by a comma, and the minimum number required for a successful indexation. If the threshold generated by the ratio is less than the minimum number, the software will use the specified minimum number as the threshold.
- Minimum ratio of indexed zone axes to recognized zone axes, separated by a comma, minimum number, and maximum number required for a successful indexation. If the threshold generated by the ratio falls below the minimum or exceeds the maximum, the software will use the specified minimum or maximum number as the threshold.

Peak Threshold: This threshold also has three operating modes:

- Minimum number of indexed diffraction peaks required for a successful indexation. Input a single value.

- Minimum ratio of indexed diffraction peaks to recognized diffraction peaks, separated by a comma, and the minimum number required for a successful indexation. If the threshold generated by the ratio falls below the specified ratio, the software will use the specified minimum number as the threshold.
- Minimum ratio of indexed diffraction peaks to recognized diffraction peaks, separated by a comma, minimum number, and maximum number required for a successful indexation. If the threshold generated by the ratio falls below the minimum or exceeds the maximum, the software will use the specified minimum or maximum number as the threshold.

Calibration Refinement: Choose the experimental geometry parameters to be refined during the optimization of experimental geometry parameters.

Clustering: Import the partitioned results of diffraction peaks from the list of theoretically possible diffraction peaks. This file is used to expedite the indexation process. Click the "Load" button on the right side of the text box, select the .mat file for your crystal from the "peak\_cluster" folder in the PYXIS software installation directory. The software already provides .mat files for some common crystals. If the crystal structure you need is not available, enter the corresponding crystal structure in the "Crystal" section, then click the "Calculate" button to perform the calculation. After the calculation is completed, the software will prompt you to save the calculation results as a .mat file in the "peak\_cluster" folder.

De-Clustering: In this box, input the parameters required for de-clustering (identifying diffraction sub-peaks from the same subgrain cluster in the indexation):

- Use the "Check all Peak Series" button to select the de-clustering mode. For the situation with many diffraction peaks (e.g., quartz), it is recommended to keep this button turned off. For situations with fewer diffraction peaks (e.g., most metals), it is recommended to turn it on. If it's turned on, you don't need to input the "Weight Ratio" parameter below.
- Weight Ratio: The ratio of positional weight to intensity weight during the de-clustering process. A larger value gives more influence to the position of subgrain identification. Typically, this value is set between -0.2 and 0.2.
- Refine Ratio: Sensitivity to potential misidentification of sub-peaks during de-clustering. A larger value results in lower sensitivity, retaining more sub-peaks that may be incorrectly identified. Conversely, higher sensitivity leads to retaining fewer sub-peaks. Typically, this value is set between 0.7 and 1.
- Intensity Ratio: Sub-peaks within a cluster with intensities lower than the "Intensity Ratio" times the intensity of the strongest sub-peak in that cluster will not be recognized.

Use the "Show Missing Reflections" button to choose whether to calculate and display (manual indexation) or export (automatic indexation) the positions of missing reflections.

Use the "Judge Dauphine twin" button to decide whether to identify Dauphine twins in quartz based on diffraction peak intensities.

Click the "Export" button to export the configured parameters and save them as a .idp file, which is an ASCII-encoded text file.

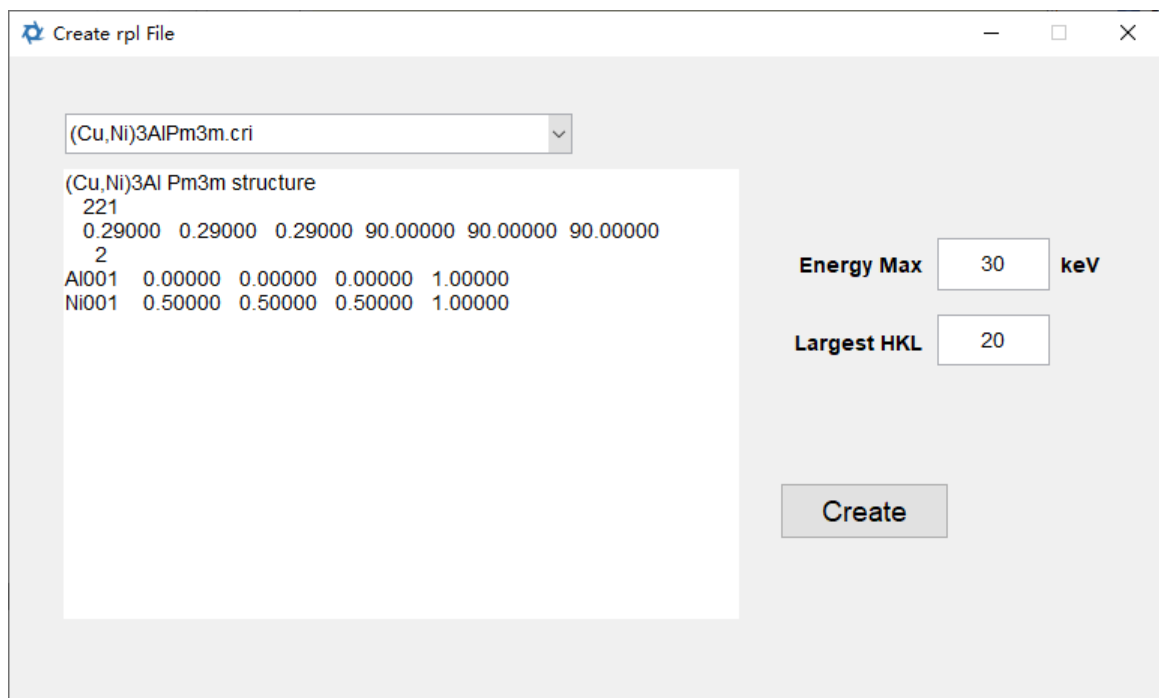
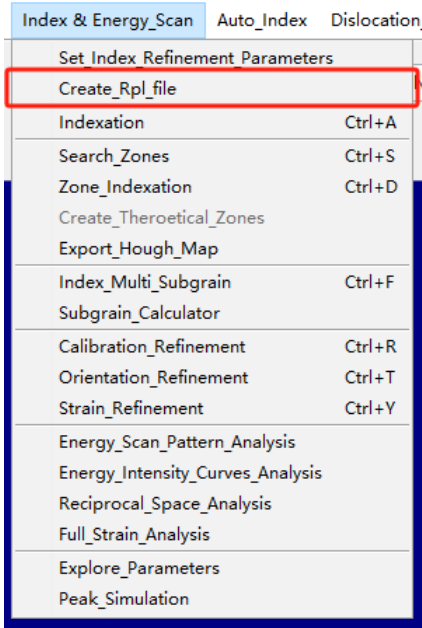
Click the "Import" button to import parameters from a .idp file.



Click the "Save" button to save the configured parameters. If you close the window, the software will automatically save the entered parameters.

## 2.3 Generation of the reciprocal lattice point list file(.rpl file)

The reciprocal lattice point list file for the material, stored in the .rpl file, contains the Miller indices and structure factors of possible diffraction peaks for this material. The interface and method for generating a new .rpl file are as follows:

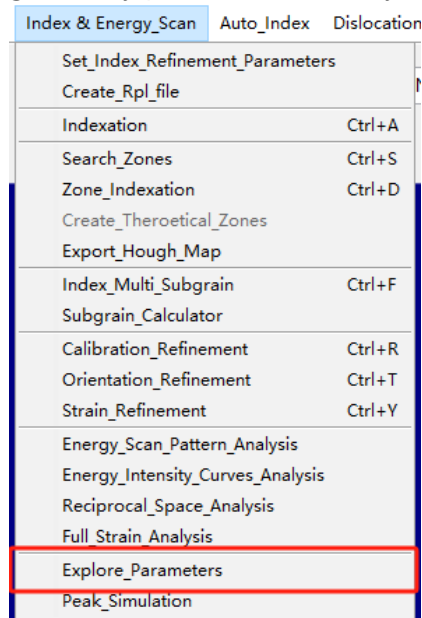


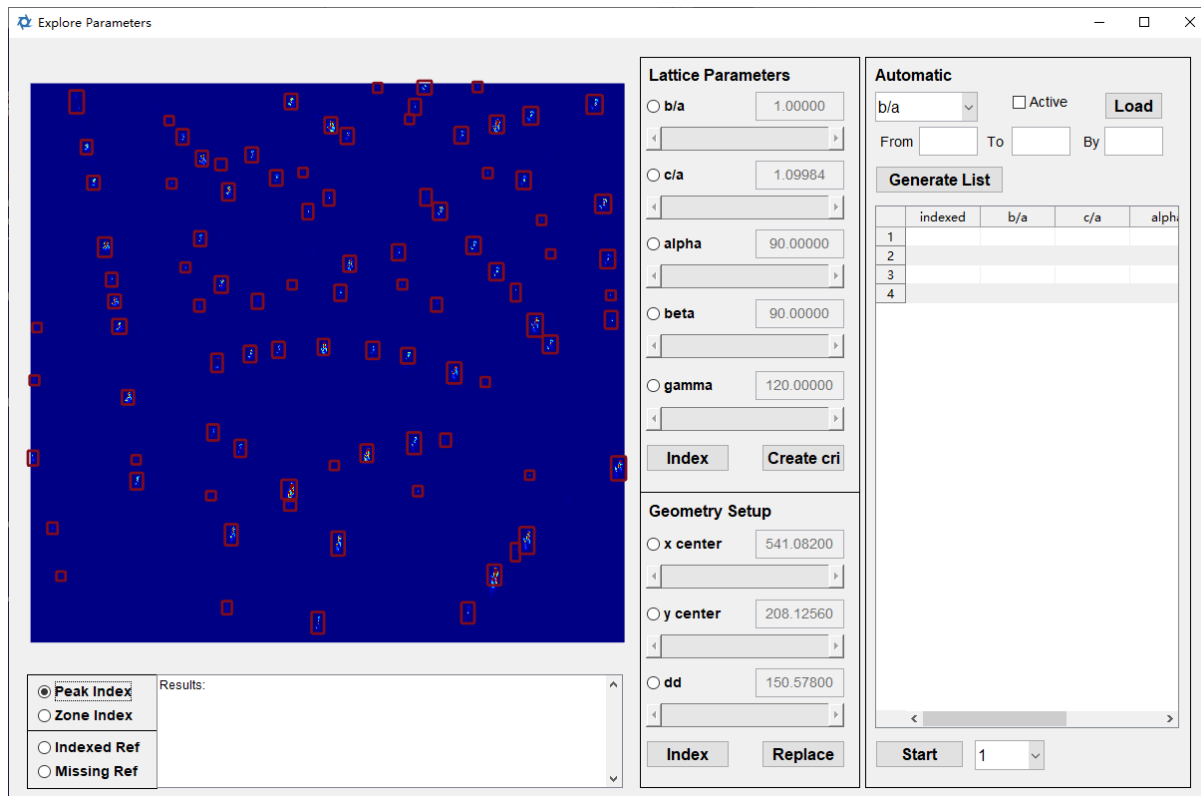
The method for generating a new .rpl file is as follows:

- From the dropdown menu, select the desired crystal structure. Once selected, the text box below will display the crystallographic information for that material.
- On the right side, enter the maximum X-ray energy and maximum Miller indices corresponding to the diffraction peaks to be included in the generated .rpl file in the "Energy\_Max" and "Largest\_HKL" fields, respectively.
- Click the "Create" button to initiate the generation process. The software will automatically save the generated .rpl file in the "rpl\_files" folder within the PYXIS software installation directory.

## 2.4 Iteration method for determining experimental geometry parameters and crystal parameters

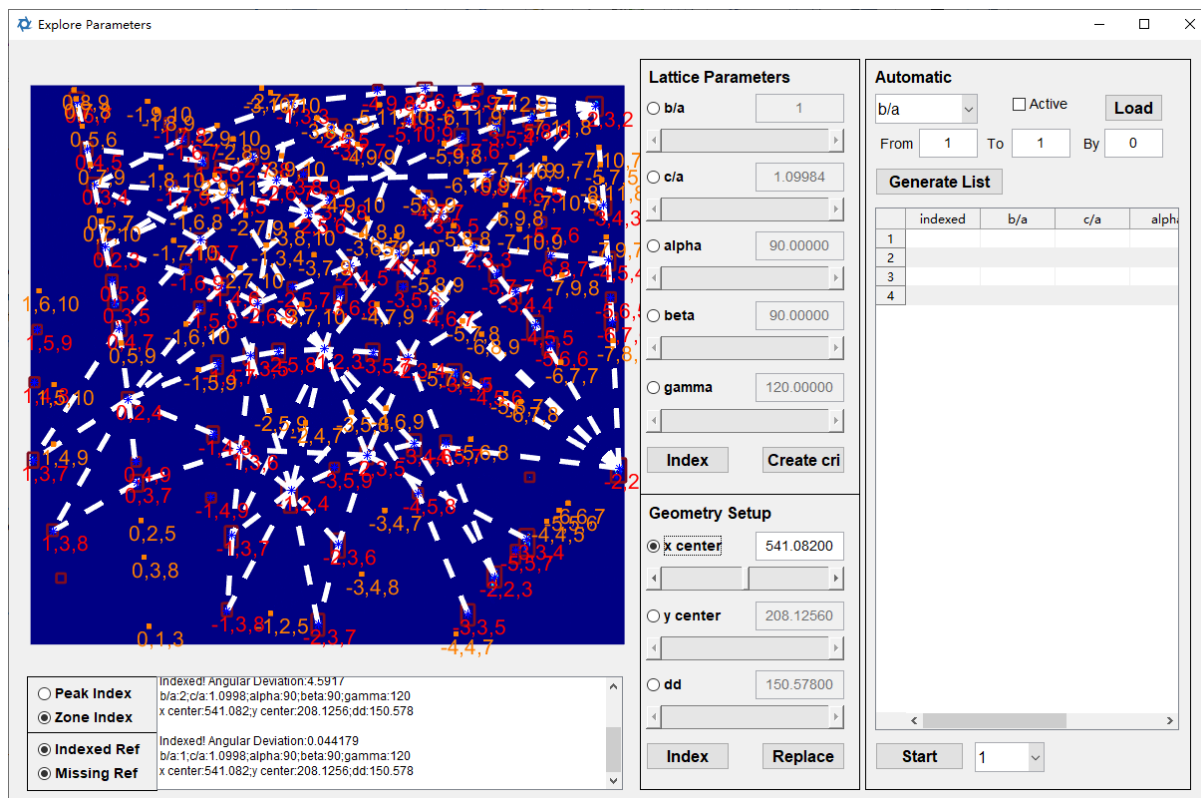
For newly adjusted experimental diffraction geometries or unknown crystals, it is not possible to determine their precise experimental geometry parameters and crystal parameters. In such cases, it is not feasible to carry out indexation and other analyses. Therefore, it is necessary to use an iterative method to approximate the experimental geometry parameters and crystal parameters in order to complete the indexation and other analyses. After peak searching (as detailed in Section 3.3) and correctly setting the indexation parameters, you can proceed with the iterative method to determine the geometry parameters and crystal parameters. The specific steps are as follows:





After opening, the software will automatically import the diffraction pattern currently displayed in the main interface and import the detected diffraction peaks. If peak clustering was used during peak detection, clustered diffraction peaks will be imported. Here is the manual parameter iteration method:

- Below the diffraction pattern, use the "Peak Index" or "Zone Index" buttons to choose whether to perform indexation based on diffraction peaks or zone axes. If you choose indexation based on zone axes, you will need to identify the zone axes in the main interface before proceeding.
- Activate the parameters in "Lattice Parameters" or "Geometry Setup" to manually iterate lattice parameters or experimental geometry parameters. The text boxes next to each parameter display the current value of that parameter. When activated, you can modify the parameters by editing the text boxes or dragging the sliders below each parameter. After making changes, click the "Index" button in "Lattice Parameters" or "Geometry Setup" to attempt indexation with the current modified parameters. If indexation is successful, the calibration results will be displayed on the diffraction pattern, and you can choose to display the indexed and missing diffraction peaks by using the "Indexed Ref" and "Missing Ref" buttons. The indexation results will also appear in the "Results" text box. If indexation fails, the "Results" text box will indicate the failure. A successful indexation interface is shown in the figure below.



When manually iterating through settings, if successful indexing is achieved, the parameters you have configured are roughly correct. If the "Lattice Parameter" parameters are activated, click the "Create cri" button to generate a crystal parameter file based on the current parameters. The software will prompt you to save this file in the "crystal\_file" folder located in the software's root directory. If the "Geometry Setup" parameters are activated, click the "Replace" button, and the software will use the currently configured parameters to replace the saved experimental geometry parameters.

The specific steps for automatic iteration are as follows:

- In the "Automatic" section, choose the parameter you want to iterate through from the dropdown menu, activate it by clicking the "Active" button, and set the starting point and step size for the iteration using the "From," "To," and "Step" fields. After activating and configuring the parameter, click the "Load" button to save the settings. Then, choose another parameter from the dropdown menu and repeat the same configuration process. Here, you can activate different lattice parameters or different experimental geometry parameters simultaneously, but you cannot activate both lattice parameters and experimental geometry parameters at the same time.
- After configuring all the settings, click the "Generate List" button. The list below will display all possible parameter combinations for the activated parameters. This is illustrated in the figure below.

**Lattice Parameters**

- b/a: 1
- c/a: 1.09984
- alpha: 90.00000
- beta: 90.00000
- gamma: 120.00000

**Geometry Setup**

- x center: 541.08200
- y center: 208.12560
- dd: 150.57800

**Automatic**

alpha: [dropdown]  Active

From: 88 To: 92 By: 1

	indexed	b/a	c/a	alp
1	0	1	0.9000	
2	0	1	0.9000	
3	0	1	0.9000	
4	0	1	0.9000	
5	0	1	0.9000	
6	0	1	1	
7	0	1	1	
8	0	1	1	
9	0	1	1	
10	0	1	1	
11	0	1	1.1000	
12	0	1	1.1000	
13	0	1	1.1000	
14	0	1	1.1000	
15	0	1	1.1000	
16	0	1	1.2000	
17	0	1	1.2000	
18	0	1	1.2000	
19	0	1	1.2000	
20	0	1	1.2000	
21	0	1	1.3000	
22	0	1	1.3000	
23	0	1	1.3000	
24	0	1	1.3000	
25	0	1	1.3000	

1 [dropdown]

**Legend:**

- Peak Index
- Zone Index
- Indexed Ref
- Missing Ref

Indexed! Angular Deviation: 4.5917  
b/a: 2; c/a: 1.0998; alpha: 90; beta: 90; gamma: 120  
x center: 541.082; y center: 208.1256; dd: 150.578

Indexed! Angular Deviation: 0.044179  
b/a: 1; c/a: 1.0998; alpha: 90; beta: 90; gamma: 120  
x center: 541.082; y center: 208.1256; dd: 150.578

- Click "Start" to begin indexation attempts for each parameter in the list. Parameters that are successfully indexed will be indicated in the "indexed" column in the first column of the list. After the iteration is completed, you can choose to display the indexation results of different parameters by selecting from the dropdown menu located to the right of the "Start" button.

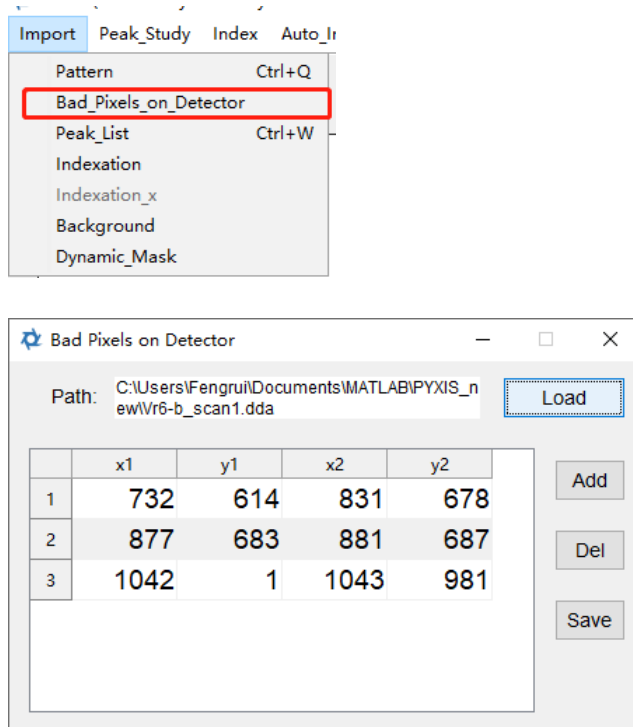
# **Basic Processing and Analysis of Patterns**

### 3 Basic Processing and Analysis of Patterns

#### 3.1

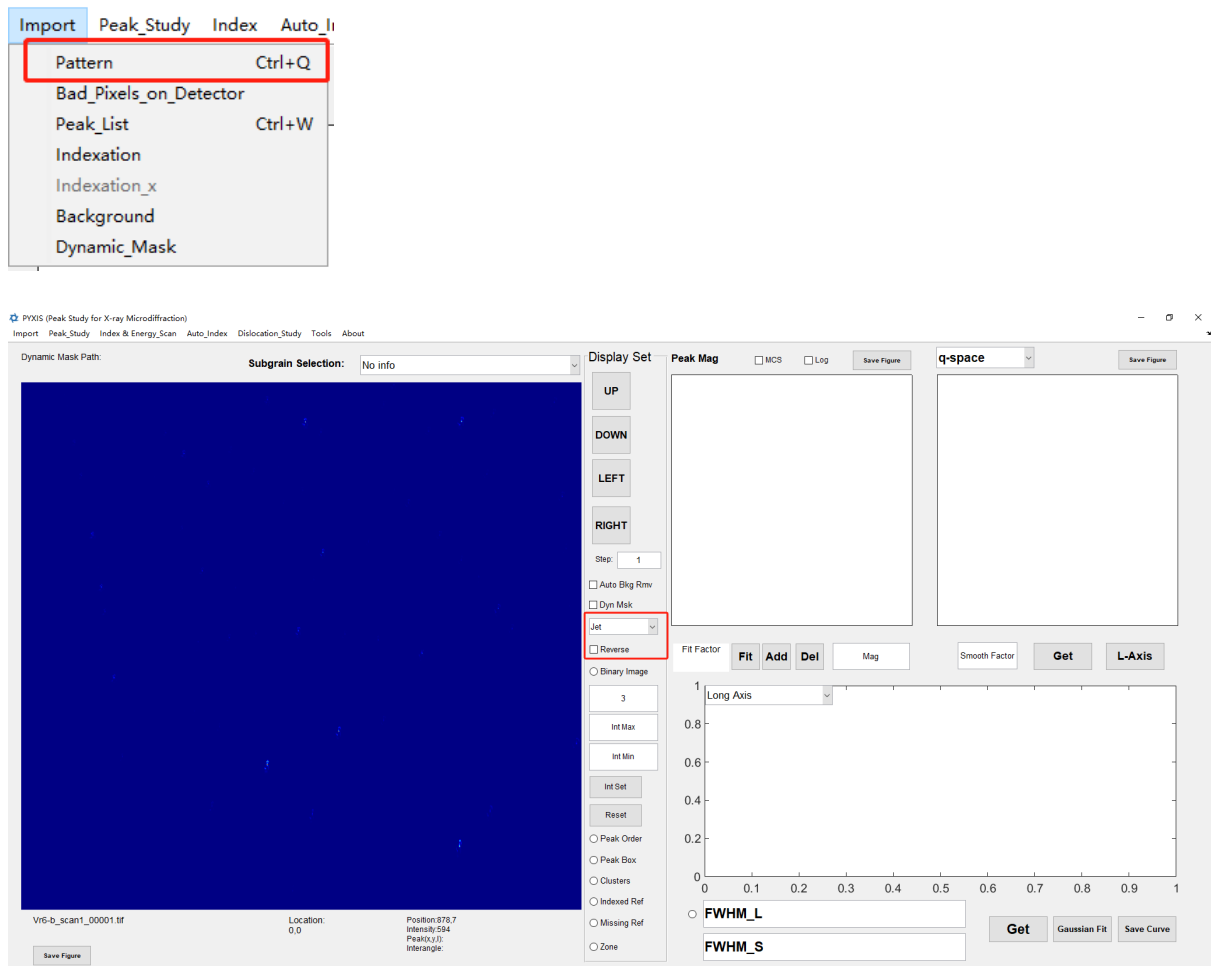
#### Pattern Import, Display Settings, Background Removal, and Binarization

- Before importing the pattern, it is necessary to set the malfunction areas on the detector. The specific method is as follows:



As shown in the figure, open the "Dead Area" window and input the coordinates of the lower-left and upper-right corners of each malfunction area in the table. Use the "Add" and "Del" buttons to add or delete rows. After entering the coordinates, click the "Save" button to save the inputted coordinates, and the software will prompt you to save the parameters as a "dda" file. When using them later, you can click the "Load" button to import the "dda" file.

- The steps for importing the pattern are as shown in the following figure:



As shown in the figure, after selecting the pattern file, the pattern will be displayed in the main window. The pattern is displayed using the "jet" colormap with pseudocolors. You can choose other pseudocolor schemes from the dropdown menu on the right side of the chart. By clicking the "Reverse" checkbox below, you can use the reversed pseudocolors. After importing the pattern in PYXIS software, the file name of the pattern and its current coordinates within the scanning area will be displayed at the bottom of the window. When the mouse is positioned over the pattern, the "Position" in the lower right corner of the pattern displays the X and Y coordinates of the mouse position (X is from left to right, and Y is from top to bottom, with the origin at the upper left corner of the pattern). "Intensity" shows the intensity at the mouse's current position, "Peak(x, y, I)" displays the x and y coordinates and intensity of the diffraction peak clicked by the mouse after peak searching (the intensity setting can be found in the experimental geometry parameter setup, as described in Section 2.1), and "Interangle" displays the angle between the diffraction vectors corresponding to two diffraction peaks clicked by the mouse after peak searching. The "Location" means the coordination of the point where the pattern was recorded in the scanned area.

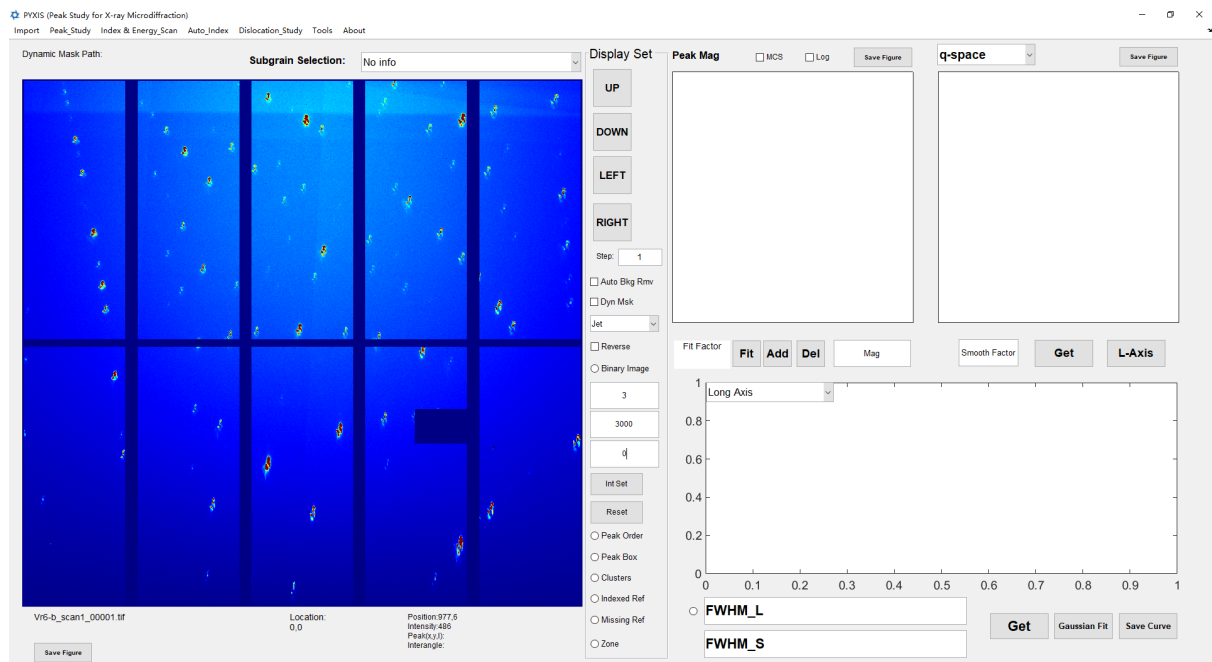


By clicking the "Save Figure" button below the pattern, you can save the pattern currently displayed on the screen. After peak searching and indexation, information about diffraction peaks, sub-peaks, indexation results, zone axes, and more will also be saved. The default resolution for saved images is 300dpi, but you can modify this resolution as described in Section 9.1.

- Display Settings

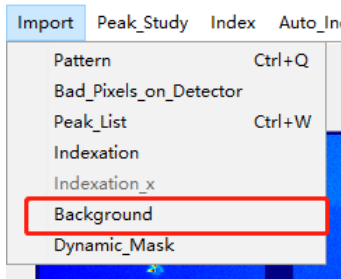
By entering the minimum and maximum intensity values in the "Int Max" and "Int Min" fields on the right side of the pattern, you can adjust the intensity levels for the pseudocolor display. For example, using the "jet" colormap as shown here, pixels with intensities higher than "Int Max" will be displayed in deep red, while pixels with intensities lower than "Int Min" will be displayed in deep blue. After adjusting the values and clicking the "Int set" button, all pixels with intensities higher than "Int Max" will be reassigned to "Int Max," and pixels with intensities lower than "Int Min" will be reassigned to "Int Min." You can click "Reset" to undo this reassignment.

The adjusted display effect is shown in the figure below:

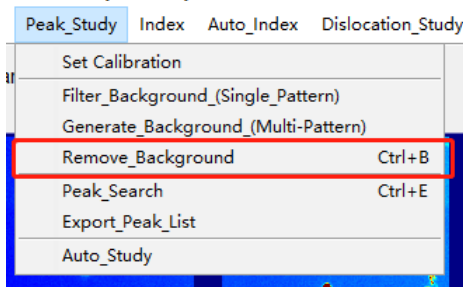


- Background Removal

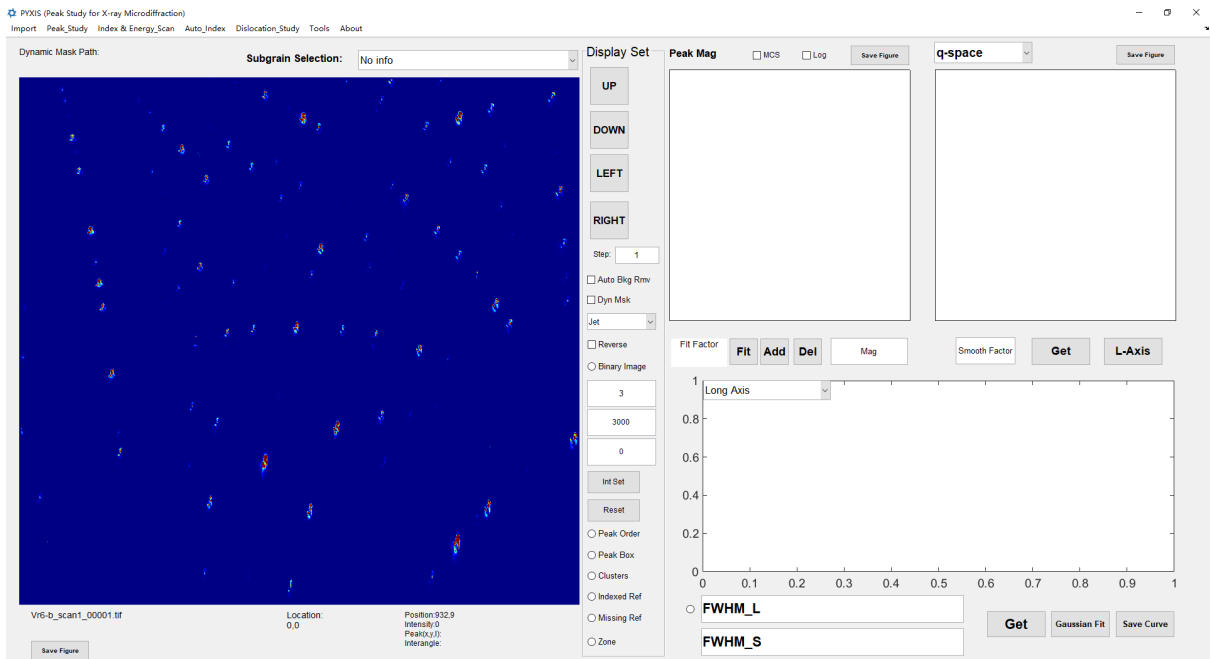
Here, background removal refers to the elimination of fluorescence background and detector noise from the pattern. Before performing background removal, it is necessary to calculate the experimental fluorescence background using typical diffraction patterns, as detailed in Section 3.2. Here, we will only introduce the methods for importing background files and performing background removal.



After clicking, select and import background files in TIFF format.



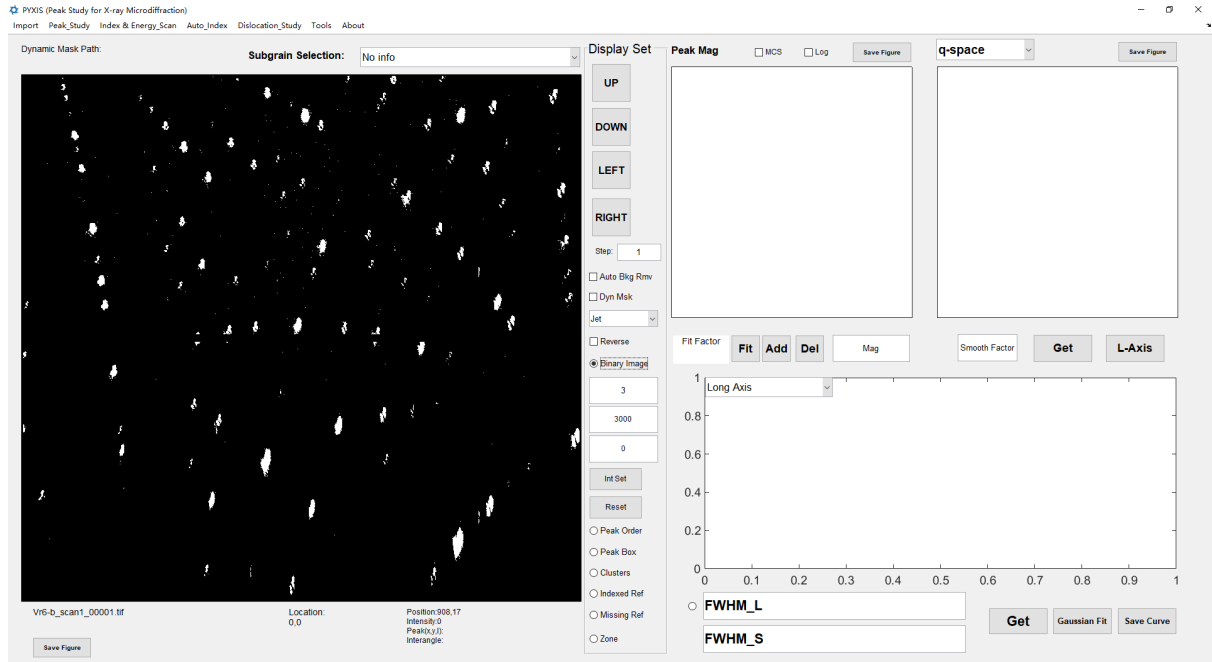
After clicking, the background removal is completed, and the effect of background removal is as shown in the figure.



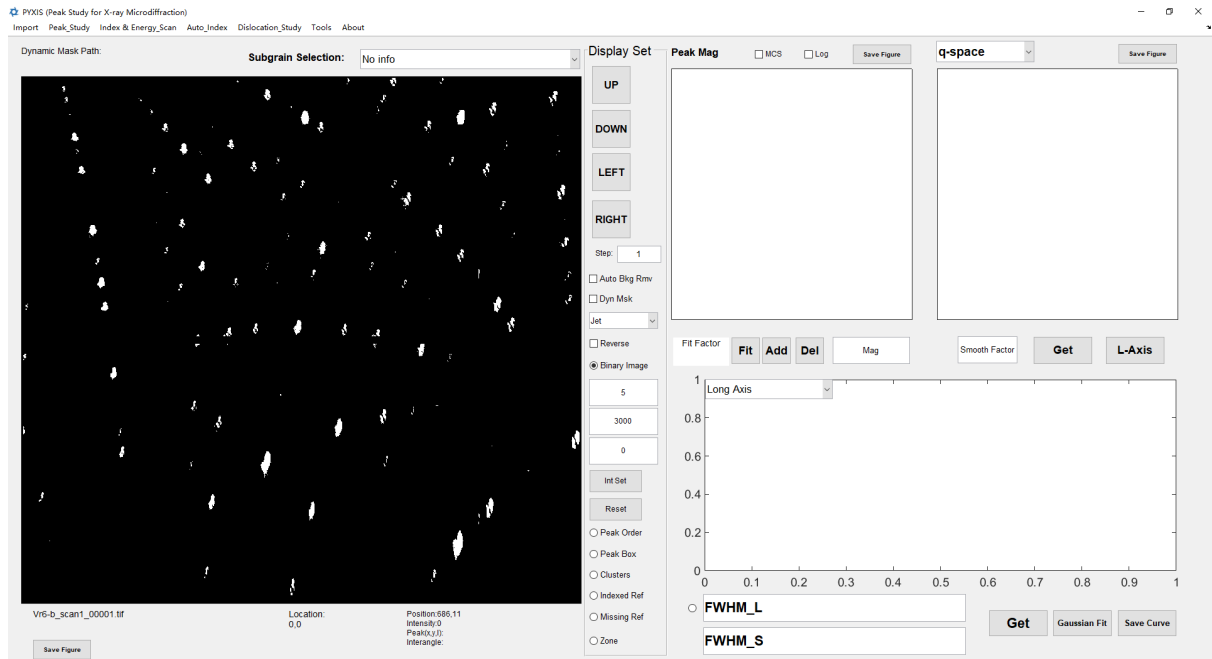
- Binarization

In PYXIS software, peak searching is performed based on binarized patterns, so appropriate binarization parameters are crucial for successful peak searching. The method for adjusting binarization parameters is as follows:

Click the "Binary Image" button on the right side of the pattern to display the binarized pattern. The effect is as shown in the figure:



Enter the appropriate binarization parameters in the "bin Filter" on the right side of the pattern. If background removal is required, please perform background removal again after each modification of the binarization parameters. The default value for binarization parameters is 3. The adjusted effect is as shown in the figure:



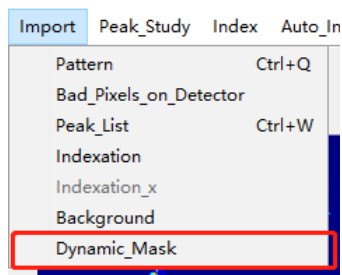
When you have adjusted the binarized pattern to a state where there is no obvious noise and the diffraction peak shapes are complete, the adjustment is complete, and you can proceed with the peak searching operation. Click the "Binary Image" button here to switch back to displaying the pattern using pseudocolors.

- Pattern Switching

By clicking the UP, DOWN, LEFT, or RIGHT buttons on the right side of the pattern, you can switch to the pattern above, below, to the left, or to the right of the current pattern. If you need automatic background removal during switching, you can check the "Auto Bkg Rmv" checkbox. Modifying the "step" parameter below allows you to choose the number of steps between pattern switches.

- Dynamic Mask

In some cases, different masks may be needed for different diffraction patterns, and the Mask function described in Section 2.1 may not meet the requirements. Dynamic masks use files saved with diffraction peak positions in formats like pkl, idx, or stn as masks. The specific operating method is as follows:



After clicking, select the file path where the dynamic mask file is located. Once selected, the file header of the dynamic mask will be displayed in the upper left corner of the pattern. The actual dynamic mask file used combines this file header with the diffraction pattern number. You can choose whether to use the dynamic mask in manual and automatic peak searching by clicking the "Dyn Msk" checkbox on the left side of the pattern.

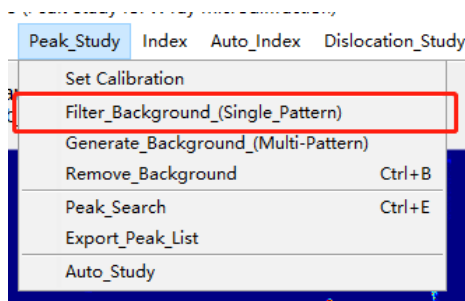
## 3.2 Background Acquisition

The software offers two methods to acquire the background of the diffraction pattern: using a single diffraction pattern and using multiple diffraction pattern. Below are the detailed instructions for using these methods.

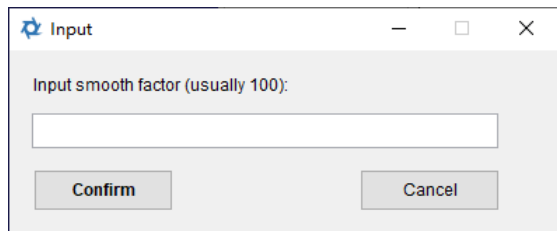
- Acquiring Background Using a Single Diffraction Pattern

This method applies median filtering to a typical diffraction pattern, filtering out the diffraction peaks and retaining only the background. Employing this method can effectively remove the background of the diffraction pattern. However, defective areas and larger diffraction peaks in the original diffraction pattern can impact the accuracy of the background. Therefore, if subsequent analysis requires examination of the shape of the

diffraction peaks, it is not recommended to use the background obtained by this method. The specific operation method is as follows.



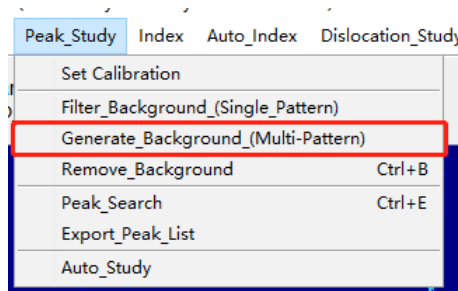
After clicking, the software prompts users to enter the size of the median filtering kernel, in pixels, typically a value of 100 is used.



After completing the median filtering, the software will prompt users to save the obtained background as a .tif file for later import and use.

- Acquiring Background Using Multiple Diffraction Patterns

In this method, diffraction peaks from several diffraction patterns, where the peaks are located differently, are eliminated, and the remaining background information is averaged to obtain background information at all positions of the diffraction pattern. The background information obtained through this method is more accurate and is not affected by defective areas and diffraction peaks in the original pattern. If the subsequent analysis requires examination of the shape of the diffraction peaks, it is recommended to use the background obtained by this method. The specific operation method is as follows.

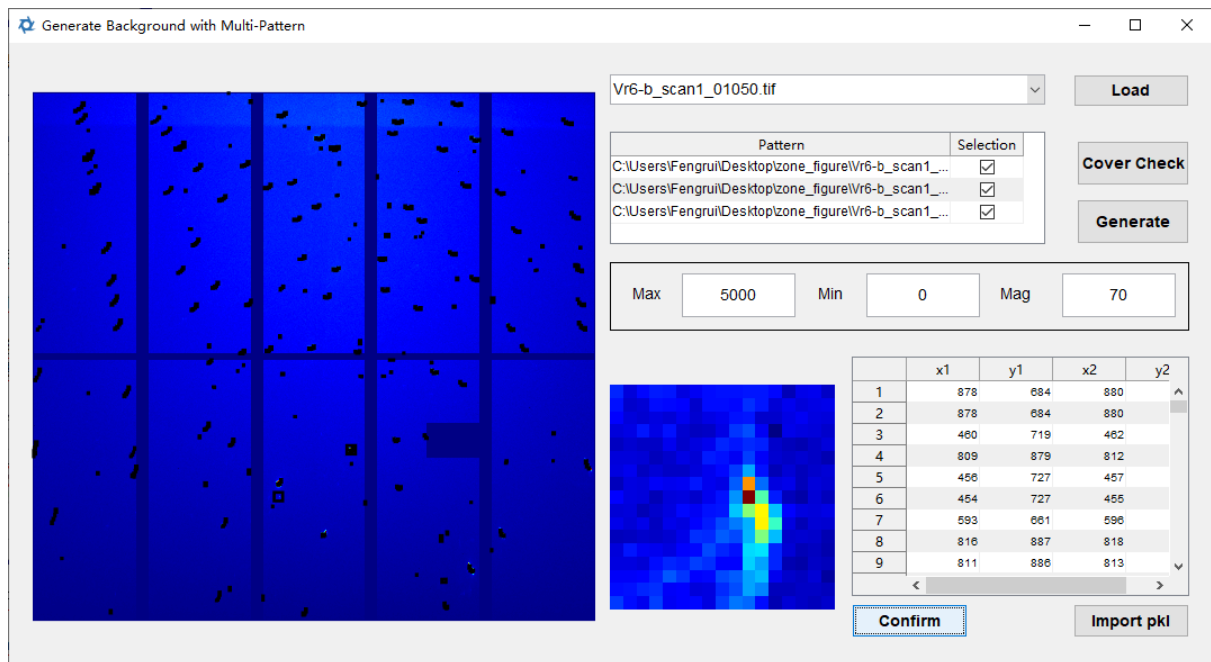


After clicking, the software opens a window for the feature that acquires background from multiple diffraction patterns.

Click the "Load" button on the right to import diffraction patterns. The names of the imported diffraction pattern files will be displayed in the list below, and you can switch the diffraction pattern displayed on the left via the dropdown list above the list. By setting the values of "Max" and "Min," you can change the range of the false-color display in the pattern to clearly show the diffraction peaks.

Click the "Import pkl" button to import a pkl file containing the peak-finding results of this diffraction pattern (for the peak-finding method, refer to section 3.3). The range information of the imported diffraction peaks will be displayed in the table above, where (x1, y1) and (x2, y2) represent the coordinates of the lower-left and upper-right corners of the diffraction peak range, respectively.

Left-click on the diffraction pattern, and you can get a magnified image of the clicked position. You can adjust the magnification by modifying the "Mag" value or using the mouse wheel on the magnified image. Click the "Confirm" button to add the range of the magnified image to the list of diffraction peak ranges, as shown in the image below.



By right-clicking on the diffraction pattern, you can delete the diffraction peaks at the clicked position from the list of diffraction peak ranges.

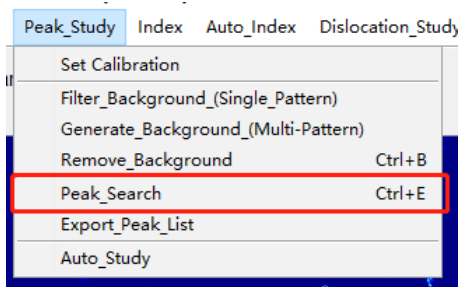
Toggle between different diffraction patterns and import the list of diffraction peak ranges for each pattern. Then, click the "Cover Check" button to verify whether every position is covered by the diffraction patterns. Overlapping diffraction peak ranges may cause some parts not to be covered; such ranges will be deleted after the check.

If the check is successful, clicking the "Generate" button will produce the background, and the software will prompt to save this background in .tif format for later import and use.

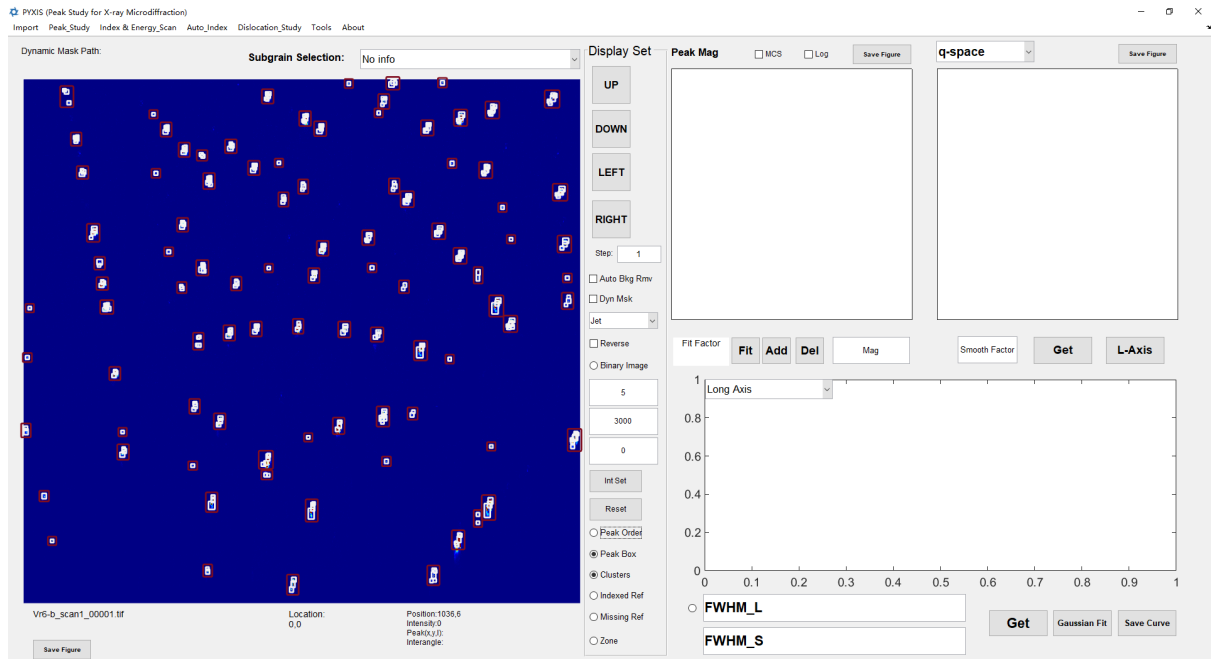
### 3.3 Peak Searching, Supplement and Deletion of Peak, and Export of Peak Searching Results

After setting appropriate binarization parameters, peak-searching parameters, and experimental geometric parameters, you can proceed with the peak-searching operation. PYXIS identifies diffraction peaks by recognizing the white patches in the binarized pattern. Among them, the peak-searching parameters, Box Size Max and Box Size Min, respectively represent the maximum and minimum lengths of one side of the bounding rectangle around a recognized patch (measured in pixels). Patches outside this range will not be recognized. When there are two sub-peaks within a patch that need to be identified separately, you can adjust the parameter Climb Level. The higher the Climb Level value, the better the precision in identifying sub-peaks, but it will also take more time. If there is no need to identify sub-peaks, Climb Level should be set to 0.

The peak-searching operation is illustrated in the image below:



After the peak-searching operation, the searched diffraction peaks will be marked with white boxes in the displayed pattern. If the number of searched diffraction peaks is less than 50, each diffraction peak will also be labeled with a number in descending order of intensity. If clustering for sub-peaks is enabled, the classes of sub-peaks will be marked with red boxes. The effect is shown in the picture:



By clicking on “Peak Order” and “Peak Box” at the bottom right side of the pattern, you can control the display of the order numbers and the boxes around the diffraction peaks, respectively. Clicking “Cluster” in the same area can control the display of the red boxes around clustered sub-peaks.

It needs to be noted that the following features mentioned above can all be modified (for the modification method, refer to Section 9.1):

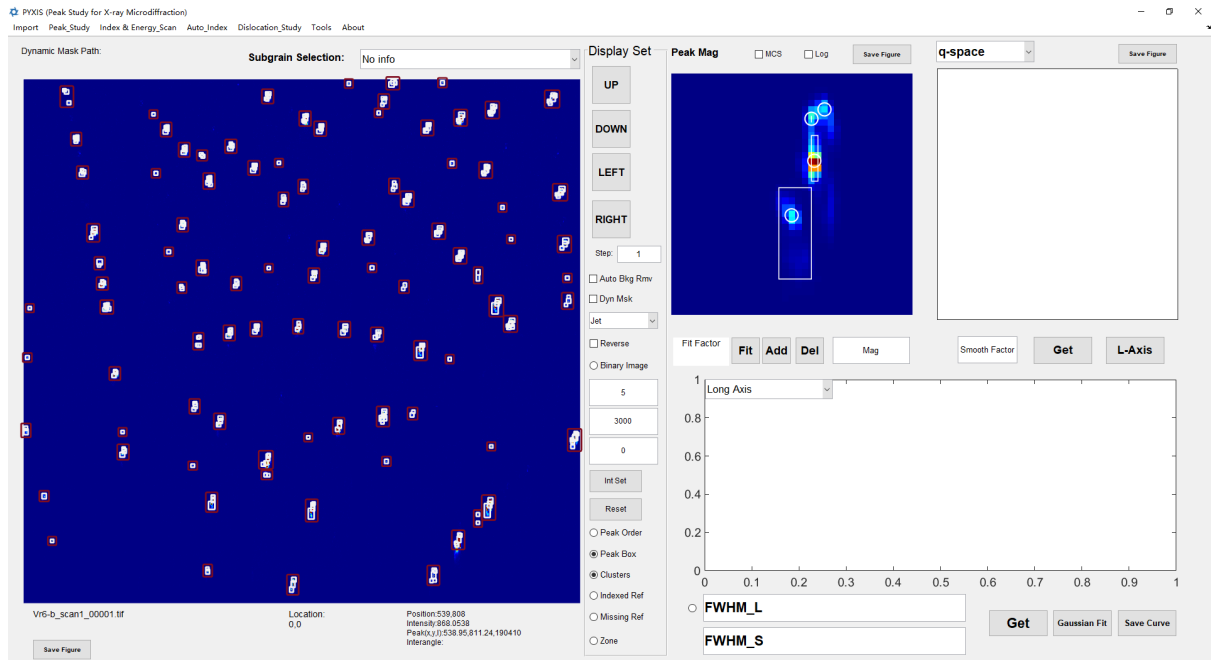
- The position, font size, and color of the text used to mark the order of diffraction peak intensity relative to the diffraction peak;
- The color of the box indicating the center of the diffraction peak;
- The line thickness and color of the box around the diffraction peak;
- The line thickness and color of the box around the clustered sub-peaks.

If any errors are found, or diffraction peaks are missed during the peak search, they can be deleted or added. The operation to delete diffraction peaks is as follows:

- Click on the erroneously found diffraction peak in the displayed pattern. At this point, a locally magnified diffraction pattern will be displayed in “Peak Mag” on the right side of the pattern. The magnification can be adjusted below the magnified image in the “Mag” column or by scrolling the mouse wheel over the magnified image (the default magnification is 30x). Clicking within the magnified frame allows for the adjustment of the magnification position. When the mouse is over the magnified image, the position and intensity displayed below the left pattern correspond to the position and intensity at the point on the magnified image where the mouse is located. The “MCS” (Modify Color Scale) checkbox above the magnified image can be used to make the color display method of the magnified image consistent with the left diffraction pattern, i.e., to change the false color range. The “Log” checkbox above the magnified image can be used to



display intensity in the magnified image in logarithmic form, highlighting weaker diffraction peaks. When the "Peak Order" display is enabled, the center of the diffraction peak in the magnified image will be represented by a circle. When "Peak Box" display is enabled, the range of the diffraction peak in the magnified image will be displayed as a box. The effect is as shown in the image:

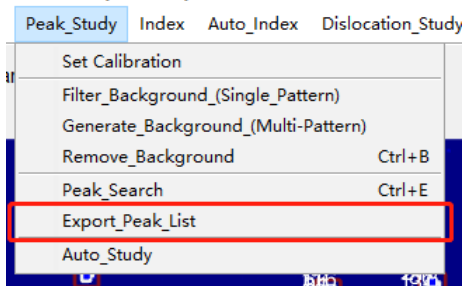


- Click the "Del" key to delete all the diffraction peaks in the magnified image.

The operation to add diffraction peaks is as follows, before manually adding diffraction peaks, you need to perform automatic peak search first.

- Click on the diffraction peak that needs to be added in the diffraction pattern, and the "Peak Mag" will display the magnified diffraction peak. If the magnification range is too large or too small, you can adjust the magnification to make the diffraction peak fully displayed properly.
- Click "Fit" to fit the diffraction peak in the magnified image; the fit's  $R^2$  value will be displayed in the "Fit Factor" column to judge the fitting effect. If the fitting is successful, click the "Add" button to the right of "Fit" to complete the addition of the diffraction peak.

After completing the peak search, you can export the results of the peak search, and the results will be stored as a .pkl file. This file uses ASCII encoding and can be opened and edited as text. The operation is as follows:



The parameters stored in the .pkl file are as follows:

X: The X-coordinate of the diffraction peak;

Y: The Y-coordinate of the diffraction peak;

Intensity: The integral intensity of the diffraction peak;

FWHM\_L: The half-width at half-maximum of the long axis of the diffraction peak\*;

FWHM\_S: The half-width at half-maximum of the short axis of the diffraction peak\*;

PB\_L/FWHM\_twotheta: Equivalent peak width of the long axis of the diffraction peak\* or the peak width of the integral in the 2theta direction (see Chapter 3.4 for details);

PB\_S/FWHM\_Chi: Equivalent peak width of the short axis of the diffraction peak\* or the peak width of the integral in the chi direction (see Chapter 3.4 for details);

BOX\_X: The X-coordinate of the upper-left corner of the bounding rectangle of the diffraction peak;

BOX\_Y: The Y-coordinate of the upper-left corner of the bounding rectangle of the diffraction peak;

BOX\_W: The width of the bounding rectangle of the diffraction peak;

BOX\_H: The height of the bounding rectangle of the diffraction peak;

R^2: The R^2 value of the diffraction peak fitting;

r^2 in long: The r^2 value of the Gaussian fitting of the peak shape of the long axis of the diffraction peak\*;

r^2 in short: The r^2 value of the Gaussian fitting of the peak shape of the short axis of the diffraction peak\*;

k1: Represents the elongation direction of the diffraction peak\*\*;

k2: Represents the elongation direction of the diffraction peak\*\*;

d\_climb: Represents the sub-peak parameters\*\*;

cluster\_num: Represents the sub-peak parameters\*\*;

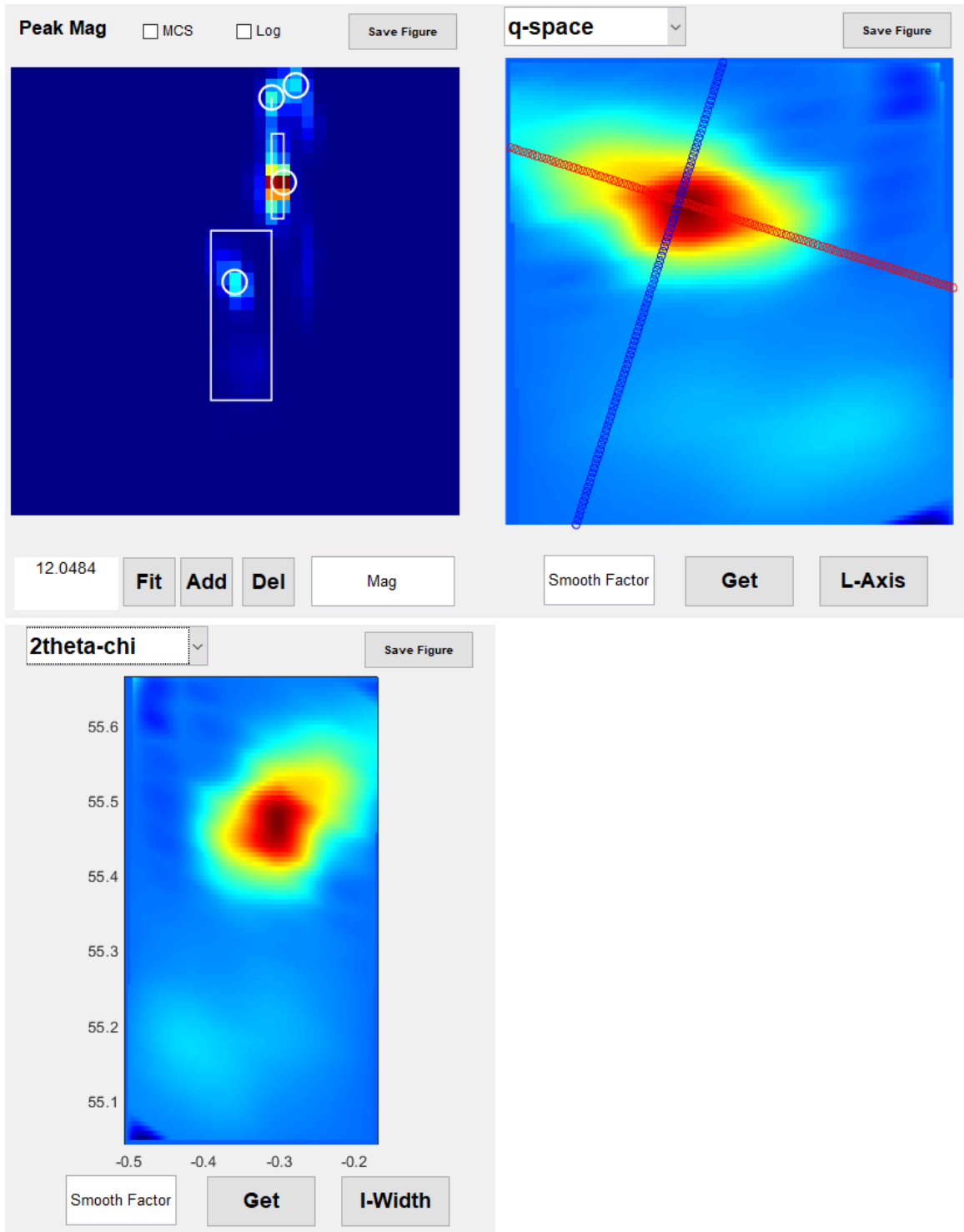
\*During manual peak searching, the elongation direction of each diffraction peak will not be sought, and the peak shapes of its long and short axes will not be extracted. Therefore, FWHM\_L and FWHM\_S in the output .pkl file here are calculated from the results of two-dimensional Gaussian fitting of the diffraction peak. PB\_L/FWHM\_twotheta and PB\_S/FWHM\_Chi are 0; r^2 in long and r^2 in short are 0;

\*\*k1, k2, d\_climb, and cluster\_num are internal parameters used for calculation. When editing the .pkl file, please do not modify them.

### 3.4 Peak Profile Analysis

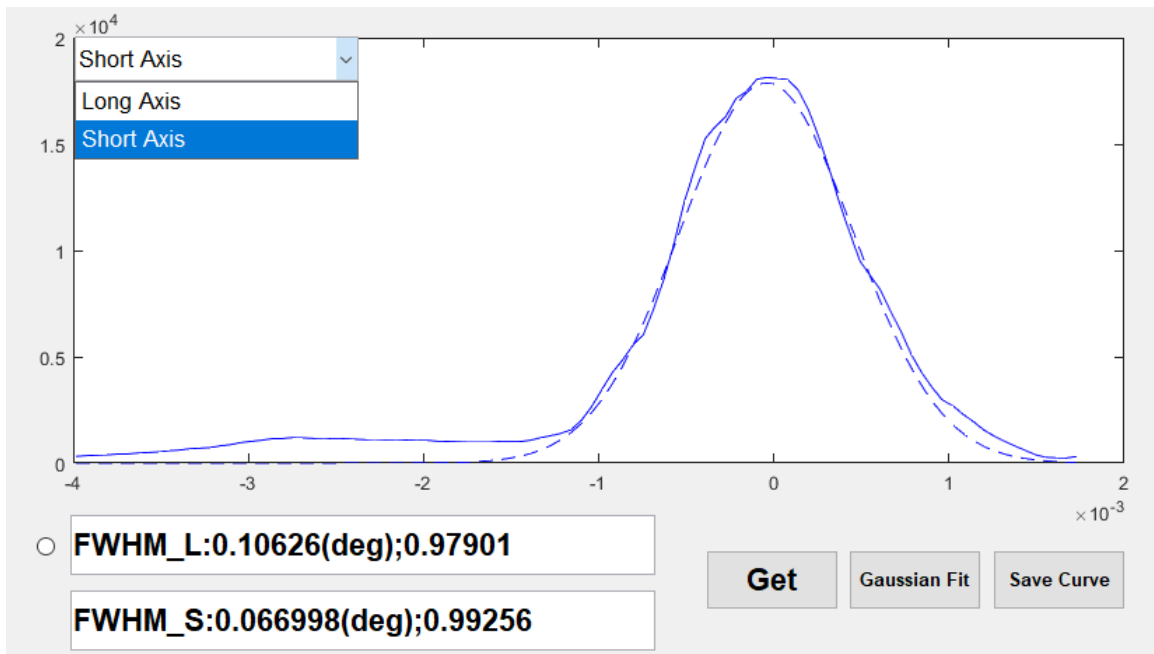
PYXIS provides the functionality to analyze the peak shape of diffraction peaks in q-space and 2theta-chi space. The operation is as follows:

- Click on the diffraction peak to be analyzed in the diffraction pattern. Adjust the magnification of Peak Mag so that the Peak Mag column displays the entire diffraction peak to be analyzed.
- Click the Get button below the box to the right of Peak Mag, and the box to the right of Peak Mag will display the peak shape in q-space. The drop-down menu above this box allows you to switch the display between the peak shape in q-space and the peak shape in 2theta-chi space.
- Click the L-Axis button to automatically find the long and short axes of the diffraction peak in the corresponding space and represent them with red and blue lines. If the automatically found long and short axes are incorrect, you can modify the direction of the long axis by clicking on both ends of the elongation direction. If the selected display is the peak shape in 2theta-chi space (with the vertical axis as the 2theta axis and the horizontal axis as the chi axis), this button becomes I-Width (Integral Width), integrating the intensity in the peak shape towards the 2theta axis and the chi axis respectively. The effect is shown in the figure:



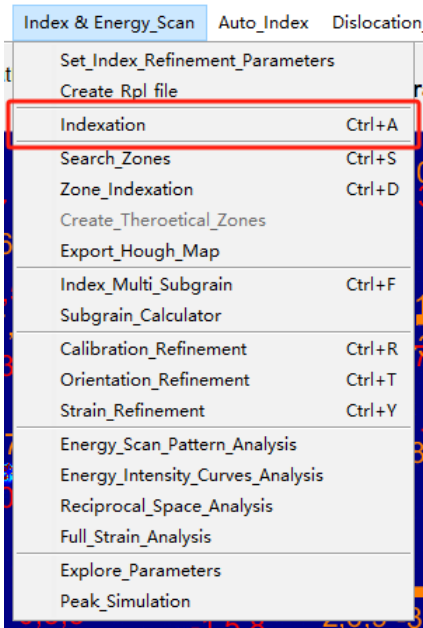
- By clicking each of the two 'Save Figure' buttons, you can store the two images on the left and right respectively.
- By clicking the 'Get' button at the bottom right corner of the window, you can display the peak shapes of the long axis or short axis in the lower right box. If you choose to display the 2theta-chi peak shape, it will show the integrated peak shape in the 2theta or chi

direction. By clicking the 'Gaussian Fit' button, you can fit the displayed peak shapes; the obtained half-height widths of the long and short axes are displayed in the text box on the left, and the  $r^2$  values from the fitting are displayed after FWHM\_L and FWHM\_S, separated by commas. By clicking the button to the left of the text box, you can toggle the display between half-height width and equivalent peak width. In the plots of the long and short axes, the horizontal axis unit is in radians. The effect is as follows:

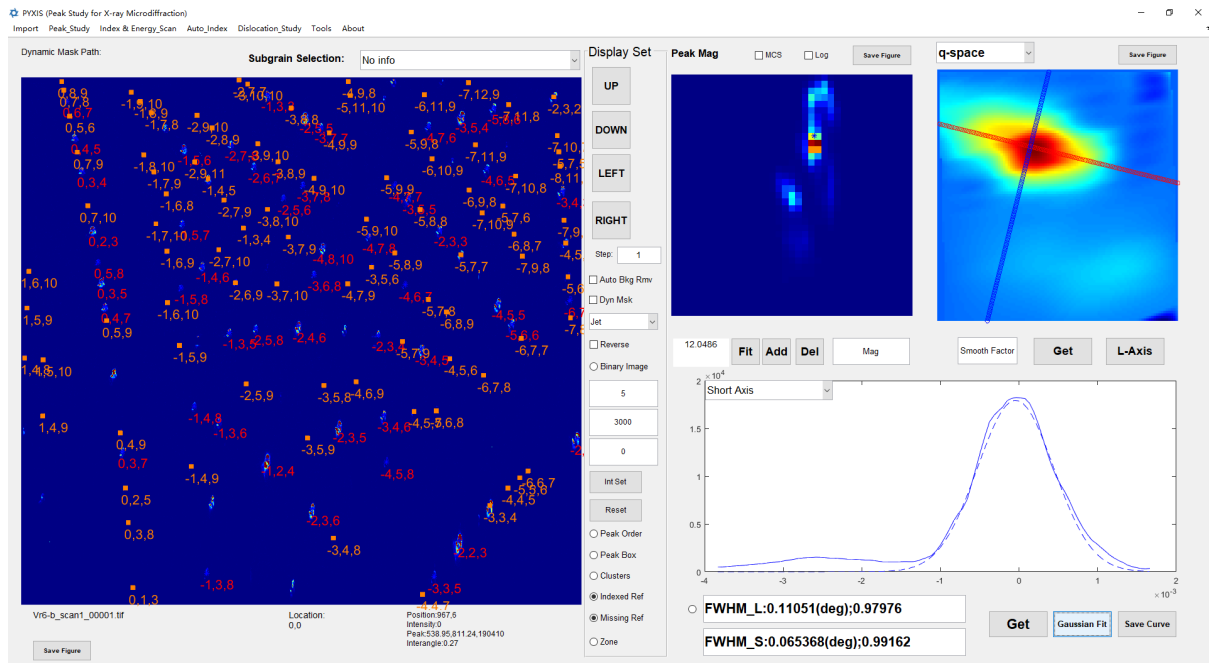


### 3.5 Indexation Based on Peak

After correctly entering the indexation parameters and completing peak searching, you can index the pattern. The specific operations are as follows:



After clicking, the software will start the indexation. Once the indexation is successful, the indexed and missing diffraction peaks will be displayed in the pattern. The effect is as follows:

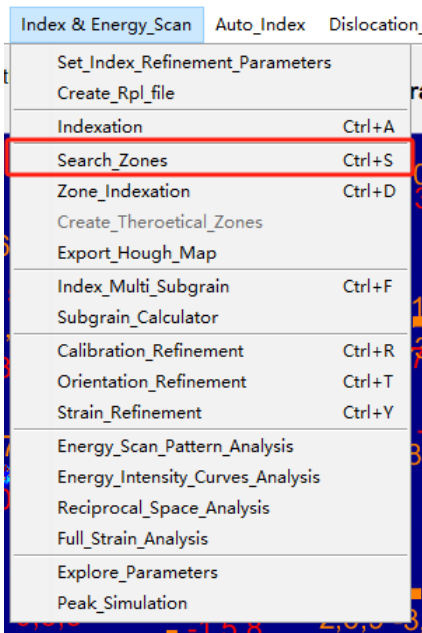


The Miller indices of the successfully indexed diffraction peaks are marked with red numbers, the positions of the diffraction peaks are marked with blue asterisks, the missing diffraction peaks are marked with orange numbers, and their theoretical positions are marked with orange squares. By clicking the 'Indexed Ref' button and the 'Missing Ref'

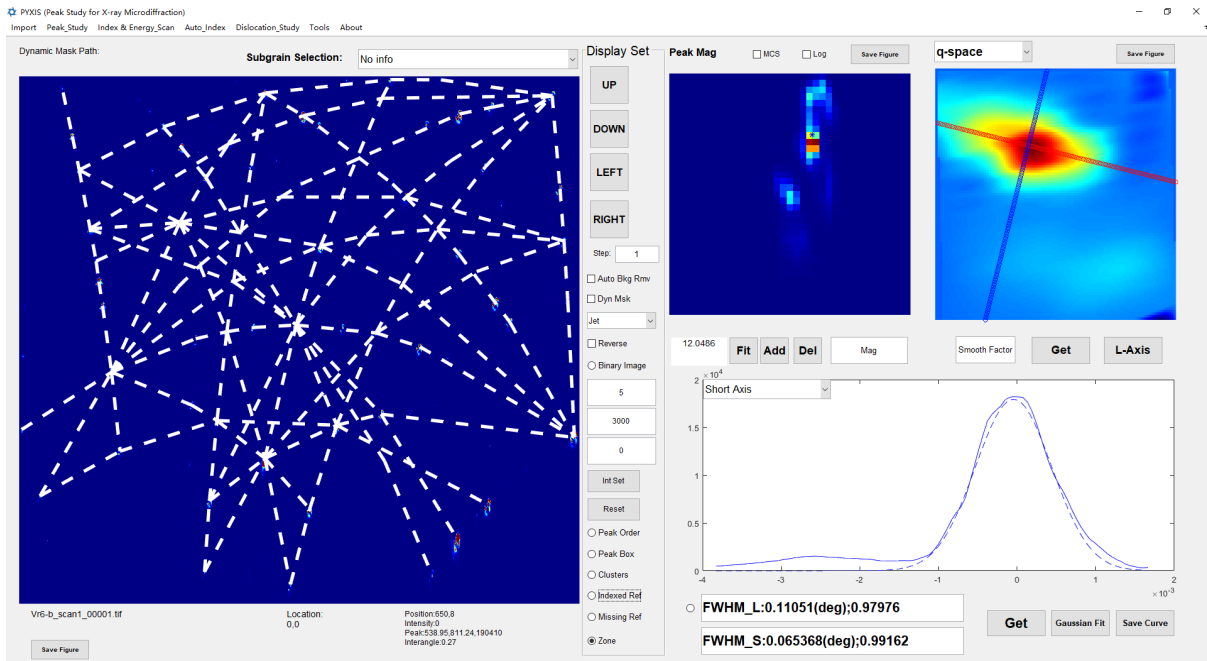
button on the right side of the pattern, you can toggle the display of the indexed diffraction peaks and the missing diffraction peaks.

### 3.6 Zone Axis Identification

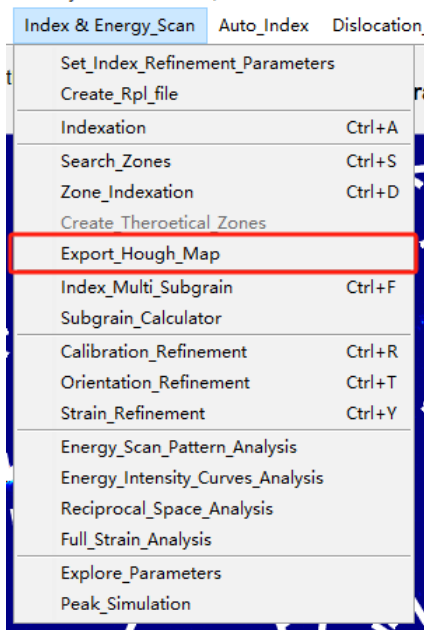
After correctly entering the indexation parameters and completing the peak search, you can proceed with the identification of the zone axis. The specific operations are as follows:



After clicking, the software will start the identification of the zone axis, and the diffraction peaks belonging to the same zone axis are connected by white dashed lines. You can choose whether to display these white dashed lines using the 'Zone' button on the right. The effect is as follows:

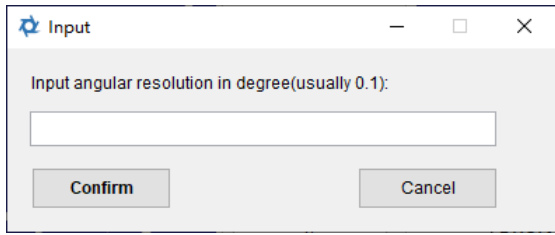


The identification of the zone axis uses the principle of the Hough transform. The following operation can be used to draw the Hough plot used during the identification of the zone axis.

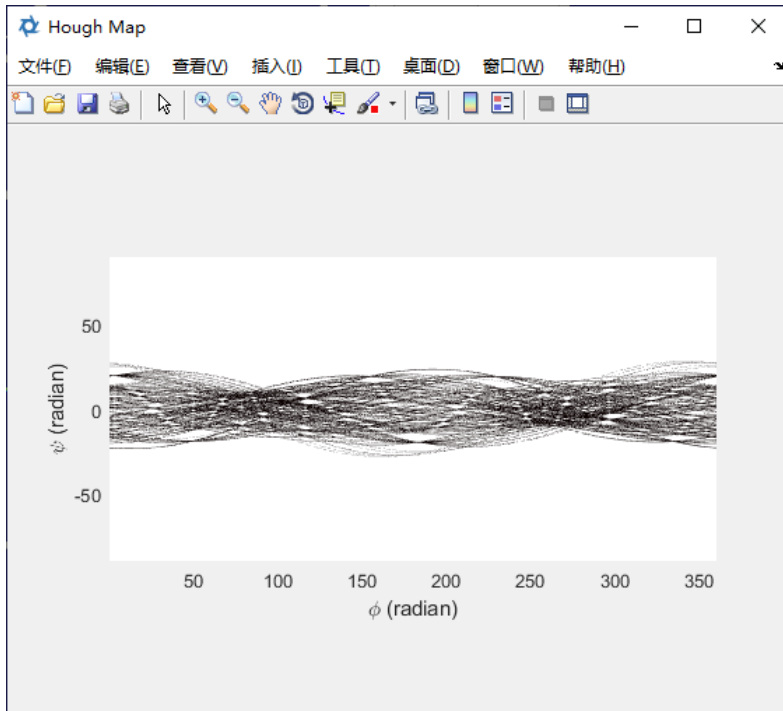


After clicking, you need to enter the resolution of the Hough plot to be drawn, generally taken as 0.1, with the unit in radians.



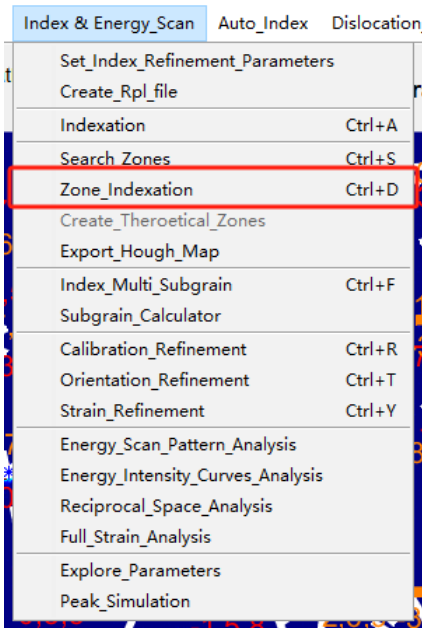


Here is the Hough map.

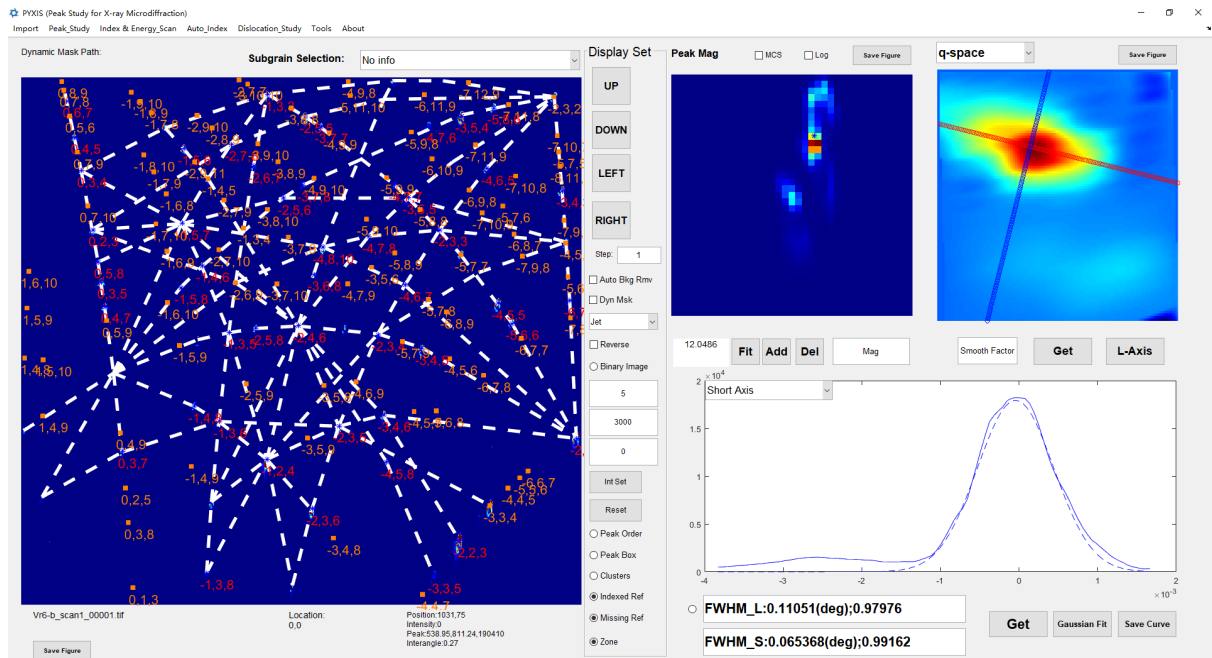


### 3.7 Zone-Axes Assisted Indexation

After correctly entering the indexation parameters and completing the identification of the zone axis, you can index the pattern. The specific operations are as follows:

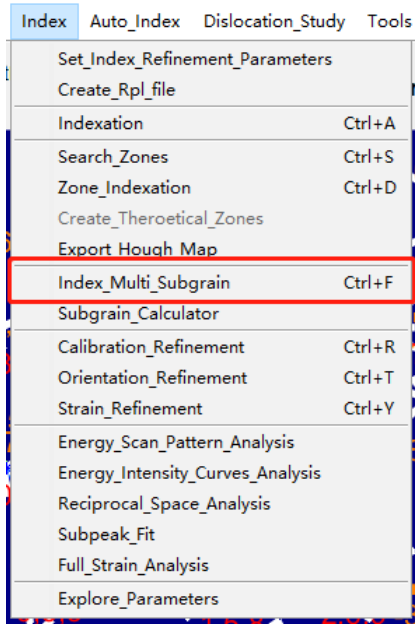


After clicking, the software will proceed with the indexation. Once the indexation is successful, the indexed and the missing diffraction peaks will be displayed in the pattern. The effect is as follows:

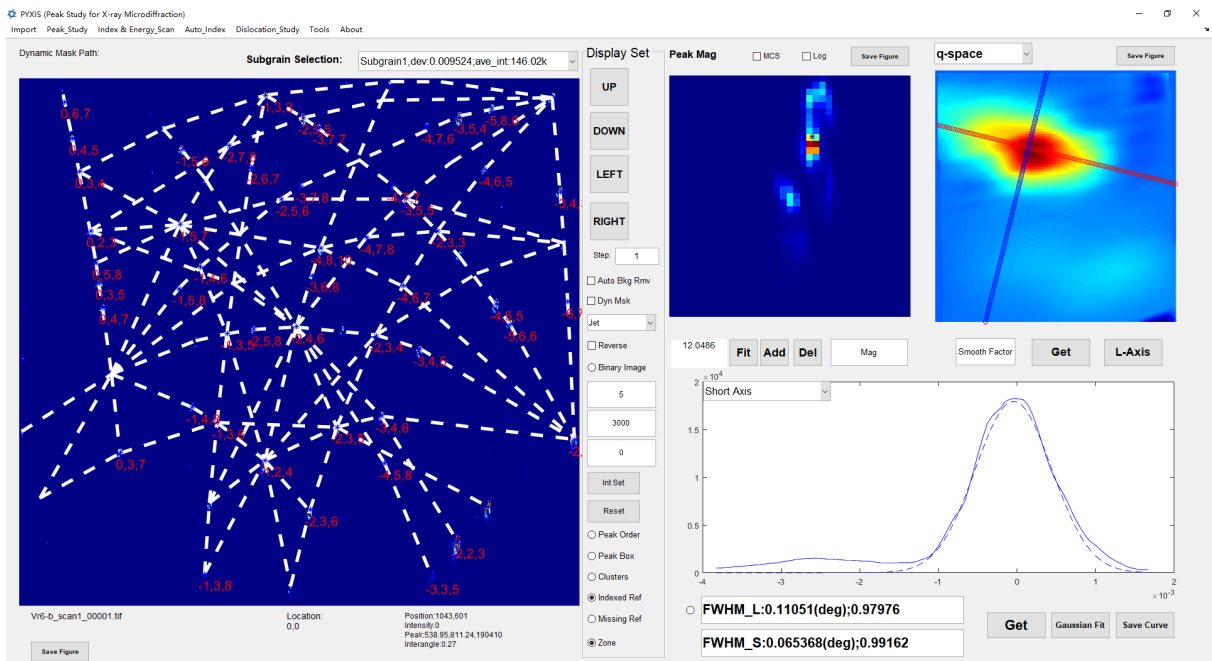


### 3.8 Multi-subgrain Indexation and Analysis

After indexing the clustered sub-peaks, multiple sets of subgrains can be indexed for different subpeaks. The specific operations are as follows:

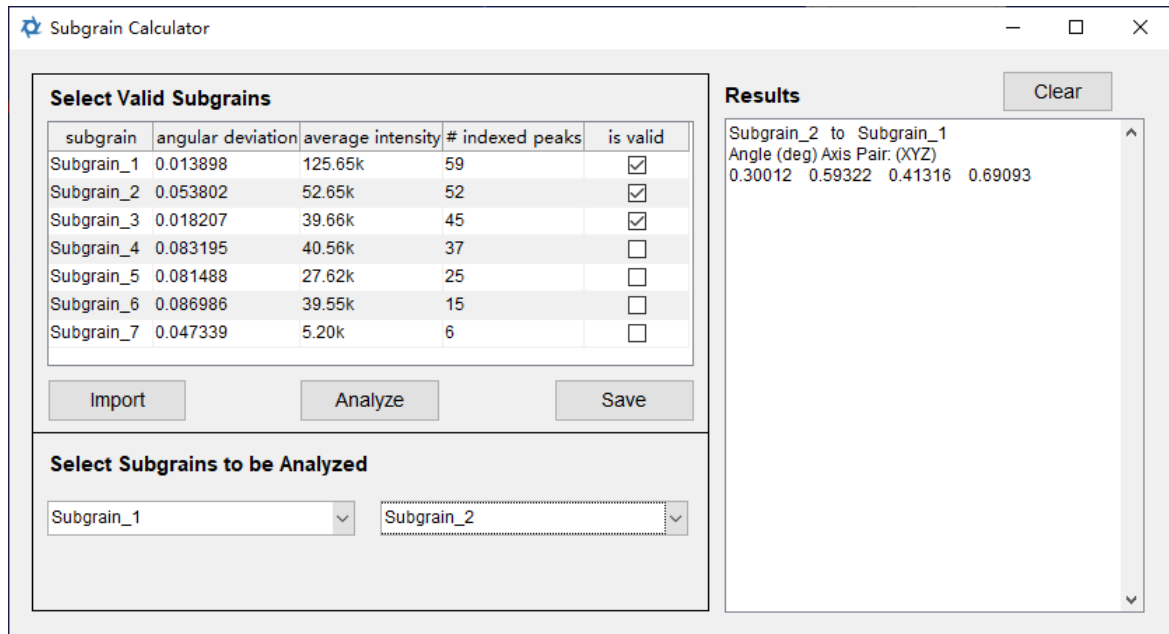
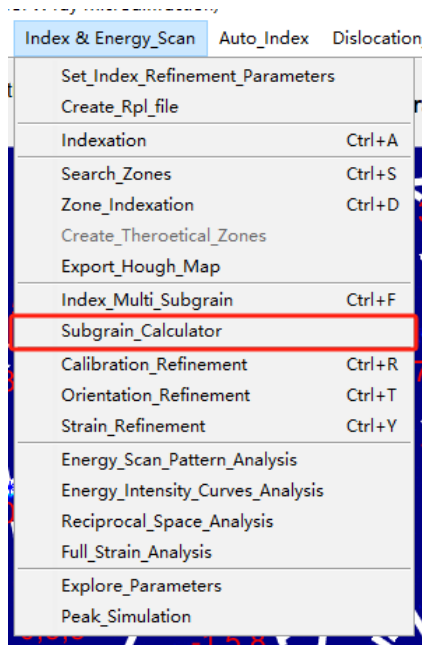


After clicking, the software will index all possible subgrans and display the indexation results in the dropdown menu above the diffraction pattern. By selecting from the dropdown menu, the oattern will display the diffraction peaks indexed for the chosen subgrain. It will look like the following after selection:



After selecting the indexed subgrain, you can perform orientation matrix and strain tensor calculations based on the diffraction peaks of the selected subgrain, with specific methods detailed in section 3.9.

After completing the indexation of multiple sub-crystals, you can use the subgrain calculator to calculate the orientation relationships between the subgrains. The specific method is as follows:



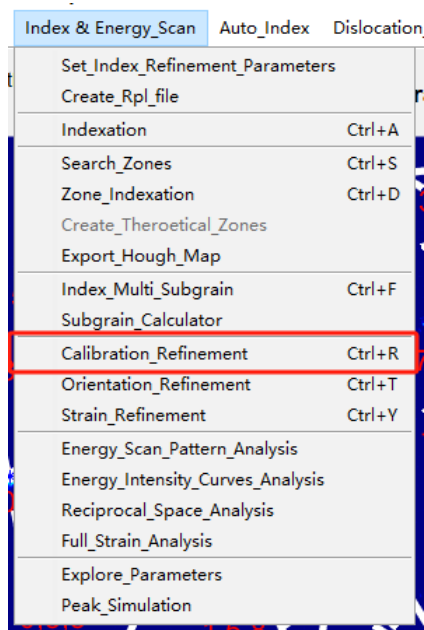
- In the table within the 'Select Valid Subgrains' box, judge whether the subgrains are valid based on the average angular deviation, average diffraction peak intensity, and the number of indexed diffraction peaks (# indexed peaks). Uncheck the invalid subgrains in the 'is valid' column.

- If you re-index multiple subgrains, click the 'Import' button to reimport the latest indexation results.
- After selecting the valid subgrains, click the 'Analyze' button to perform orientation and strain tensor fitting for each subgrain.
- After the fitting is complete, the two dropdown menus in the 'Select Subgrains to be Analyzed' box will import all the valid sub-crystals. By selecting subgrains in the two dropdown menus, the 'Results' box on the right will display the angular difference and rotation direction under the sample coordinate system between the two selected subgrains. Click the 'Clear' button above to clear the 'Results' box.
- Click the 'Save' button to save the results of the orientation refinement and strain tensor refinement in 'mid' and 'mst' files respectively.

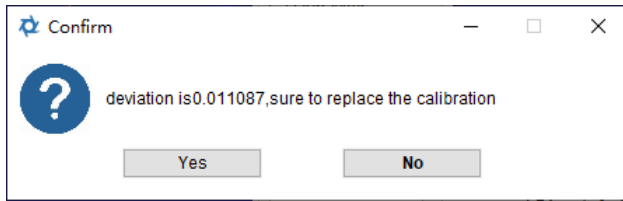
### 3.9 Calibration, Orientation, Strain Refinement

After completing the indexation of the diffraction peaks, you can refine the experimental geometric parameters, orientation matrices, and strain tensors.

- The operation for calibration refinement on experimental geometric parameters is as follows:

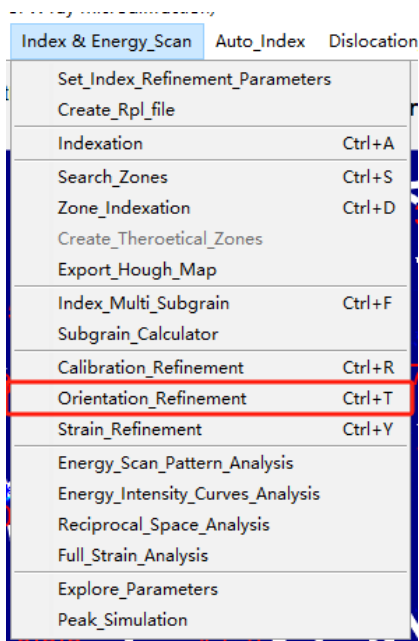


After clicking, the software will perform optimization calculations on the experimental geometric parameters. Upon completion of the calculation, the following dialog box will appear:



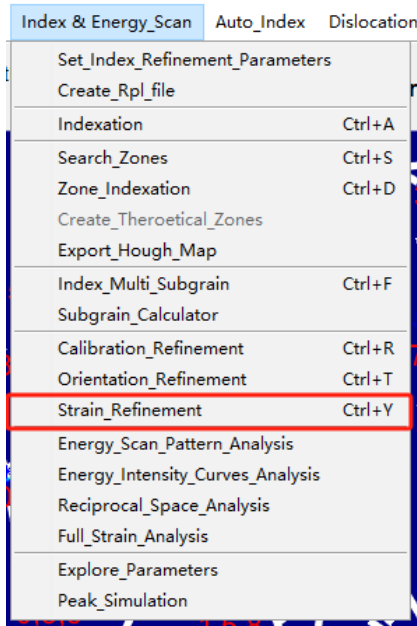
Here, 'deviation' refers to the average difference in angle between each diffraction peak after refinement and the theoretical value. If this value is small enough, it indicates that the refinement was successful; selecting 'Yes' can replace the previously entered experimental geometric parameters with the refined results. You can reopen the interface for entering experimental geometric parameters to view the final results. The settings for the experimental geometric parameters involved are specifically introduced in Section 2.1.

- The operation for orientation refinement is as follows:



After clicking, the software will perform refinement on the orientation. Upon completion of the calculation, the software will prompt to save the results as an 'idx' file. This file stores the indexation results of the diffraction pattern and the orientation matrix.

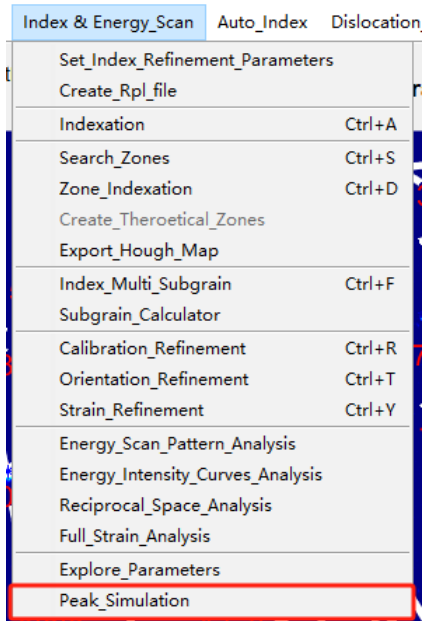
- The operation for strain refinement is as follows:



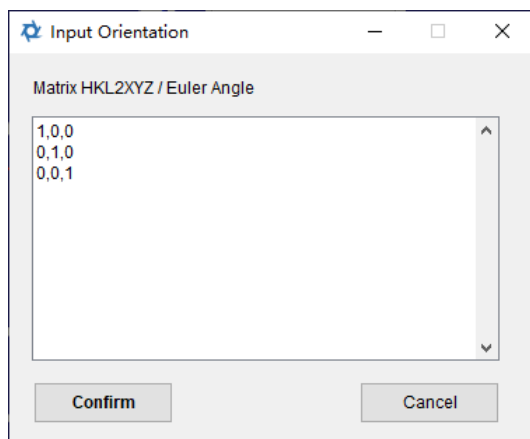
After clicking, the software will perform refinement on the strain tensors. Upon completion of the calculation, the software will prompt to save the results as an 'stn' file. This file stores the indexation results of the diffraction pattern and the strain tensor.

### 3.10 Simulated Peaks Generation

After completing the input of crystal information in experimental geometric parameters and indexation parameters, you can generate simulated diffraction peaks. The specific method is as follows:



After clicking, crystal orientation is required. The input format is either the orientation hkl to xyz matrix or Euler angles, with the three values of Euler angles separated by commas:



After clicking 'Confirm', the simulated peaks will be displayed on the pattern in the form of Missing Reflections.

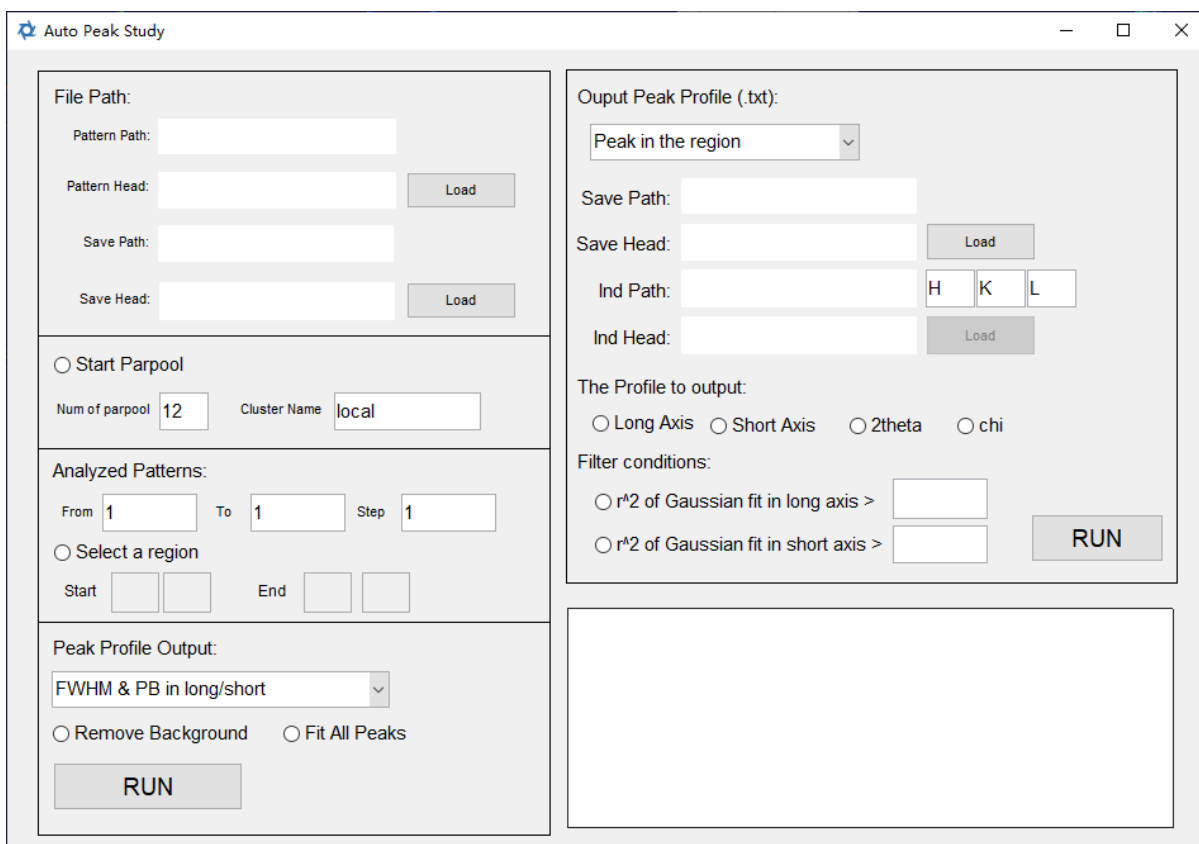
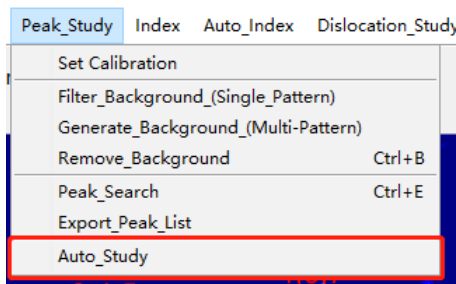


# Auto Peak Analysis

## 4 Auto Peak Analysis

### 4.1 Batch Peak Searching

Upon completing the settings for the experimental geometric parameters, peak search parameters, and binarization parameters for the diffraction patterns, you can proceed with the automatic peak search. The specific operations are as follows:



The interface can be divided into 5 regions. The specific steps to set up automatic peak searching are as follows:

1. In the File Path region, click the Load button at the top to select a pattern for automatic peak searching. The software will automatically record its path and filename prefix\*. All

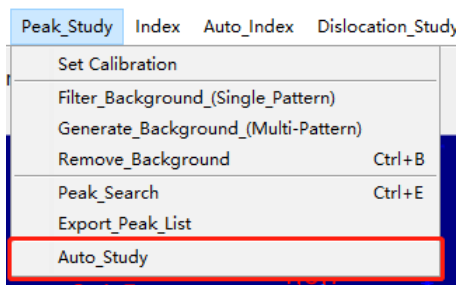
diffraction patterns that require automatic peak searching need to be in the same path and have the same filename prefix as this pattern.

2. In the File Path region, click the Load button at the bottom to set the save path for the pkl file, which will store the peak search results. The contents of the pkl file is detailed in Section 3.3.
3. If parallel computing is needed, click the Start Parpool button to enable parallel computing. Once enabled, the automatic peak searching process will use parallel computing. After parallel computing is enabled, no progress bar will be displayed. Num of parpool represents the number of parallel computations started, and Cluster Name represents the name of the cluster where parallel computing is located. These two parameters are determined by the hardware parameters of the computer running the software; please do not modify them unless necessary.
4. If you need to sequentially compute several patterns, you can directly enter the number of the first pattern\*, the number of the last pattern, and the interval between them in the From, To, and Step fields in the Analyzed Patterns region.
5. If you need to search peaks for diffraction patterns located in a certain region, you can enable the Select a region button in the Analyzed Patterns region and input the coordinates of the lower-left corner and upper-right corner of the desired peak searching area in Start and End, respectively.
6. Through the dropdown menu in the Peak Profile Output region, select whether to output the half-height width and peak width of the long and short axis in peak shape analysis or the half-height width of the long and short axis and peak width in the 2theta and chi directions.
7. In the Peak Profile Output region, click Remove Background to choose whether to remove the background from the pattern during peak searching.
8. In the Peak Profile Output region, use the Fit All Peaks button to decide whether to analyze the peak width of all diffraction peaks.
9. After completing the above settings, click the RUN button in the Peak Profile Output region to start automatic peak searching. If Select a region is enabled but Start Parpool is not, the white box on the right will display the progress of automatic peak searching synchronously.

\*When using all automatic analysis functions of PYXIS software, it is required that files of the same type (such as diffraction patterns, pkl files) be saved under the same path and have the same filename prefix. The naming convention for files is: filename\_prefix\_number.file\_type. For example, for a file named ALS\_Pure\_Ni\_00001.tif, the filename prefix is ALS\_Pure\_Ni\_, the number is 00001, and the file type is tif.

## 4.2 Output of Selected Peak Profile

After the automatic peak search is completed, this feature can be used to output the peak profile of certain selected diffraction peaks. The specific operating method is as follows:



 A screenshot of the 'Auto Peak Study' dialog box. The dialog is divided into several sections:
 

- File Path:** Contains four text input fields: 'Pattern Path', 'Pattern Head', 'Save Path', and 'Save Head'. Each field has a 'Load' button to its right.
- Start Parpool:** Includes a radio button, a 'Num of parpool' field with the value '12', and a 'Cluster Name' field with the value 'local'.
- Analyzed Patterns:** Includes a radio button, 'From' (1), 'To' (1), and 'Step' (1) fields, and a 'Select a region' section with 'Start' and 'End' fields.
- Peak Profile Output:** Includes a dropdown menu set to 'FWHM & PB in long/short', two radio buttons for 'Remove Background' and 'Fit All Peaks', and a 'RUN' button.
- Output Peak Profile (.txt):** Includes a dropdown menu set to 'Peak in the region', 'Save Path' and 'Save Head' fields with 'Load' buttons, 'Ind Path' and 'Ind Head' fields with 'H', 'K', and 'L' buttons and 'Load' buttons, and radio buttons for 'The Profile to output' (Long Axis, Short Axis, 2theta, chi).
- Filter conditions:** Includes two radio buttons for 'r^2 of Gaussian fit in long axis >' and 'r^2 of Gaussian fit in short axis >', each with a text input field, and a 'RUN' button.

Before performing peak profile parameters output, it is necessary to first import the path information of the diffraction patterns and the corresponding .pkl file path. The import method is as follows:

1. In the File Path area, click the upper Load button to import the path and filename prefix of the diffraction pattern file. Details regarding the diffraction pattern file path and filename prefix are specifically explained in section 4.1.
2. In the File Path area, click the lower Load button to import the file path and filename prefix of the .pkl file.
3. In the Analyzed Patterns area, enter the start, end diffraction pattern numbers, and step in the text boxes following From, To, and Step.

After successful import, select which method to use for selecting diffraction peaks from the dropdown menu at the top of the Output Peak Profile (.txt) area. The three methods for

selecting diffraction peaks and their corresponding setting methods are explained individually as follows:

1. Peak in the region: After selecting this method, switch to the main window and click on the location where the selected diffraction peak appears in the diffraction pattern, then check in the Peak Mag on the right whether the selected region includes the area where the diffraction peak appears. The software will finally output the peak profile curve of the diffraction peaks found by automatic peak searching in the Peak Mag area displayed, for each diffraction pattern.
2. Peak with highest Intensity: After selecting this method, the software will output the peak shape data of the diffraction peak with the highest integrated intensity found in each diffraction pattern during automatic peak searching.
3. Peak with particular HKL: After selecting this method, the software will automatically output the peak profile curve of a diffraction peak with a particular Miller index. After selecting this method, the lower Load in this area will be activated; click it and import the file path and filename prefix of the corresponding .idx or .ind file produced by XMAS software. Then, enter the HKL values of the diffraction peaks that need to be output in the three consecutive text boxes to the right of Ind Path.

Once the method of selecting diffraction peaks is determined and related settings are completed, the following steps are:

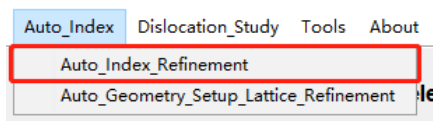
1. Select the storage path and filename prefix for peak shape data by clicking the upper Load button in this area.
2. Choose the peak profile curve that need to be output by clicking the Long Axis, Short Axis, 2theta, chi buttons. The specific peak profile curve refers to:
  - i. Long Axis: Intensity data on the long axis of the diffraction peak in q-space, output in the form of ASCII-encoded text data.
  - ii. Short Axis: Intensity data on the short axis of the diffraction peak in q-space, output in the form of ASCII-encoded text data.
  - iii. 2theta: Integrated intensity data of the diffraction peak in the 2theta direction, output in the form of ASCII-encoded text data.
  - iv. chi: Integrated intensity data of the diffraction peak in the chi direction, output in the form of ASCII-encoded text data.
3. If only the peak shape data that can be well fitted need to be output, click the  $r^2$  L or  $r^2$  S buttons and enter the critical value in the text box to the right. After setting, if the  $r^2$  value of the Gaussian fit of the peak profile on the long or short axis in q-space of the diffraction peak is less than this critical value, the peak shape data of this diffraction peak will not be output.
4. After completing all the above settings, click the RUN button in this region to start outputting the peak shape data of the selected diffraction peaks.

# Auto Peak Indexation

## 5 Auto Peak Indexation

### 5.1 PPC Assisted Indexation

After correctly inputting the experimental geometric parameters and completing the automatic peak searching, automatic indexation assisted by PPC can be used. The operating method is as follows:



As shown, the interface is divided into 5 areas. The steps for PPC-assisted indexation are:

1. Input File Path and Indexation Parameters.
  - Load the .pkl file obtained from automatic peak searching in the upper 'Load' button in the 'File Path' area. For definitions and requirements of the file path and prefix, refer to section 4.1.
  - If some diffraction patterns in the experiment are of extremely poor quality due to being outside the sample area or other reasons, click the 'Judge Valid' button to activate the diffraction pattern quality check. The software will exclude clearly unreasonable diffraction patterns during indexation.

- To set the storage path and prefix for indexation results, click the lower 'Load' button in the 'File Path' area. Possible files include:
    - i. .pkc file: stores PPC pre-indexation results
    - ii. .idx file: stores indexation results and orientation matrix
    - iii. .stn file: stores indexation results and strain tensor
2. Set PPC Related Indexation Parameters.
- Enter relevant parameters in Phase I. To index two phases simultaneously, activate the Phase II area by clicking the Phase II button and enter parameters for Phase II. Specific methods are as follows:
    - i. Load the idp file storing indexation parameters in the upper 'Load' button in Phase I. The software will auto-load the mat file based on the imported idp file. The method to generate idp file is included in section 2.2. If the mat file is not loaded automatically, it can be loaded manually by click "Load" button on the right side. The basic PPC parameters are AR and Nc. If the "Intensity Check" function is on, Nr and Ns are also required to be entered. The meaning of the PPC related parameters are explained in section 8.13.
    - ii. If the two phases indexed simultaneously have the same space group, 'Critical' and 'Missing' parameters also need to be entered for both phases.
3. Setting Experiment Area for Non-Distributed Calculation:
- Enter the coordinates of the lower-left and upper-right corners of the auto-indexation experiment area in 'Start' and 'End' in the 'PPC Analysis' area respectively. The coordinate of the lower-left corner of the whole scan area is set as (0,0).
  - Input the coordinate to start PPC in "Seed". The pattern at the coordinate will be indexed first. It is required that this pattern has high quality.
  - Decide whether to use 'Search All Peaks' to check for any missing reflections in the pattern indexed using PPC. If there is a searched peak at the location of a missing reflection, the peak will be indexed. It is recommended to turn it on in the case the scan step is large.
  - Decide whether to calculate the orientation and strain tensor and export idx and stn files by clicking 'Orient Refine' and 'Strain Refine'. It is not recommended to turn them on. The refinement will elongate the time consuming of PPC. Once PPC indexation is finished, the orientation and strain refinement can be executed in parallel computing based on the pkc file generated by PPC, which is much faster.
  - To index a single grain, activate 'Scan One Grain'. The PPC will stop after one grain is indexed.
  - Decide whether to execute PPC indexation based on the subpeak clusters by clicking "Base on Clusters" button. If the peaks are split into subpeaks, it is recommended to turn it on.
  - Decide whether to index the seed pattern by zone axes assisted indexation by click "Zone Index" button in the area "File Path".



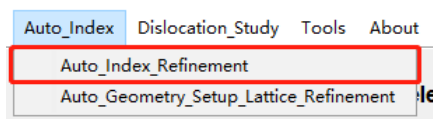
4. Setting Experiment Area for Distributed Calculation:
  - In the distributed calculation, the whole scan area will be divided into several part and execute PPC indexation at different computing pools simultaneously.
  - Start the distributed computing feature by clicking 'Start Distributed Computation'.
  - Each computing pool will auto-index a different area. After completing the 'Start', 'End', and 'Seed' settings, click 'Load' and then set up the next computing pool.
  - Suitable computing pool number is hardware-dependent and is automatically determined by the software.
  - The features "Search All Peaks", "Base on Clusters", and "Zone Index" can also be turned on.
5. Starting Automatic Indexation:
  - After completing all settings, click the 'Start' button in the 'PPC Analysis' area to begin automatic PPC assisted indexation.

If you only output the .pkc file during auto-indexation, you can use the parallel computing feature to calculate the orientation matrix and strain tensor and output .idx and .stn files. The specific methods are as follows:

1. Choose 'Input PKC' from the dropdown menu in the 'Refinement & Sequent Index' area.
2. Load the .pkc file's path and prefix in the area.
3. If analyzing two phases, choose 'Use Phase Map' and load the Phase map outputted from PPC Analysis. If only analyzing one phase, select 'Use Phase I'.
4. Open parallel computing by clicking 'Start Parpool'. If already open, no further action is needed.
5. Click 'Strain Refine' if needed to calculate the strain tensor and output the .stn file.
6. Click 'Search Missing Refl' to output the .idx file containing information about missing reflections.
7. After completing all settings, click 'Start' in the area to begin calculations, with results outputted according to the path and prefix name entered in area "File Path". If the 'Ignore Existing Files' button is activated, existing files won't be replaced.

## 5.2 Sequent Indexation

After correctly entering the experimental geometric parameters and completing the automatic peak searching, you can proceed with automatic sequent indexation. The operating method is as follows:



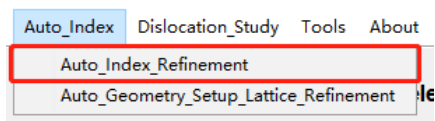
The specific operational steps are as follows:

1. In the area of Refinement & Sequent Index, select Sequent Index from the dropdown menu.
2. Click the upper Load button in the File Path area to import the save path and filename prefix of the pkl file obtained by automatic peak searching. The definition and requirements of the file path and filename prefix are detailed in Section 4.1.
3. If, during the experiment, some diffraction pattern collection areas are outside the sample or for other reasons, causing extremely poor quality of diffraction patterns, click the Judge Valid button to enable the pattern validation checking, and the software will exclude obviously unreasonable diffraction patterns during indexation. If you need to use a dynamic mask, click the Dyn Msk button to enable the dynamic mask feature, the setting method of the dynamic mask is detailed in Section 3.1.
4. Click the lower Load button in the File Path area to set the storage path and filename prefix for the indexation result file, such as idx files and stn files.
5. Click the upper Load button in the Phase I area to import the idp file storing indexation parameters; automatic indexation of this phase will use the indexation parameters stored in the idp file. If there is no suitable idp file, refer to Section 2.2 to generate a suitable idp file.
6. Click the lower Load button in the Phase I area to import the mat file; the software will generally automatically import the mat file based on the imported idp file. If there is no suitable mat file, refer to Section 2.2 to generate a suitable mat file.

7. If you need to index multiple subgrains for each diffraction patterns, select Multi-grain from the dropdown menu in the Refinement & Sequent Index area. Then click the Load button in this area to import the path and filename prefix of the diffraction pattern. Then enter the minimum number of diffraction peaks required for valid subgrains in Threshold. Selecting multiple subgrains requires clustering sub-peaks during peak searching.
8. Click the Start Parpool button in the Refinement & Sequent Index area; if it is already opened, there is no need to open it again. The automatic indexation function only supports parallel computing.
9. To choose the patterns by number, select By Num from the dropdown menu, and enter the starting, ending diffraction pattern number, and step in From, To, Step respectively; if you need to index patterns of a certain area, select By Region from the dropdown menu and enter the coordinates of the lower-left and upper-right corners of the to be indexed area in Start and End.
10. If needed, click Strain Refine to simultaneously calculate the strain tensor and output the stn file.
11. Click the Start button in the Refinement & Sequent Index area to start automatic indexation. If Multi-grain is selected, the output orientation, and strain tensor files are mid and mst files, respectively. It should be noted that if the Ignore Existing Files button is lit, and the target output folder already contains the corresponding idx file or mid file, the software will no longer output this idx file and the corresponding stn file or mst file, i.e., it will not replace existing files.

### 5.3 Batch Strain Refinement

If strain tensor refinement is not performed during indexation, it is possible to fit the strain tensor by importing the idx file obtained from automatic indexation. The operation method is as follows:



The specific operation steps are as follows:

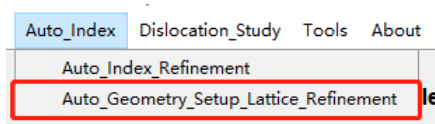
1. In the dropdown menu of the Refinement & Sequent Index area, select Input IDX/MID.
2. Click the lower Load button in the File Path area to set the storage path and filename prefix for the indexation result file.
3. Click the upper Load button in the Phase I area to import the idp file storing indexation parameters; the automatic indexation of this phase will use the indexation parameters stored in this idp file. If there is no suitable idp file, refer to Section 2.2 to generate a suitable idp file.
4. Click the lower Load button in the Phase I area to import the mat file; generally, the software will automatically import the mat file based on the imported idp file. If there is no suitable mat file, refer to Section 2.2 to generate a suitable mat file.
5. Click the Load button in the Refinement & Sequent Index area to import the path and filename prefix of the .idx file or .mid file.
6. If you need to select patterns for analysis based on the record in the Phase Map, select Use Phase Map in the dropdown menu and click the Load Phase Map button within this area to import the Phase map outputted by PPC Analysis. Once imported, the button in front of it will light up. After importing the Phase map, the software will use the diffraction pattern numbers recorded in the Phase map to import idx files and perform strain analysis. If you need to select patterns for analysis, you can choose Use Phase I in the dropdown menu, then the By Num dropdown menu on its left will light up, allowing you to enter the start, end, and step of the diffraction patterns numbers for strain

refinement. If you need to analyze pattern in one certain area, select By Region in the dropdown menu, and enter the coordinates of the lower-left and upper-right corners of the area in Start and End.

- Click the Start Parpool button to enable parallel computing. If it's already enabled, no further action is needed.
- After completing all the above settings, click the Start button in this area to begin calculation; the results will be output according to the save path and filename prefix entered in the File Path area. It should be noted that if the Ignore Existing Files button is lit, and if the output folder already contains the corresponding stn files, the software will not output new stn files, i.e., it will not replace existing files.

## 5.4 Batch Calibration/Lattice Refinement

For the indexation data (that is, the obtained idx, pkc, or mid files), you can fit its experimental geometric parameters and lattice parameters together or separately. The operation method is as follows:



Specific operation steps are as follows:

- Within the Indexation area, click the Load button to set the storage path and filename prefix for the indexation result file (idx, pkc, or mid files).
- If the input is indexation results containing multiple subgrains (i.e. mid files), you need to enter filtering criteria in Multi-grain Filter to screen the subgrains used for refinement. Here, Deviation < represents choosing subgrain with an angular deviation (the average value of the angular difference between each diffraction peak and its theoretical position) less than a certain value, Intensity Order represents choosing subgrain, which

are ranked in terms of average intensity of indexed diffraction peaks, under the condition that they meet the angular deviation filtering criteria. If Deviation < is not entered, angular deviation filtering will not be conducted; if Intensity Order is not entered, it will default to choosing the subgrain with the strongest average intensity.

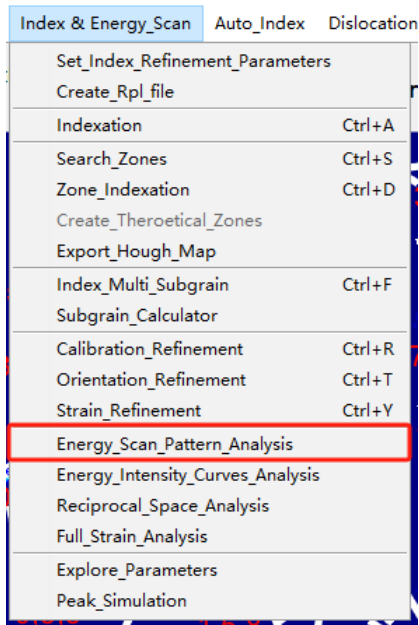
3. In the Output Path area, click the Load button to set the storage path and filename prefix for the saved gsr file.
4. In Refined Constants, select the parameters to be refined by clicking the buttons in front of each parameter.
5. Enter the starting, ending diffraction pattern number, and step length respectively in From, To, Step.
6. If parallel computing is needed, click to open the Start Parpool button. Here, Num of par represents the number of parallels opened, and Cluster Name represents the cluster performing the calculation. These two parameters will be automatically configured by the software based on the computer's configuration; please do not modify them unless needed. After parallel computing is enabled, the progress bar will not be displayed during the automatic fitting process.
7. Click the Start button to begin automatic refinement.

# Energy Scan Analysis

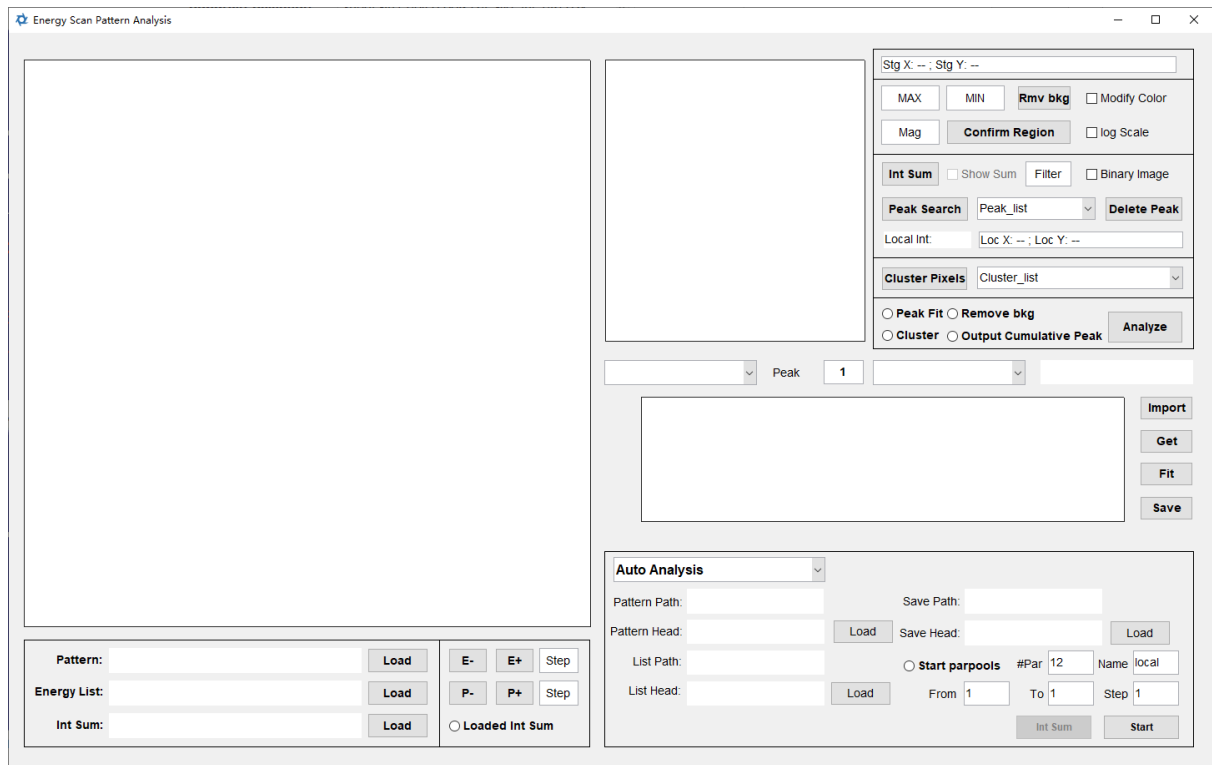
## 6 Energy Scan Analysis

### 6.1 Peak Intensity Collection

For the energy scan data, it is first necessary to collect data on the intensity of diffraction peaks. After completing the input of experimental geometry parameters and peak search parameters, the collection of diffraction peak intensity data can be carried out. The specific method is as follows:







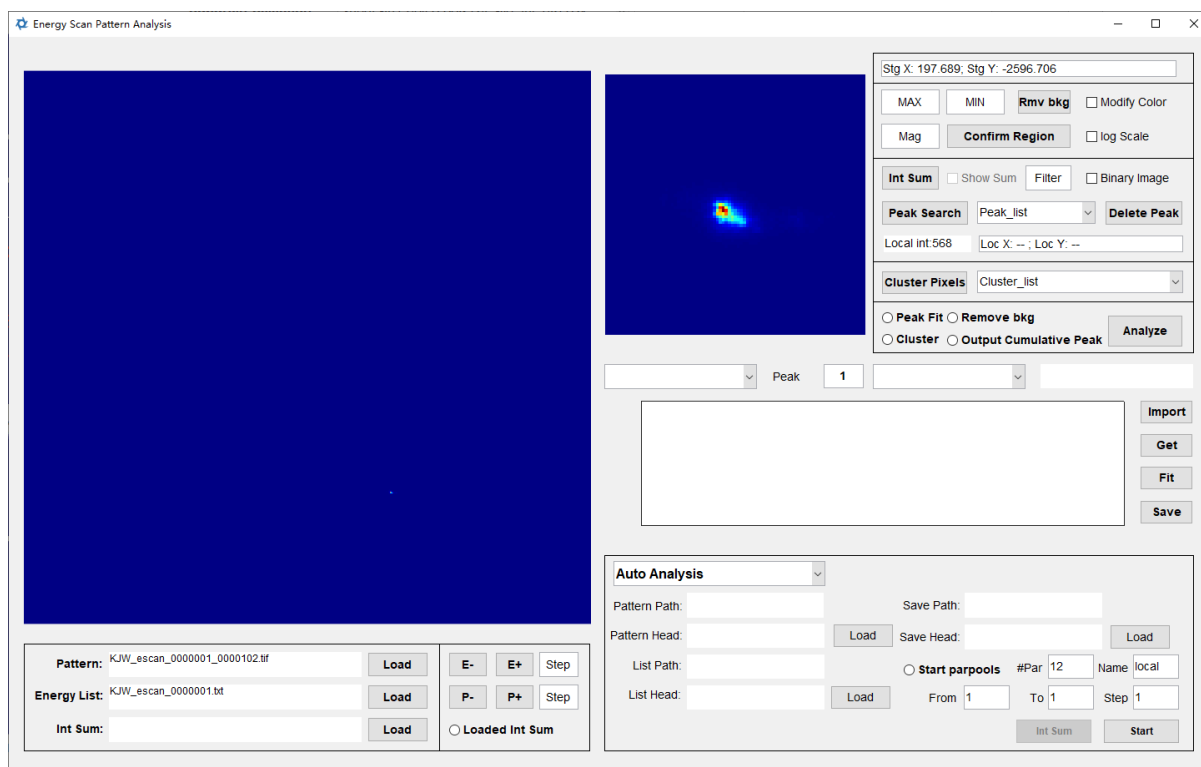
The specific method for manually collecting diffraction peak intensity data from a set of energy scan data is as follows:

1. Click the Load button to the right of "Pattern" below the pattern, and select a diffraction pattern from a set of energy scan data to import. After importing, the pattern is displayed in jet pseudo-colormap.
2. Click the Load button to the right of "Energy List" below the pattern, and import the parameter record file of this set of energy scan data. This file records the incident X-ray intensity and energy of each diffraction pattern in this set of energy scan data. This version of PYXIS only supports importing parameter record files of energy scan data collected at the Taiwan Photon Source (TPS) 21A beamline. The position of the sample stage during this energy scan is displayed in the top right columns of Stg X and Stg Y. PYXIS also provides tools to convert energy scan data collected at the Advanced Photon Source (APS) 34-ID-E beamline to the TPS 21A beamline energy scan data format, see Section 8.11 for details.
3. Clicking the E- and E+ buttons allows you to toggle the display to the diffraction pattern at the previous or next energy at this point. By entering the step value in the Step box to the right, you can change the interval quantity each time you switch.
4. Clicking the P- and P+ buttons allows you to toggle to the diffraction pattern at the previous or next point at the current energy. By entering the step value in the Step box to the right, you can change the interval quantity each time you switch.
5. Enter the intensity values corresponding to the darkest and lightest in the color map in the Max and Min on the right side of the pattern. For example, using the jet color map

here, pixel points in the pattern with intensity above Max will all be displayed in deep red, and those below Min will be displayed in deep blue.

6. If the diffraction pattern needs to remove background, click the Remove bkg button to remove the fluorescence background of the diffraction pattern. Before removing the background, you need to import the fluorescence background in advance.
7. Click on the location of the diffraction peak in the diffraction pattern, and a local magnified image of the clicked location will be displayed on the right side of the diffraction pattern. You can change the magnification of the magnified image by entering the magnification number in the Mag box or scrolling the mouse wheel on the magnified image.
8. Click the Modify Color button to modify the false color range displayed in the magnified image to be consistent with the diffraction pattern, i.e., pixel points with intensity above Max are all displayed in deep red, and those below Min are displayed in deep blue. Click the Log Scale button to display the intensity in the magnified image in logarithmic form, highlighting the lower intensity parts.

After completing the above operations, the effect is as shown in the figure:



In actual analysis, it is often necessary to collect diffraction peaks from a single subgrain. Therefore, depending on whether the diffraction peaks are split, there are different operation steps. Below, the situation where the diffraction peaks are not split is introduced first:

- After selecting the magnified image that precisely contains the diffraction peak that needs to be collected, switch diffraction pattern of different energies and click the Confirm Region button to confirm that the now-selected magnification location and magnification can completely contain the diffraction peak for diffraction patterns of different energies.
- Choose the fitting and output that need to be performed during collection. Among them, click the Peak Fit button to perform Gaussian fitting on the magnified image to determine the center of the diffraction peak; click the Remove bkg button to remove the background of the diffraction pattern during collection; click Output Cumulative Peak to output the intensity information of all pixel points, if it is necessary to reconstruct the intensity distribution in reciprocal space, the intensity information of all pixel points must be output. Split diffraction peaks require more settings for clustering recognition; here, the Cluster button cannot be opened.
- Click the Analyze button to start analyzing the collection.

If the diffraction peak is split, the selected magnified image often contains multiple subpeaks during collection, so it is able to perform clustering recognition of the diffraction sub-peaks in the magnified image to collect and analyze different diffraction subpeaks. **It should be noted that the clustering recognition can also be performed in the three dimensions and will be introduced in Section 6.3 in details. Thus, it is recommended to performed the clustering recognition in 3D.** For the situation with over 5 subpeaks, the clustering recognition in 2D, introduced here, has higher robustness, and is recommended. The specific operations are as follows:

- Click the Int Sum button to accumulate diffraction pattern from all energies at the current point. After the accumulation is complete, click Show Sum to display the accumulated diffraction pattern.
- Click on the diffraction pattern to get a magnified image containing the diffraction peak. When the mouse is placed on the magnified image, the intensity at the current mouse position will be displayed in Local int. Click the Binary Image button to display the binarized magnified image, and input the intensity value of the background in Filter based on the intensity obtained in Local int. The software will distinguish between the diffraction peak and the background based on this standard, so the intensity value entered in Filter should make the binarized magnified image just completely display the diffraction peak. As shown in the picture:

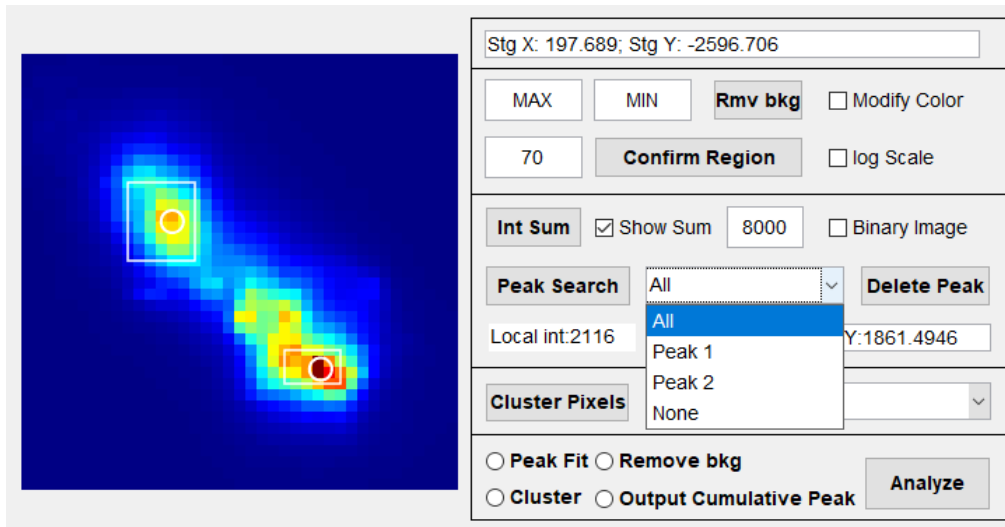
The top screenshot shows a color-coded diffraction pattern on the left. The control panel on the right includes the following elements:

- Stg X: 197.689; Stg Y: -2596.706
- Buttons: MAX, MIN, **Rmv bkg**,  Modify Color
- Buttons: 70, **Confirm Region**,  log Scale
- Buttons: **Int Sum**,  Show Sum, Filter,  Binary Image
- Buttons: **Peak Search**, Peak\_list (dropdown), **Delete Peak**
- Local int: 1565, Loc X: --; Loc Y: --
- Buttons: **Cluster Pixels**, Cluster\_list (dropdown)
- Radio buttons:  Peak Fit,  Remove bkg,  Cluster,  Output Cumulative Peak
- Analyze** button

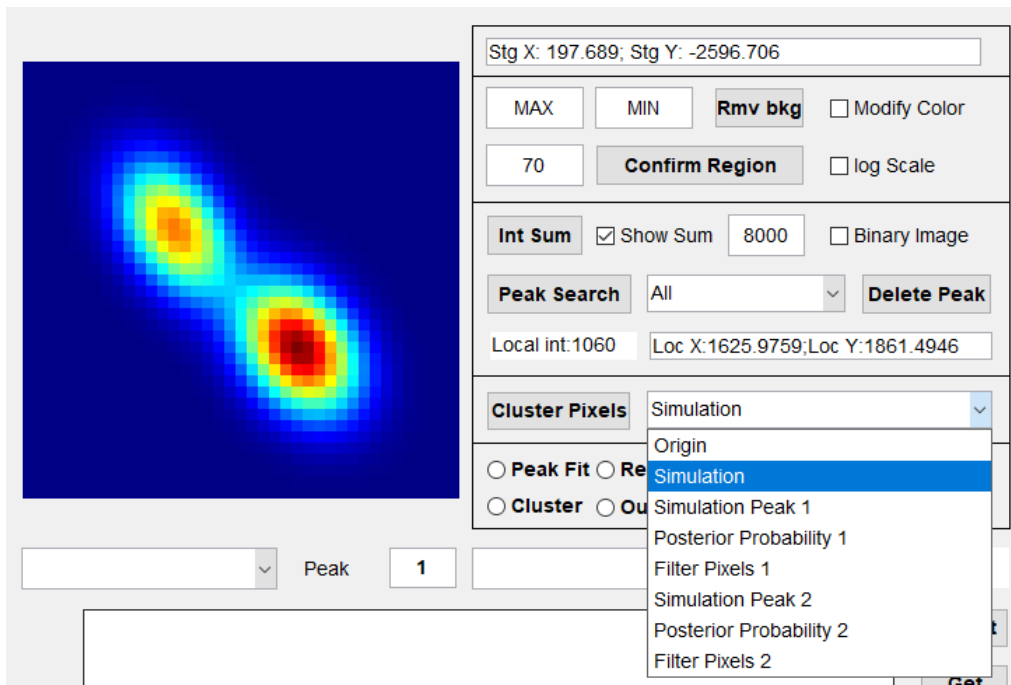
The bottom screenshot shows the same diffraction pattern converted to a binary image (white on black). The control panel settings are updated as follows:

- Stg X: 197.689; Stg Y: -2596.706
- Buttons: MAX, MIN, **Rmv bkg**,  Modify Color
- Buttons: 70, **Confirm Region**,  log Scale
- Buttons: **Int Sum**,  Show Sum, 8000,  Binary Image
- Buttons: **Peak Search**, Peak\_list (dropdown), **Delete Peak**
- Local int: 324, Loc X: --; Loc Y: --
- Buttons: **Cluster Pixels**, Cluster\_list (dropdown)
- Radio buttons:  Peak Fit,  Remove bkg,  Cluster,  Output Cumulative Peak
- Analyze** button

- Click the Peak Search button, and the software will perform peak search in the magnified image of the current displayed accumulative diffraction pattern, with the search results shown in the image. The searched diffraction peak range is framed in white, and the center of the diffraction peak is marked with a circle. The diffraction peak to be displayed can be selected through the dropdown menu on the right, and the coordinates of the center of the selected diffraction peak will be displayed in the Loc X and Loc Y columns. Clicking the Delete Peak button to its right will delete the diffraction peak selected in the dropdown menu.



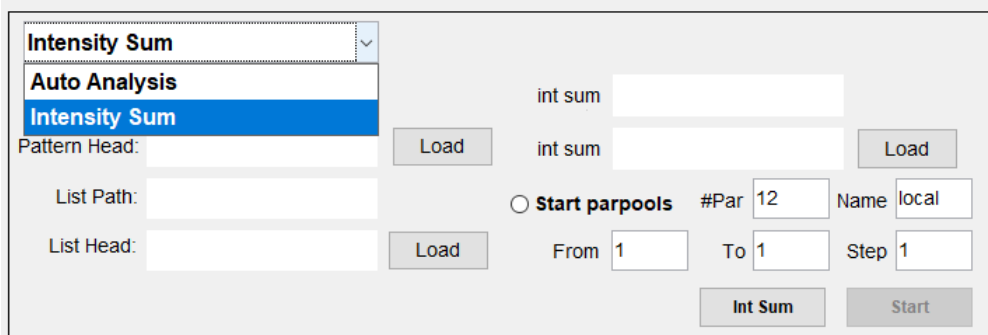
After confirming the correct peak search, click the Cluster Pixels button to perform clustering recognition of the diffraction peaks to assign the intensities to each diffraction peak. After completion, the content to be displayed in the magnified image can be selected through the dropdown menu. Here, Simulation represents the diffraction peaks simulated according to the fitting parameters after clustering recognition, Simulation Peak represents each simulated diffraction peak, Posterior Probability represents the probability that the photons on each pixel point in the magnified image come from a certain diffraction peak, and Filter Pixels represents the magnified image drawn using pixel points where the probability that photons come from a certain diffraction peak is greater than 75%. If the Posterior Probability distribution corresponding to different diffraction peaks can exactly separate different diffraction peaks, it means that the clustering recognition is correct.



- After completing the above settings, click Analyze to collect diffraction peak intensity data. Here, the Cluster button must be activated. The meanings represented by other buttons are completely consistent with the data collection steps for diffraction peaks without splitting, refer to the above text.

It should be noted that the accumulation process after clicking Int Sum may take a long time. All energy scan data can be accumulated in advance for direct importation and use during analysis. The specific method is as follows:

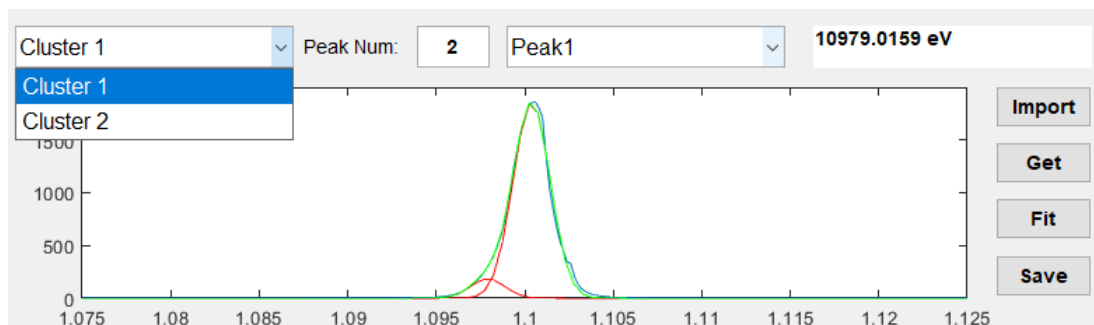
In the dropdown menu in the automatic analysis frame, select Intensity Sum, then import the patterns and parameter record files separately, and import the storage path of int sum. In From, To, and Step, enter the starting, ending energy scan number, and interval step length. If parallel computing is needed, activate the Start Parpools button. After completing the settings, click the Int Sum button to start accumulating. The accumulation results are stored as tif format.



After the accumulation is completed, the patterns obtained by accumulation can be imported into the pattern and parameter record file import bar below the pattern display. After importing the accumulated pattern, the Loaded Int Sum to its right will be activated.

After completing the intensity analysis collection, the collected results can be displayed and saved, and the specific methods are as follows:

- As shown in the picture, select the (clustered) diffraction peak to be drawn in the dropdown menu on the left. If the collected one is an unsplit diffraction peak, there is only Cluster 1. Click the Get button on the right to draw its energy and intensity distribution.
- Enter the number of peaks to be fitted after Peak Num and click the Fit button to perform Gaussian fitting. The fitted diffraction peak will be displayed in red, and the sum of the fitting curves of all diffraction peaks will be displayed in green. Select the fitted diffraction peak through the dropdown menu on the right, the right will display the peak center position of the selected diffraction peak, click Import at this time to import the peak center of the current selected peak, this peak center can be exported for use when calculating the full strain tensor, see Section 6.5 for details.
- Click the Save button to store the collected data. Among them, the diffraction peak center of different energies (Peak Fit activated during collection) and energy data will be stored as esc files. If Output Cumulative Peak is activated during collection, the intensity of each pixel point will be stored as an esf file.



This interface also provides the function of automatically collecting diffraction peak intensity data for multiple groups of energy scan data, and the specific operating methods are as follows:

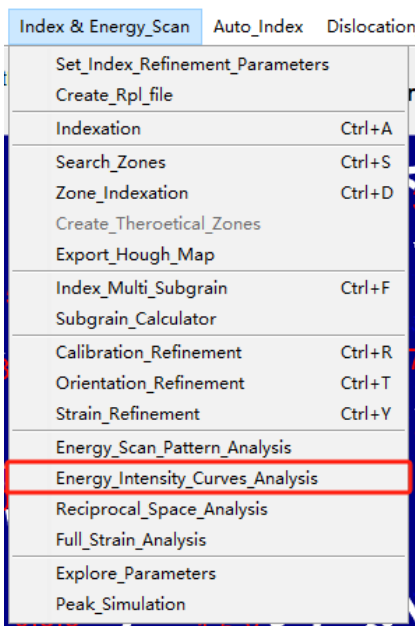
1. Complete all settings for manual collection. Select Auto Analysis in the dropdown menu in the automatic analysis column.
2. Click the Load button to the right of Pattern Head in Auto Analysis to import the file path and filename prefix of the diffraction pattern. The file path and filename prefix of all diffraction patterns must be the same.
3. Click the Load button to the right of List Head in Auto Analysis, to import the file path and filename prefix of the energy scan parameter record file. The file paths and filename prefix of all parameter record files must be the same.

4. Click the Load button to the right of Save Head in Auto Analysis to import the path and filename prefix for saving data.
5. In From, To, and Step, set the starting energy scan data group number, ending number, and step length.
6. If parallel computing needs to be enabled, click Start parpools to enable parallel computing. #Par and Name are determined by the hardware of the running computer, the software will choose the optimal parameters, please do not modify if not needed.
7. Click the Start button to start automatic analysis.

\*: The naming rule for the diffraction patterns of energy scans is: prefix\_group number\_pattern number.tif. For example, a diffraction pattern named: ML\_receive\_mono1\_0000011\_0000125.tif, indicates a spectrum with a filename prefix of ML\_receive\_mono1\_, a group number of 11, and a spectrum number of 125.

## 6.2 Peak Profile Curve Analysis

In the Peak Shape Curve Analysis interface, you can import the obtained esc files containing energy and diffraction peak intensity information from energy scans, to perform single (or multiple) peak Gaussian fitting, as well as operations such as converting energy to Bragg angle. The specific operating methods are as follows:





Energy-Intensity Curve Analysis

File Path:

Curve Path:

Curve Head:

Saving Path:

Select Patterns:

From  To  Step

Add 2theta to Each Curve Files

Peak Fit

Peak Num:  HKL:

Energy Range (eV):

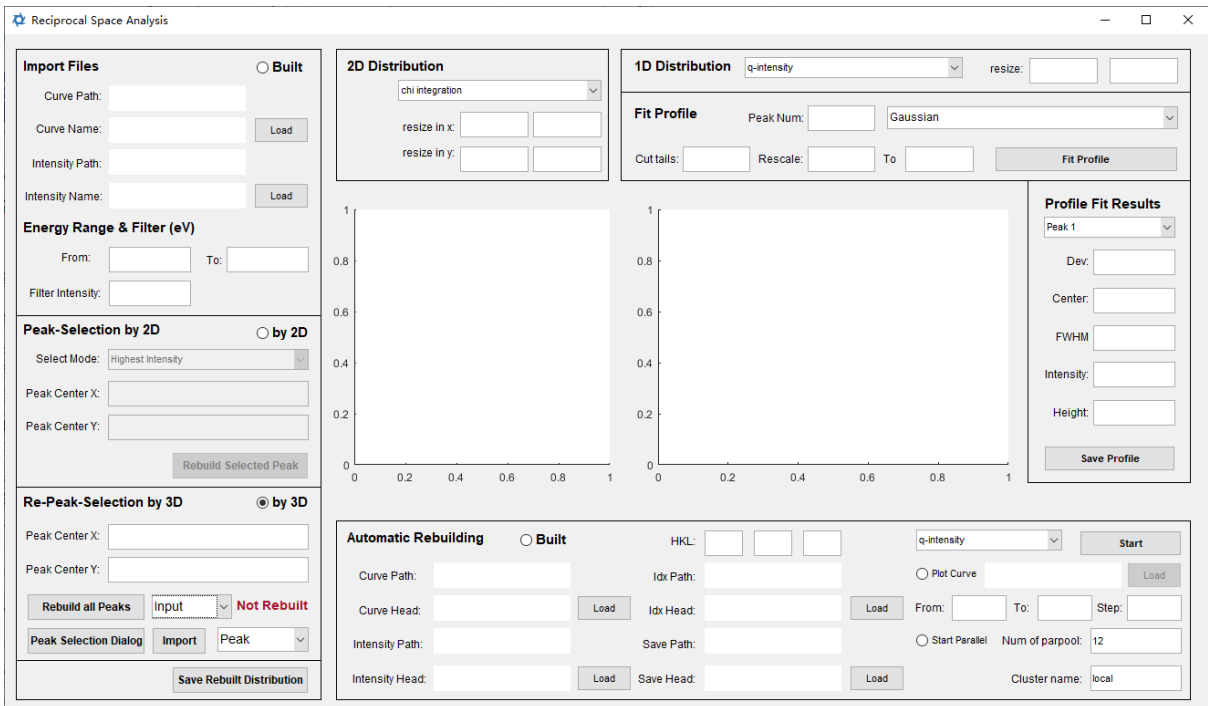
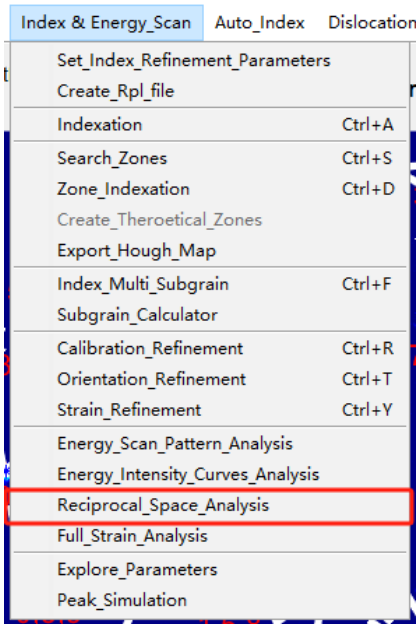
From  To

Plot Curves

1. Click the Load button next to Curve Head in File Path to import the file path and filename prefix of the esc file.
2. Click the Load button next to Saving Path in File Path to set the storage path for the curve fitting results.
3. In Select Pattern, enter the starting, ending file numbers, and step size of the esc file in From, To, and Step.
4. Enter the number of peaks for Gaussian fitting next to Peak Num in Peak Fit.
5. Enter the Miller index for this diffraction peak after HKL.
6. If Gaussian fitting needs to be specified within a certain energy range, enter the energy range in From and To next to Energy Rescale in Peak Fit; the unit is eV.
7. If you need to plot the curves and draw the fitted curves at the same time, open the Plot Curves button in Peak Fit and click the Load button next to it to set the save path for the curve pictures.
8. After completing all the above settings, click the Start button in Peak Fit to automatically perform Gaussian fitting on all curves and output and store the results.
9. After completing the settings in steps 1 to 7, click the Start button in Add 2theta to Each Curve Files. The software will calculate the Bragg angle, interplanar spacing, and the energy-related integrated intensity data for each stored file of the integrated intensity versus energy curve and save it in the original path.

## 6.3 Reciprocal Space Reconstruction & Analysis

After completing the collection of diffraction peak intensity data and saving the files with integrated intensity related to energy data (esc files) and the files with intensity information of all pixel points (esf files), you can proceed with the reconstruction and analysis of intensity distribution in reciprocal space. The specific method is as follows:



The manual method for reconstructing and analyzing the intensity distribution in reciprocal space is as follows:

1. Click the Load button next to Curve Name in the Import Files section to import esc files, and the Load button next to Intensity Name to import esf files. The esc and esf files here must come from the same set of energy scan data.
2. In Energy Range & Filter (eV), enter the energy range for reciprocal space reconstruction in From and To. Intensity from diffraction patterns exceeding this energy range will not be reconstructed in this set of energy scan data. If not entered, the software will reconstruct all data in the imported files. In Filter Intensity, enter the intensity screening standard; intensity below this value will not be reconstructed. If not entered, the software will not filter any data.
3. If using the diffraction peak selection result in two-dimensional space, enable the by 2D button in the Peak-Selection by 2D area. If clustering recognition of diffraction peaks was performed when generating the imported esc and esf files, four selection modes provided by the software can be used. The selection mode is chosen from the Select Mode dropdown menu in this area. The specific meanings of different options are:
  - i. Highest Intensity: reconstruct the subpeak with the highest intensity among the split diffraction peaks.
  - ii. Near Input Peak: enter the center of the diffraction subpeak to be reconstructed in Peak Center X and Peak Center Y below, the software will select the diffraction subpeak closest to the input point for reconstruction, and the peak center used for reconstruction is the peak center fitted when generating the esc file.
  - iii. Input Peak: input the center of the diffraction subpeak to be reconstructed in Peak Center X and Peak Center Y below, the software will select the diffraction sub-peak closest to the input point for reconstruction, using the peak center coordinates entered here for reconstruction.
  - iv. Re-Fit: directly accumulate the intensity of the recorded area and perform 2D Gaussian fitting to obtain a single peak center. This method is not recommended for use when diffraction peaks are split; splitting will result in reduced accuracy of its results.
  - v. Non-Rotation: directly output the absolute values of  $\kappa$  and  $\theta$ .If the diffraction peaks in the imported esc and esf files have not undergone clustering identification, only Input Peak and Re-Fit modes can be chosen. When using Input Peak mode, the diffraction peak center needs to be input, and it will be used during reconstruction.
4. Click the Rebuild Selected Peak button in this area to reconstruct the intensity distribution in reciprocal space. During the reconstruction, data import will be performed first, displaying a progress bar during import. After import is complete, if the number of data points is more than 10,000, the software will ask whether to reconstruct using interpolation. Using interpolation will achieve higher reciprocal space resolution but will take longer. If interpolation is not used, the software will reduce reciprocal space resolution to allocate data points. This method is faster but will sacrifice reciprocal space resolution.

5. If using the diffraction peak selection result in three-dimensional space, enable the by 3D button in the Re-Peak-Selection by 3D area. Similar to when selecting 2D diffraction peaks, three modes can be chosen to determine the center of the diffraction peak. If the Input mode is selected from the dropdown menu, the software will read the Peak Center X and Peak Center Y entered above as the peak center; if the esc file mode is chosen, the imported esc and esf files are required to have undergone diffraction peak clustering identification, and the software will fill the strongest diffraction peak center saved in the esc file into the Peak Center X and Peak Center Y text boxes in this area. If the Re-fit mode is selected, the software will re-acquire a single diffraction peak center using a 2D Gaussian distribution. If the Non-Rotation mode is selected, the software will directly use the absolute values of  $\kappa$  and  $\theta$  to reconstruct the reciprocal space.

**Re-Peak-Selection by 3D**  by 3D

Peak Center X:

Peak Center Y:

Re-fit   
Input  
esc file  
Re-fit  
Non-Rotation

After filling in Peak Center X and Peak Center Y, click the Rebuild all Peaks button inside this area to start the reconstruction of all diffraction peaks. Once the reconstruction is complete, it will indicate the completion of the reconstruction in this area. After the reconstruction is complete, this area will appear as shown in the figure:

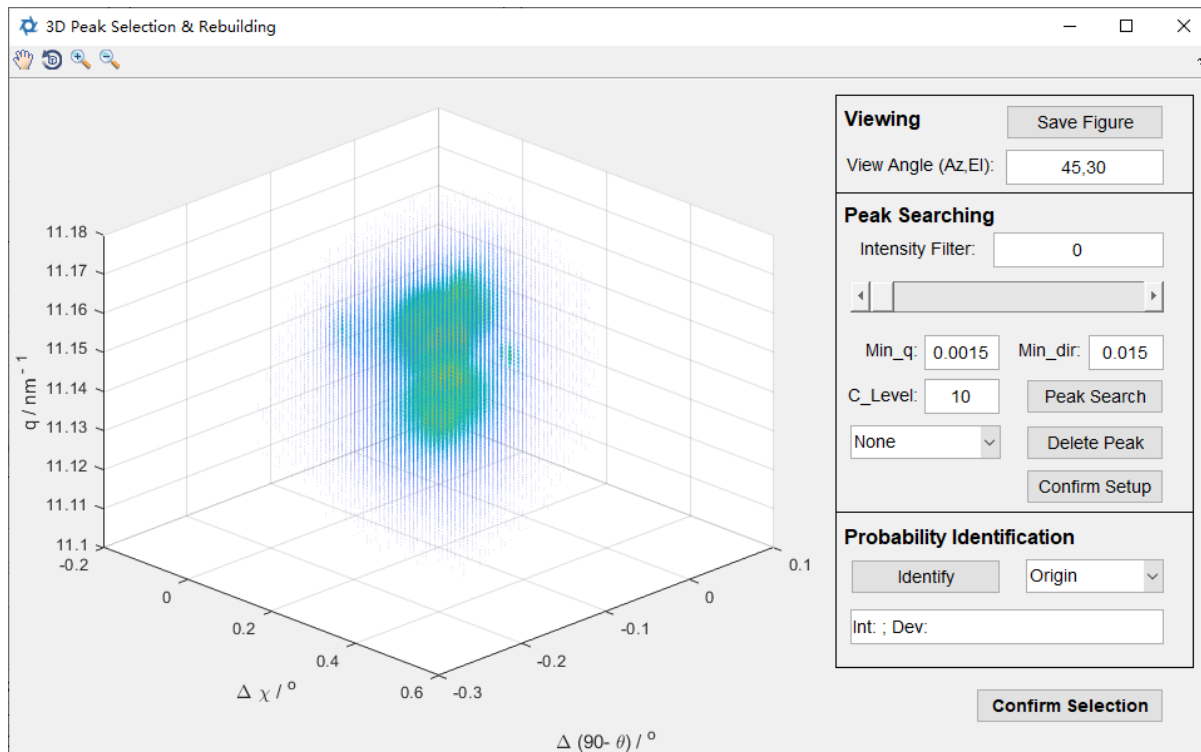
**Re-Peak-Selection by 3D**  by 3D

Peak Center X:

Peak Center Y:

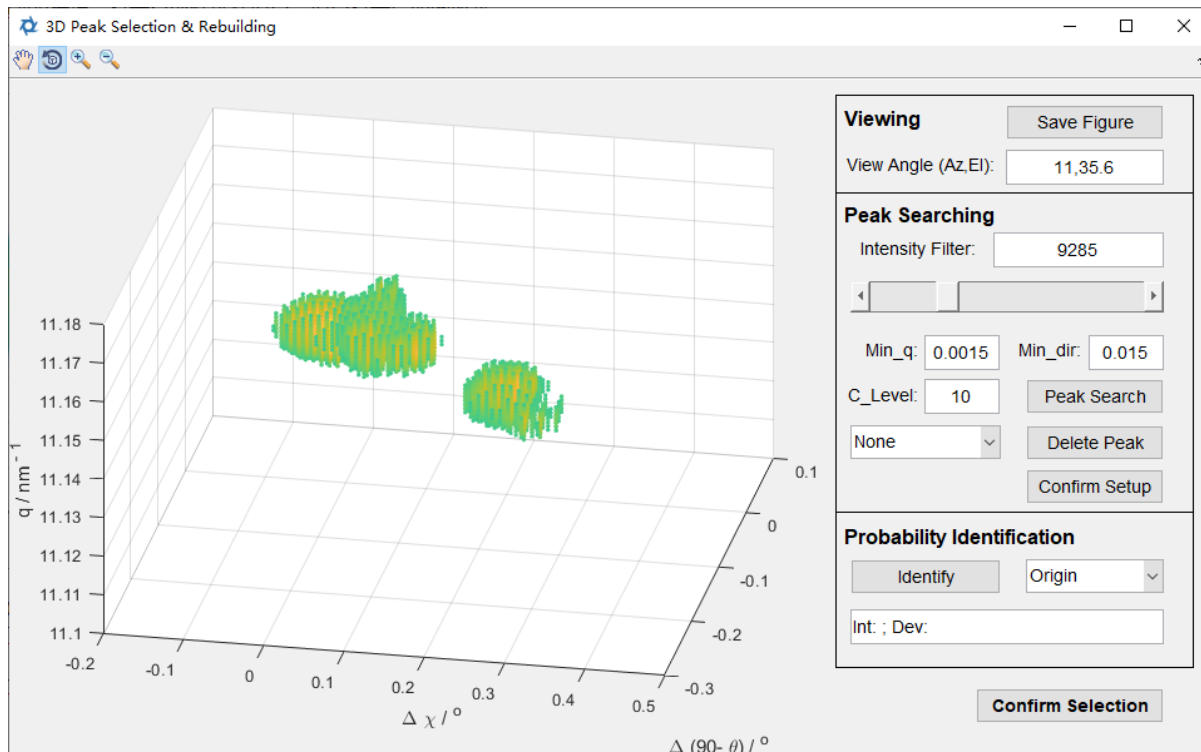
Re-fit   
Peak

After completion, click the Peak Selection Dialog button to open the diffraction peak selection window. After opening the window, it will appear as shown in the figure:



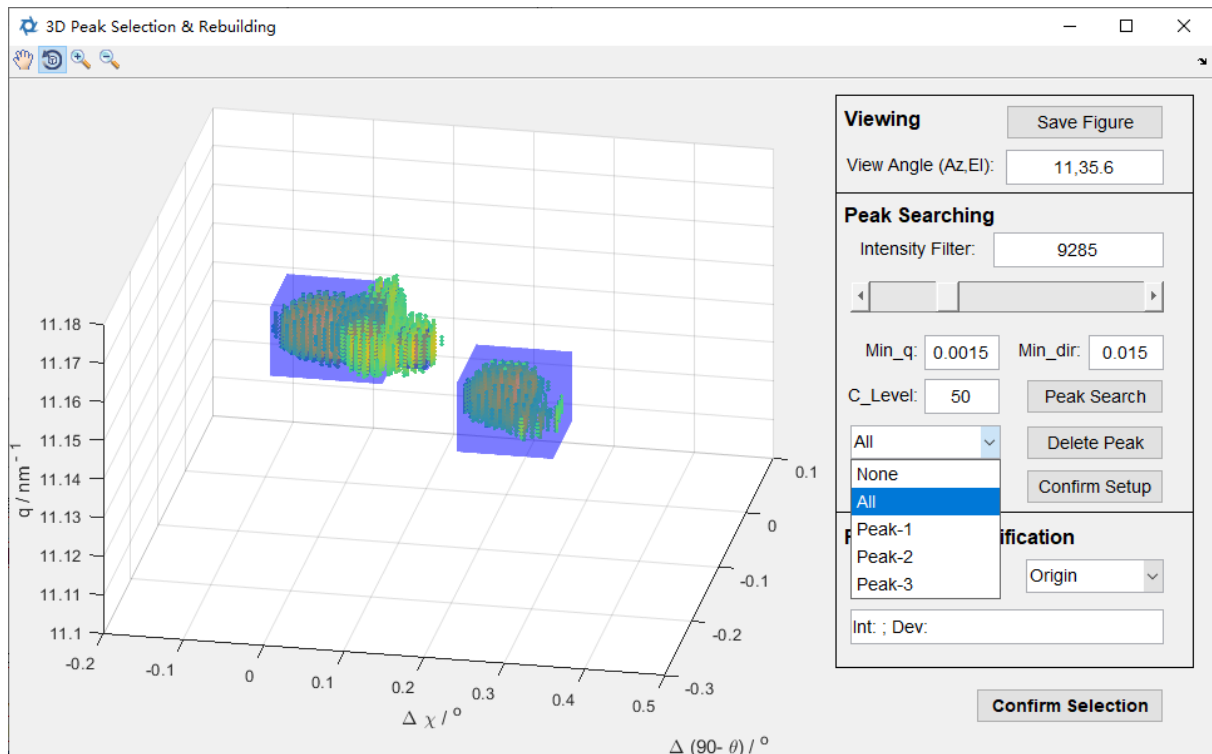
In the Viewing area, entering the view angle in the View Angle (Az, El) text box can change the display angle of the three-dimensional diffraction peaks. The two values in this angle need to be separated by a comma. The tools in the toolbar can also be used to change the display angle of the three-dimensional diffraction peaks. Clicking the Save Figure button in this area can save the currently displayed three-dimensional diffraction peak.

In the Peak Searching column, adjust the Intensity Filter parameter by entering parameters in Intensity Filter or by dragging the slider below it; intensity values below this parameter will be removed. The window after adjusting the display angle and Intensity Filter appears as shown in the figure:

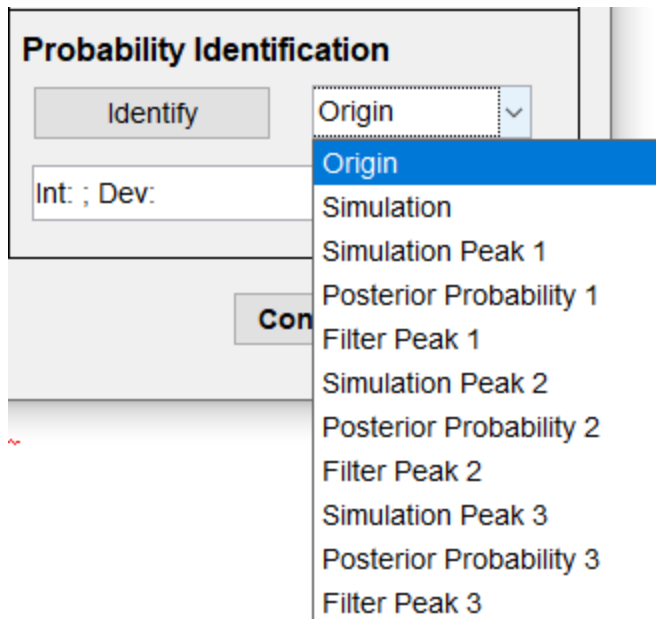


Enter the peak search parameters in Min\_q, Min\_dir, and C\_Level, where Min\_q represents the minimum length of the diffraction peak in the q dimension, Min\_dir represents the minimum length of the diffraction peak in the other two dimensions, and C\_Level represents the recognition sensitivity to identify subpeaks during peak searching, the higher the value, the more sensitive it is to identify sub-peaks. After completing the settings, click the Peak Search button in this area to start searching for peaks. After the peak search is completed, the software will frame the searched diffraction peaks with a semi-transparent blue rectangle, and the effect is as shown in the figure below. The dropdown menu in this area can be used to select the marked diffraction peaks. After selecting the corresponding diffraction peaks, click the Delete Peak button to delete the currently displayed diffraction peak. Clicking the Confirm Setup button, the software will save the current Peak Searching parameters, which will be used for the automatic reconstruction feature.

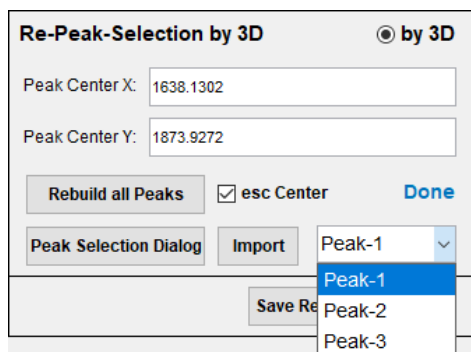
It should be noted that the color and size of the scatter points in the displayed diffraction peak distribution scatter plot can be adjusted through the corresponding parameters, the specific method is detailed in Section 9.1. The color, transparency, and whether to display the edge of the square indicating the peak search results can also be adjusted, the method is detailed in Section 9.1.



After completing the peak search, in the Probability Identification column, click the Identify button to identify the diffraction peaks to which each intensity belongs by the mean of 3D clustering recognition. After the identification is completed, you can select the content to be displayed from the dropdown menu in this column. Among them, Simulation represents the diffraction peaks simulated according to the fitted parameters after identification, Simulation Peak represents each simulated diffraction peak, Posterior Probability represents the probability that the photons at each location come from a certain diffraction peak, and Filter Peak represents the intensity distribution of a certain diffraction peak modified according to probability.



6. After completion, click 'Confirm Selection' to save the identification results. You can close the interface after saving. When reopened, the software will prioritize loading the saved peak search and identification results and display them on the interface.
7. Back to the interface, click the 'Import' button in the 'Re-Peak-Selection by 3D' area, read the saved identification results, and then select the diffraction peak to be analyzed from the dropdown menu.



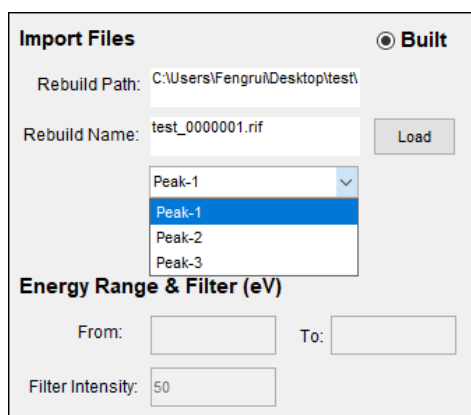
8. After completing the above operations, click the 'Save Rebuilt Distribution' button in this area to store the reconstructed file, i.e., the rif file.
9. In the '2D Distribution' area, select which kind of two-dimensional intensity distribution map to draw from the dropdown menu and enter the range in x and y directions in 'resize in x' and 'resize in y' to select the drawing area. Three plotting methods provided are:
  - i. chi integration: Integrates all intensities in the 2theta-q// plane.
  - ii. 2theta integration: Integrates all intensities in the chi-q// plane.
  - iii. q integration: Integrates all intensities in the chi-2theta plane.



10. In the '1D Distribution' area, select which kind of one-dimensional distribution graph to draw from the dropdown menu and select the drawing range by entering the range of the x-axis in 'resize'. Three plotting methods provided are:
  - i. q-intensity: Integrates all intensities in the q// direction.
  - ii. 2theta-intensity: Integrates all intensities in the 2theta direction.
  - iii. chi-intensity: Integrates all intensities in the chi direction.
11. After the one-dimensional distribution graph is drawn, select which function is needed for fitting in the dropdown menu in the 'Fit Profile' area. Enter the number of peaks to be fitted in 'Peak Num'; enter the Cut tails value in 'Cut tails', the intensity below this value in the one-dimensional distribution graph is assigned a value of 0. Enter the fitting range in 'Rescale', fitting is only done for the part of the one-dimensional distribution graph where the horizontal axis value is within this range. 'Cut tails' and 'Rescale' can be left blank.
12. Click the 'Fit Profile' button to perform peak shape fitting and analysis. The fitting results will be displayed in the 'Peak Fit Results' area. You can select which peak's information to display from the dropdown menu here. The information displayed includes:
  - i. Peak Center: Center of the peak
  - ii. Integrated Intensity: Integrated intensity
  - iii. FWHM: Full width at half maximum of the peak
  - iv. Peak Height: Height of the peak
  - v. Deviation: Fitting deviation
13. Click the 'Save Profile' button in the 'Fit Curve' area to save the data used for drawing the one-dimensional distribution graph, i.e., the ric file. This data can be used for subsequent line profile analysis.

If the reciprocal space distribution has already been reconstructed, you can import the ric file and then proceed with the analysis. The specific method is as follows:

1. Open the 'Built' button in the 'Import Files' area, the area will change as shown in the figure below:



**Import Files**  Built

Rebuild Path: C:\Users\Fengru\Desktop\test\

Rebuild Name: test\_0000001.rif

Peak-1  
Peak-1  
Peak-2  
Peak-3

**Energy Range & Filter (eV)**

From:  To:

Filter Intensity:

2. Click the 'Load' button in this area. Import the rif file. If the imported rif file is obtained by selecting three-dimensional diffraction peaks, the dropdown menu below will be activated, and you can select the diffraction peak to be analyzed.
3. The steps for analysis are the same as steps 9 to 13 of the method for manually performing inverse space intensity distribution reconstruction and analysis.

The method for automatically performing reciprocal space reconstruction and analysis is as follows:

1. Click the 'Load' button in the top left of the 'Automatic Rebuilding' area to import the file path and filename prefix of the esc file.
2. Click the 'Load' button in the bottom left of the 'Automatic Rebuilding' area to import the file path and filename prefix of the esf file.
3. Click the 'Load' button in the bottom right of the 'Automatic Rebuilding' area to set the storage path for the reconstructed rif file, ric file, and fitting results.
4. If you have selected 2D-Peak Selection and chosen Near Input Peak or Input Peak, or selected 3D-Peak Selection and chosen Input, you need to click the 'Load' button in the top right of the 'Automatic Rebuilding' area, import the indexation data of the white beam pattern corresponding to each set of energy scan data, i.e., .idx data, and enter the Miller indices of the diffraction peaks analyzed in HKL. The numbering of .idx data needs to correspond to the numbering of esc files and esf files. Otherwise, there is no need to import idx files or enter Miller indices.
5. If necessary, follow the method described in the manual above, enter the parameters in 'Energy Range & Filter (eV)'.
6. Select which kind of one-dimensional distribution graph to output from the dropdown menu. If necessary, enter the drawing range through 'resize'.
7. Click the 'Plot Curve' button in the 'Automatic Rebuilding' area, choose whether to output the one-dimensional distribution graph in picture form, if output is needed, light up the button, and then click the 'Load' button to the right to set its output path and filename prefix.
8. Enter the start analysis, the last analysis file number, and step in 'From', 'To', and 'Step'.
9. If parallel computing is needed, open the 'Start Parallel' button. The value of 'Cluster Num' is determined by the hardware of the running computer, the software has automatically selected the best value, please do not modify it unless necessary.

- Click the 'Start' button to start automatic reconstruction and analysis. If 3D-Peak Selection is used, generating one rif file may simultaneously generate multiple ric files corresponding to multiple diffraction peaks.

If the reconstruction has been completed and a large number of rif files have been generated, only automatic analysis is needed to generate ric files. The specific operation is as follows:

- Open the 'Built' button in the 'Automatic Rebuilding' area, the area will change as shown in the figure below:

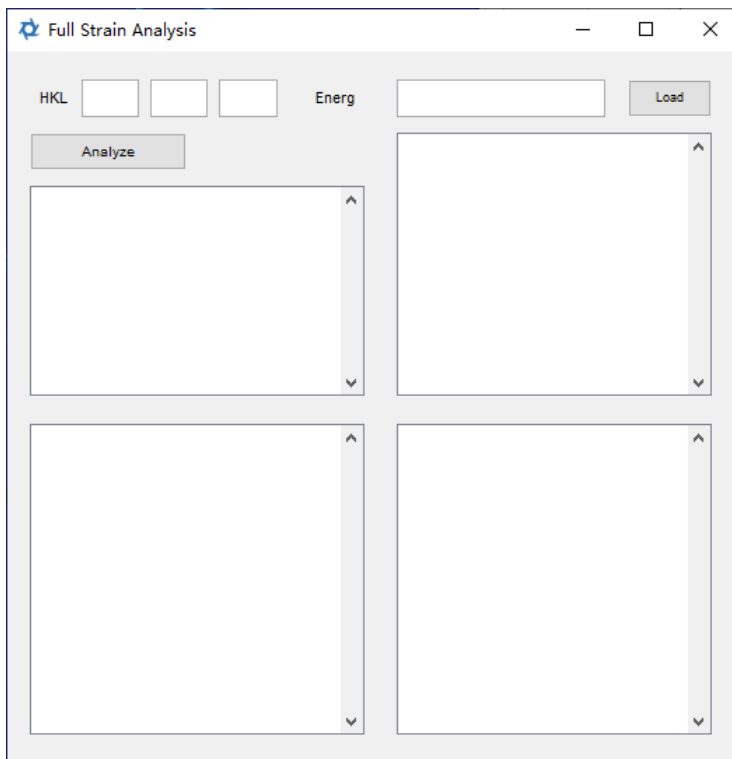
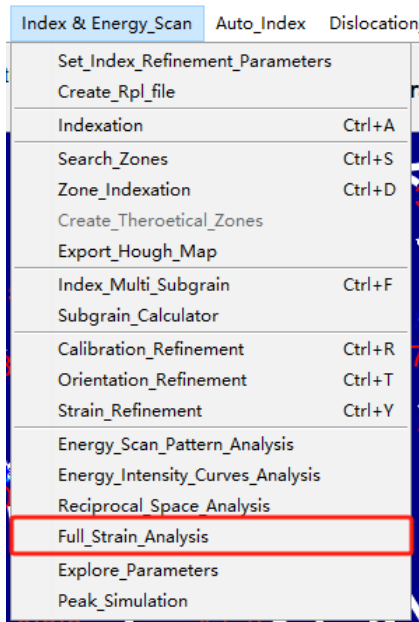
The screenshot shows the 'Automatic Rebuilding' section of the software interface. The 'Built' button is selected, indicated by a blue circle. The interface contains several input fields and buttons:

- Rebuild Path:** Input field with a 'Load' button to its right.
- Rebuild Head:** Input field with a 'Load' button to its right.
- Intensity Path:** Input field with a 'Load' button to its right.
- Intensity Head:** Input field with a 'Load' button to its right.
- Idx Path:** Input field with a 'Load' button to its right.
- Idx Head:** Input field with a 'Load' button to its right.
- Save Path:** Input field with a 'Load' button to its right.
- Save Head:** Input field with a 'Load' button to its right.
- HKL:** Three empty input boxes.
- q-intensity:** A dropdown menu.
- Start:** A button.
- Plot Curve:** A radio button.
- From:** Input field.
- To:** Input field.
- Step:** Input field.
- Start Parallel:** A radio button.
- Num of parpool:** Input field with the value '12'.
- Cluster name:** Input field with the value 'local'.

- Click the 'Load' button on the left in this area to import the file path and filename prefix of the rif files.
- Click the 'Load' button in the middle of this area to set the storage path for one-dimensional distribution graph data and fitting results.
- Other operations are the same as steps 6 to 10 of the method for manually performing inverse space intensity distribution reconstruction and analysis.

## 6.4 Full Strain Tensor Calculation

After obtaining the peak center position in the energy curve through diffraction peak intensity data collection or other methods (for specific methods, see Section 6.1) and after performing strain tensor calculations in the main window (for specific methods, see Section 3.5), you can proceed with the calculation of the full strain tensor. The specific method is as follows:



1. Enter the Miller indices of the diffraction peaks at known energy in HKL.
2. Enter the energy of the diffraction peaks at known energy in Energy, the unit is eV. If the energy data has already been stored in the software by clicking the Import button in the diffraction peak intensity data collection interface (see Section 6.1), you can directly click the Load button to import it.

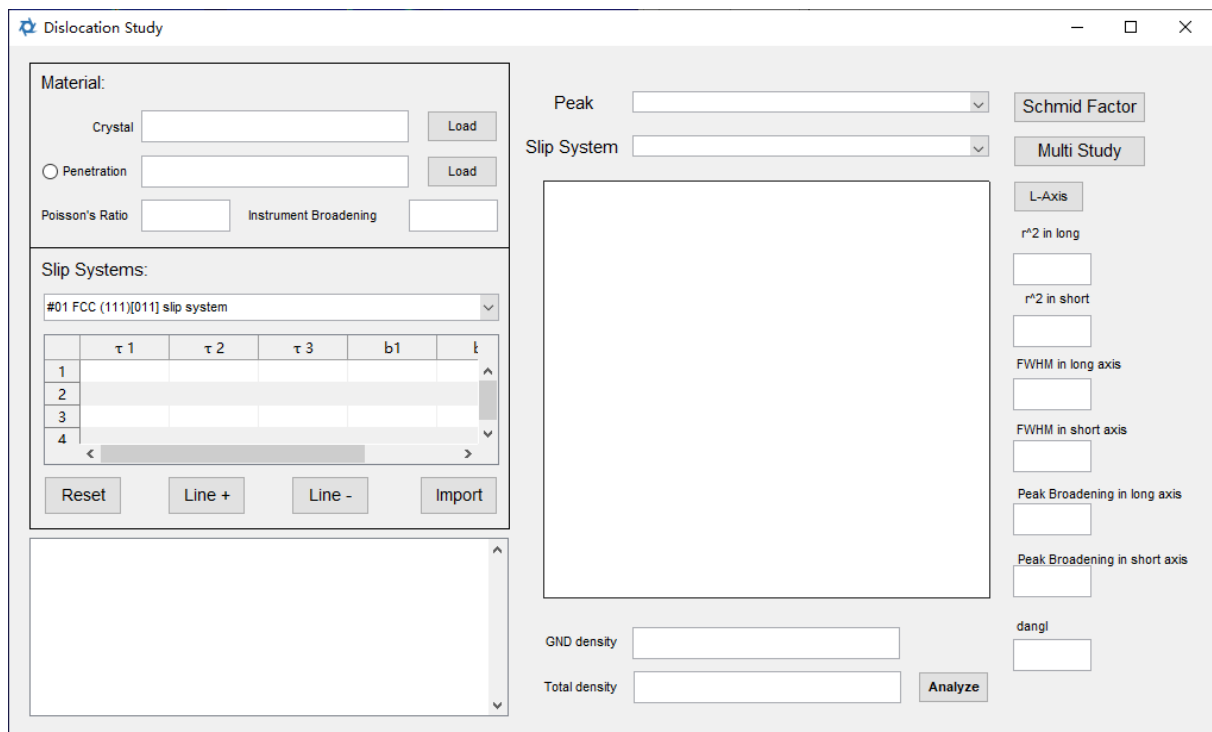
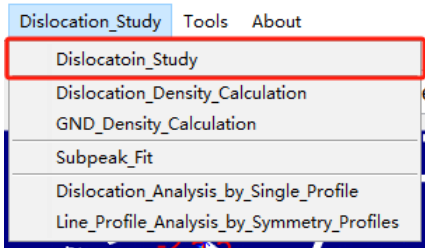
3. Click the Analyze button, and the software will start performing full strain tensor calculations. The calculation results will be displayed in the four text boxes on the interface.

# **Dislocation Analysis based on Peak Profile**

## 7 Dislocation Analysis based on Peak Profile

### 7.1 Manual Dislocation Analysis based on Laue Peak Profile

After completing the calculation of the orientation matrix for the diffraction pattern in the main window (for specific methods, see Section 3.5), you can proceed with manual analysis of dislocation density for the diffraction peak profile generated in the main window. The specific method is as follows:



The specific method for conducting a manual analysis of dislocation density is as follows:

1. Click the Load button next to Crystal in the Material region to import the .rpl file of the crystal structure of the experimental material under analysis. If there is no suitable .rpl file, refer to the content in Section 2.3 to generate one.
2. Click the Load button next to Penetration in the Material region to import the X-ray penetration data for the material under analysis; the penetration data is an ASCII-encoded .pnt text file. If there is no suitable penetration data, please contact the software provider to obtain appropriate data. If using fixed penetration, click the button

to the left of Penetration and enter the penetration value in micrometers in the text box to the right of Penetration.

3. Enter the Poisson's ratio of the material under analysis in Poisson's Ratio. Enter the value of instrument broadening in Instrument Broadening; its unit is degrees.
4. Enter all slip systems of the material under analysis in the list in the Slip System region; you need to input the dislocation line direction and the corresponding Burgers vector. You can reset, add lines to the table, and delete lines from the table using the Reset, Line+, and Line- buttons. Various materials' slip system data are preset in the dropdown menu above the table; you can import the corresponding slip system data directly by selecting it from the dropdown menu. After entering the slip system data, click the Import button to import the diffraction peak information from the main window and the entered slip system information.
5. Select a diffraction peak marked in the main window from the dropdown menu next to Peak on the right side. Its diffraction intensity distribution in q-space will be displayed in the box.
6. Click L-Axis; the software will automatically acquire the long and short axes of the displayed diffraction peak and represent them with red and blue lines respectively. If there is a deviation in the automatically acquired long and short axes, you can redefine them by continuously clicking on the two ends of the elongated diffraction peak. After obtaining the long and short axes, the fitting information of the long and short-axis peaks will be displayed on the right side in region 2, which includes:
  - i.  $r^2$  in long:  $r^2$  value of Gaussian fit to the long-axis peak shape.
  - ii.  $r^2$  in short:  $r^2$  value of Gaussian fit to the short-axis peak shape.
  - iii. FWHM in long axis: Full width at half maximum of the long-axis peak shape.
  - iv. FWHM in short axis: Full width at half maximum of the short-axis peak shape.
  - v. Peak Broadening in long axis: Equivalent peak width of the long-axis peak shape.
  - vi. Peak Broadening in short axis: Equivalent peak width of the short-axis peak shape.
7. Choose a slip system from the dropdown menu located lower in the Slip System on the right side; the number of the slip system corresponds to the list of slip systems entered in region 1. After choosing the slip system, the theoretical elongation direction of the diffraction peak will be displayed in black lines in the graph, and at the same time, the software will calculate the angle between the theoretical elongation direction and the actual long-axis direction and display it in dangle on the right side; its unit is degrees. Determine the slip system closest to the actual elongation direction by selecting the slip system.
8. After selecting the slip system closest to the actual elongation direction, click the Analyze button. The geometrically necessary dislocation (GND) density and the total dislocation density calculated by the software will be displayed in GND density and Total density, respectively; their units are per square meter. Each time you click Analyze, the calculated results will also be recorded in the text box in the lower-right corner of the interface.

The effect after completing the above operations is as shown in the figure below:



**Material:**  
 Crysta: ni.rpl [Load]  
 Penetration: DD407.pnt [Load]  
 Poisson's Ratio: 0.375 Instrument Broadening: 0

**Slip Systems:**  
 #01 FCC (111)[011] slip system

	$\tau_1$	$\tau_2$	$\tau_3$	b1	b2	b3
1	-0.5000	-0.5000	1	0.5000	-0.5000	-0.5000
2	1	-0.5000	-0.5000	0	0.5000	-0.5000
3	0.5000	-1	0.5000	0.5000	0	0
4	-0.5000	-1	0.5000	0.5000	0	0
5	0.5000	-0.5000	1	0.5000	0.5000	0

Slip system: 9 dangle: 7.5626 GND: 1.9593\*10<sup>11</sup> Total: 9.4917\*10<sup>13</sup>

Peak: 0 0 2  
 Slip: 9

**Schmid Factor**  
 Multi Study

L-Axis  
 r<sup>2</sup> in long: 0.82601  
 r<sup>2</sup> in short axis: 0.99711  
 FWHM in long axis: 0.064486  
 FWHM in short axis: 0.03739  
 Peak Broadening in long: 0.1135  
 Peak Broadening in short axis: 0.056488

dangle: 7.5626

GND density: 1.9593\*10<sup>11</sup>  
 Total: 9.4917\*10<sup>13</sup> [Analyze]

If Schmid factor calculations are required, after completing steps 1 to 4 of the manual dislocation density analysis, click the Schmid Factor button to open the Schmid factor calculation interface, as shown in the figure below:

**Slip System**  
 #1: (1 1 1)[1 -1 0]

Level: 100 [Calculate]  
 Colormap: 1. Blue-Green-Red

Level: 200 [Reverse]  
 Show Slip Plane & Slip Dir  
 Indices [Save Figure]

Load dir: [ ]

Min: 0 Max: 0.5 [Plot] [Undo] [Reset]

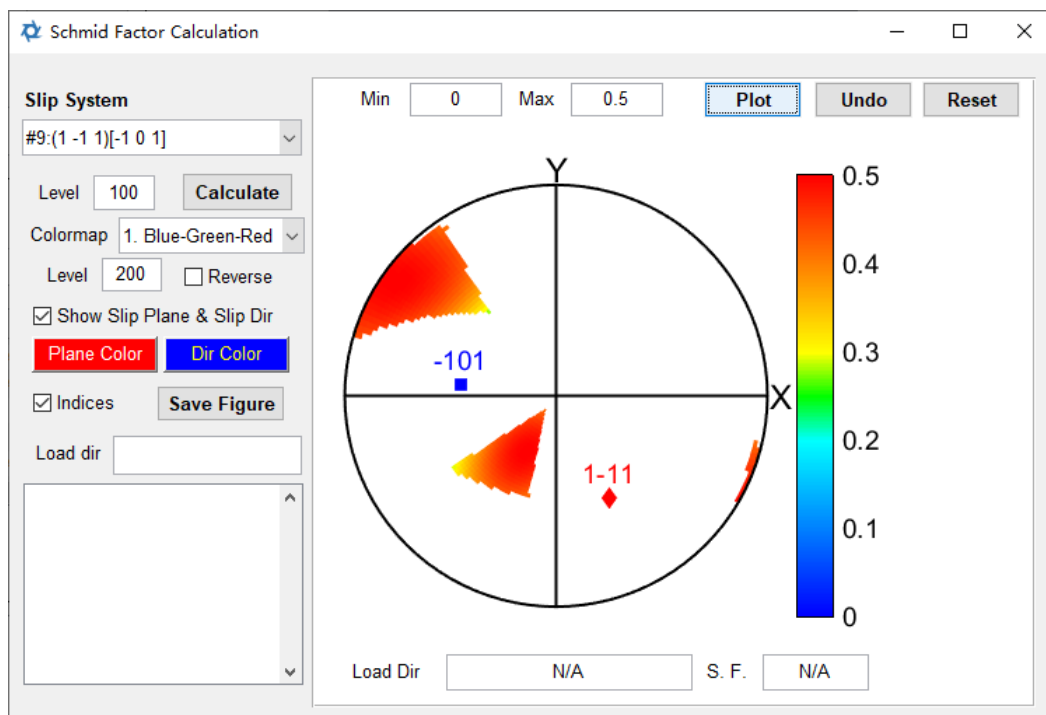
Y  
 X

Load Dir: [ ] S. F.: [ ]

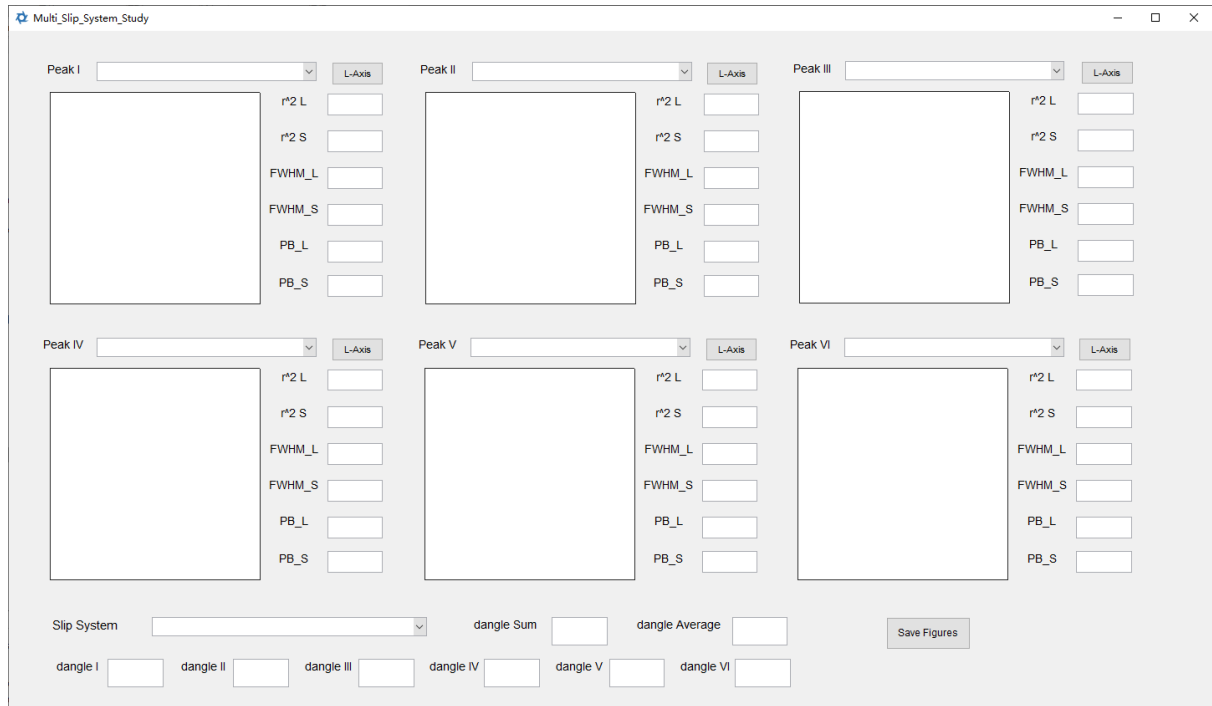
The specific operations are as follows:

1. In the Slip System dropdown menu, select a slip system and enter the calculation precision Level for the Schmidt factor, typically set to 100. Click Calculate to compute the Schmidt factor.
2. After completing the calculation, enter the plotting precision Level in the Level field below, typically set to 200. Click the Plot on the right side to complete drawing the Schmidt factor distribution in the polar plot on the right.
3. When the Show Slip Plane & Slip Dir on the left side is checked before plotting, the polar plot will display the slip plane and slip direction. Clicking Plane Color and Dir Color allows you to change the display colors of the slip plane and slip direction. If Indices are checked, the Miller indices for the slip plane and slip direction will also be displayed in the polar plot.
4. Click Save Figure to save the image.

The effect after completing the above operations is as shown in the figure below:



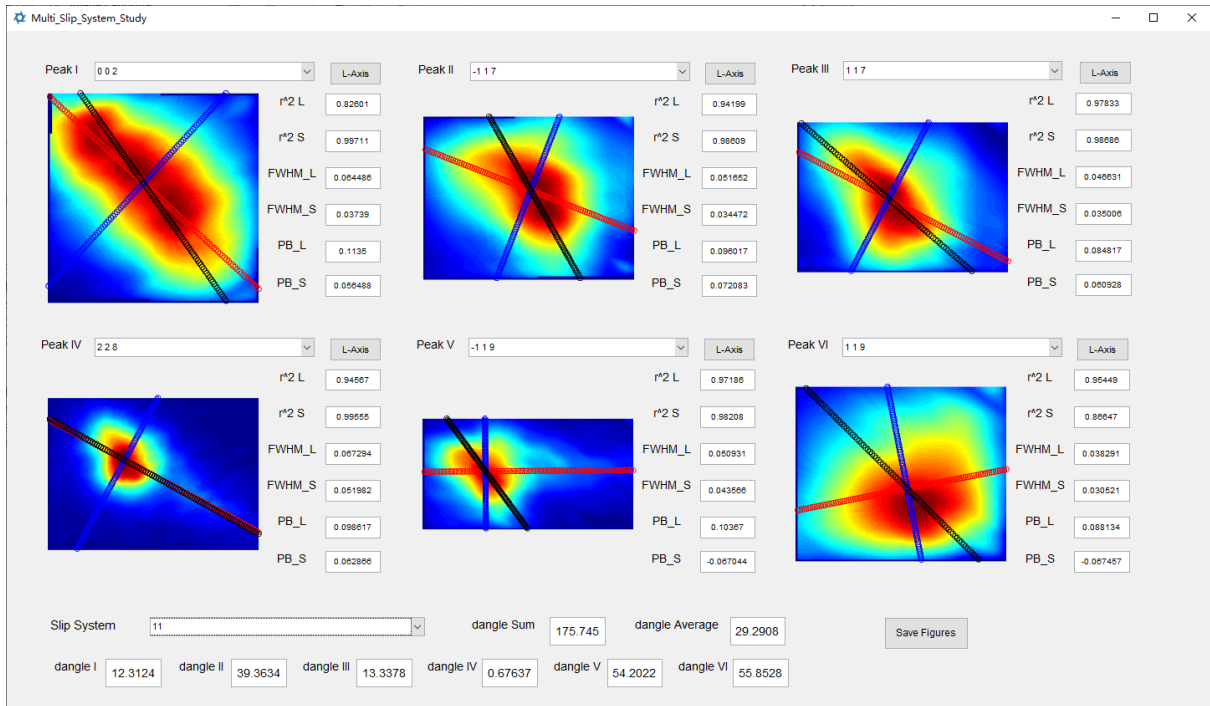
If there is a need to compare the actual long-axis directions of multiple diffraction peaks with the theoretical elongation direction of a certain slip system simultaneously, after completing steps 1 to 4 of the manual dislocation density analysis, click the Multi Study button to open the multi-peak analysis interface, as shown in the figure below:



The specific operations are as follows:

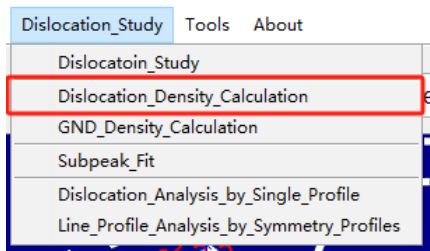
1. In the dropdown menus from Peak I to Peak VI, select different diffraction peaks and successively click the L-Axis buttons to the right of each dropdown menu to automatically acquire their long and short axes, represented by red and blue lines. The peak width fitting data for the long and short axes will be displayed to the right of the diffraction peaks.
2. In the Slip System dropdown menu, select a slip system; its theoretical elongation direction will be displayed on the diffraction peaks. The angle differences between the actual elongation directions and theoretical elongation directions of each diffraction peak are displayed from dangle I to dangle VI. The sum of the angle differences is displayed in dangle Sum, and the average angle difference is displayed in dangle Average.
3. Clicking the Save Figure button allows you to save images of each diffraction peak.

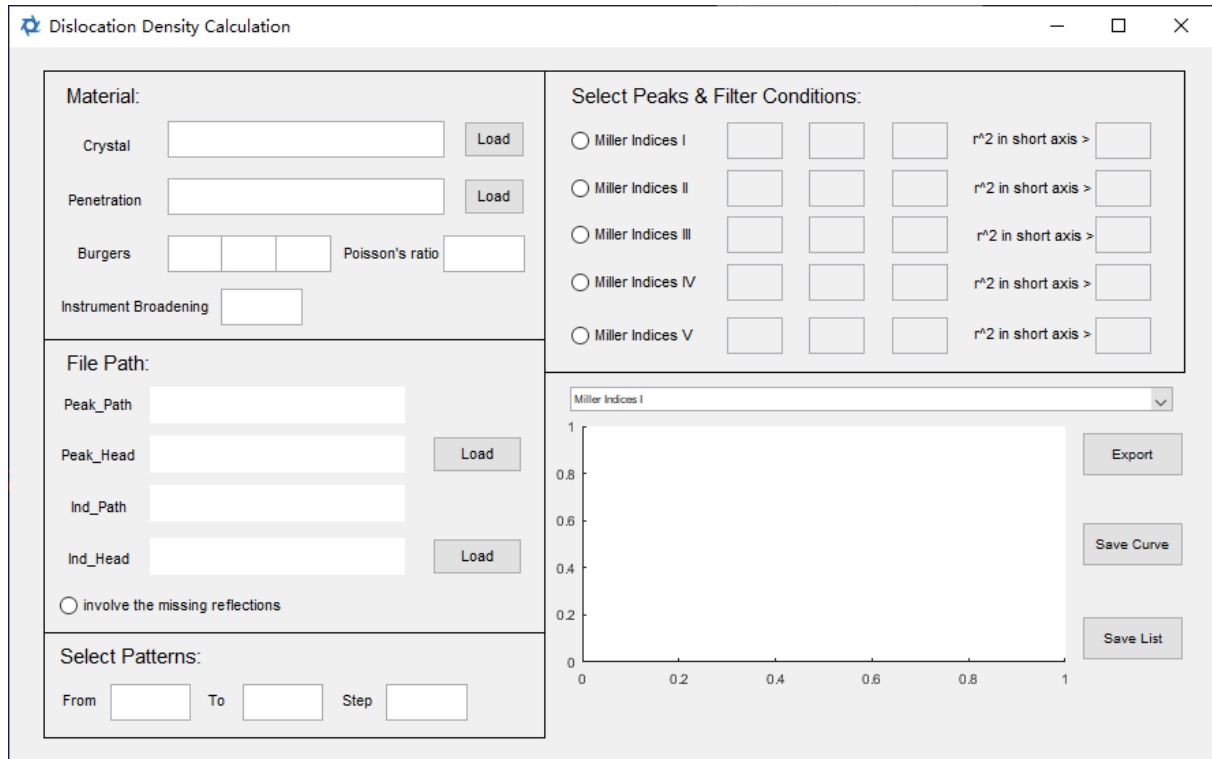
The effect after completing the above operations is as shown in the figure below:



## 7.2 Auto Analysis for Total Dislocation Density

After inputting experimental geometric parameters and completing automatic peak searching and indexation for a large number of diffraction patterns, you can carry out an automatic analysis of the total dislocation density. The specific operation methods are as follows:





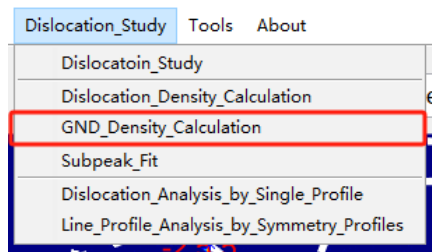
1. Click the Load button to the right of Crystal to import the .rpl file of the crystal structure of the analyzed material. If there is no suitable .rpl file, please refer to section 2.3 to create one.
2. Click the Load button to the right of Penetration to import the penetration data .pnt file of the analyzed material. If there is no suitable .pnt file, please contact the software provider.
3. Click the Load button to the right of Peak\_Head to import the file path and filename prefix of the .pkl file storing diffraction peak information. When creating this .pkl file, a peak shape analysis must be performed on all diffraction peaks, i.e., the Fit All Peaks button needs to be clicked when creating; the method is detailed in section 4.1.
4. Click the Load button to the right of Ind\_Head to import the file path and filename prefix of the .idx file or .ind file generated by XMAS, storing the indexation information of the diffraction peak. The numbers of .idx or .ind files need to correspond one-to-one with the .pkl file numbers.
5. If importing .ind files generated by XMAS, you can click the involve the missing reflections button. After clicking, the software will match the missing diffraction peaks in the .ind file with the diffraction peak positions in the .pkl file and re-index the matched diffraction peaks.
6. Click the buttons to the left of Miller Index I to Miller Index V to activate the Miller indices input. After activation, input the Miller indices of the diffraction peaks used for total dislocation density analysis and successively input the critical values of  $r^2$  for short-axis peak shape fitting to the right of  $r^2$  in short axis >. If the  $r^2$  value of short-axis peak shape fitting is below the entered critical value, it is considered that the

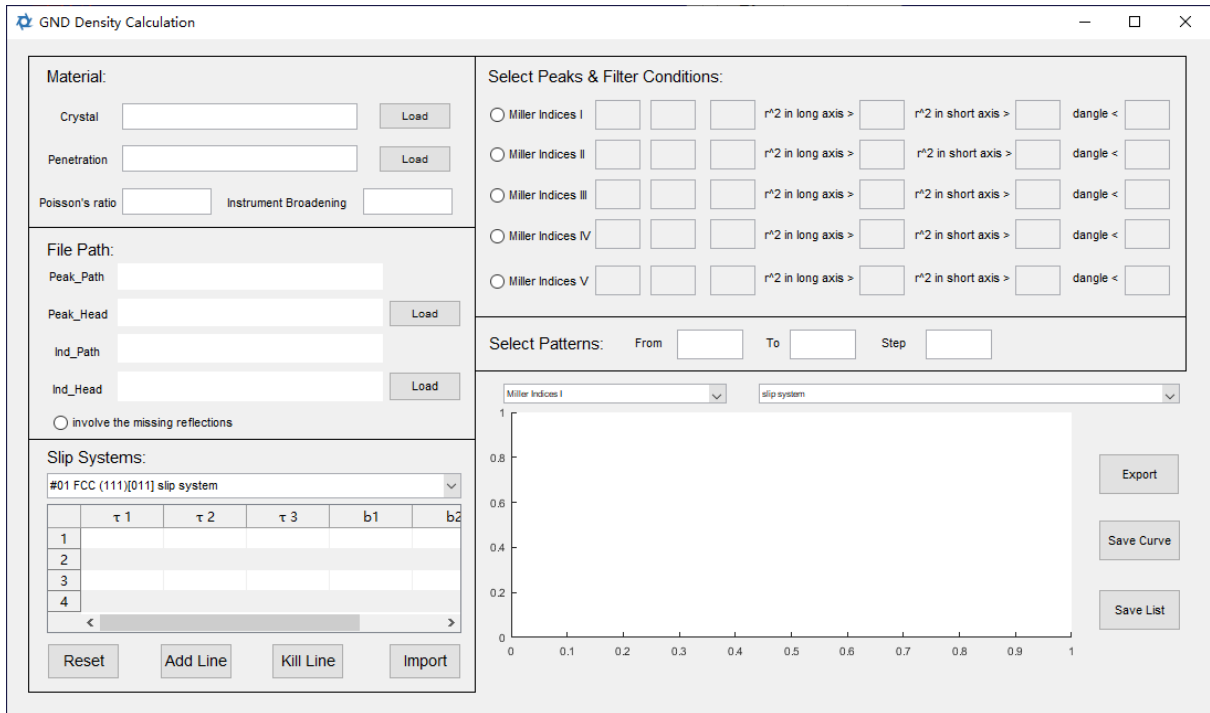
diffraction peak has not been successfully fitted and will not be used for calculating the total dislocation density.

7. Enter the Burgers vector in the Burgers Vector field.
8. Enter the Poisson's ratio of the analyzed material in the Poisson's ratio field.
9. Enter the instrument broadening in the Instrument Broadening field, in the unit as degree.
10. Enter the start number, end number, and step length for calculations in the From, To, and Step fields.
11. Click Export to start the calculation.
12. After the calculation is completed, select different diffraction peaks through the dropdown menu to view the total dislocation density calculated. The relationship graph between the total dislocation density and the numbers will be drawn below the dropdown menu.
13. Select different diffraction peaks in turn and click Save List to store the total dislocation density data calculated. The saved file is an ASCII-encoded .txt file, including numbers, Bragg angles, short-axis peak width of diffraction peaks, X-ray penetration, and total dislocation density data. Click the Save Curve button to save the pictures drawn below the dropdown menu. Here, different diffraction peaks need to be selected in turn, and data should be saved for each diffraction peak.

### 7.3 Auto Analysis of GND & Total Dislocation Density

After inputting the experimental geometric parameters and completing the automatic peak search and indexation of numerous diffraction patterns, you can proceed to automatic analysis of geometric necessary dislocations and total dislocations. The specific operation method is as follows:





1. Click the Load button on the right side of Crystal to import the .rpl file of the crystal structure of the analyzed material. If there is no suitable .rpl file, refer to section 2.3 to generate one.
2. Click the Load button on the right side of Penetration to import the .pnt file of the penetration data of the analyzed material. If there is no suitable .pnt file, please contact the software provider.
3. Enter the Poisson's ratio of the analyzed material in the Poisson's ratio field.
4. Enter the instrument broadening in the Instrument Broadening field, in the unit as degree.
5. Click the Load button on the right side of Peak\_Head to import the file path and filename prefix of the .pkl file storing diffraction peak information. When generating this .pkl file, all diffraction peaks must undergo peak shape analysis, i.e., click the Fit All Peaks button during generation; the method is detailed in section 4.1.
6. Click the Load button on the right side of Ind\_Head to import the file path and filename prefix of the .idx file or the .ind file generated by XMAS, storing diffraction peak indexation information. The numbers of .idx or .ind need to correspond one-to-one with the numbers of the .pkl file.
7. If importing an .ind file generated by XMAS, click the involve the missing reflections button; after clicking, the software will match the missing reflections in the .ind file with the positions of the diffraction peaks in the .pkl file and re-index the matched diffraction peaks.
8. In the list at the lower left of the interface, enter all slip systems of the analyzed material, including the dislocation line direction and the corresponding Burgers vector. Through the Reset, Add Line, and Kill Line buttons, you can reset, add rows, and delete

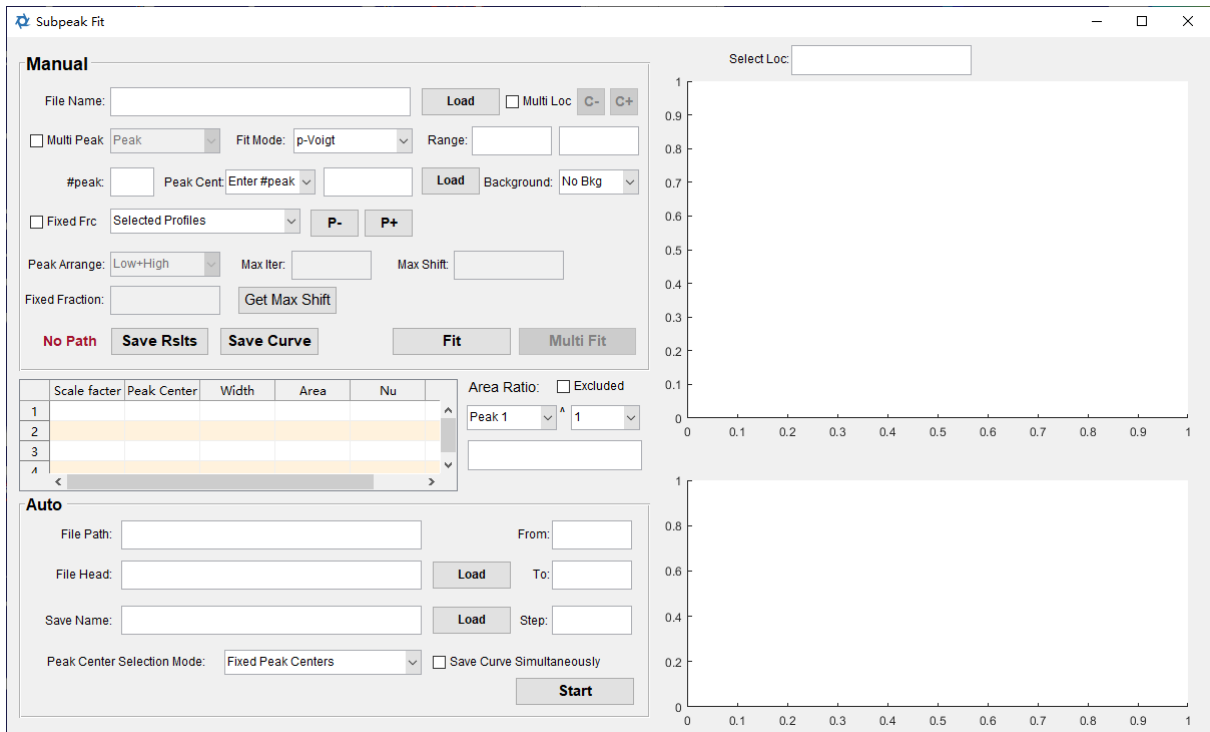
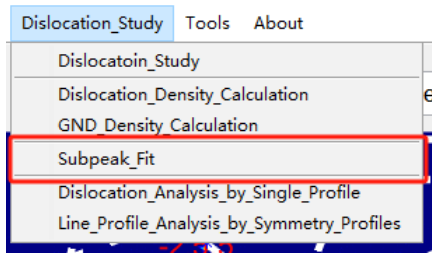
rows in the table. Various slip system data for different materials are preset in the dropdown menu above the table; select the corresponding slip system data directly from the dropdown menu. After completing the slip system data input, click the Import button to import the slip system information.

9. Click the buttons to the left of Miller Indices I to Miller Indices V to activate the Miller indices input, and after activation, enter the Miller indices of the diffraction peaks used for analyzing the total dislocation density.
  - i. To the right of  $r^2$  in long axis  $\lambda$ , successively enter the critical values of  $r^2$  for the long-axis peak profile fitting of the diffraction peaks. If the  $r^2$  value is below the input threshold, it is deemed that the diffraction peak has not been successfully fitted, and it will not be used for calculating dislocation density.
  - ii. To the right of  $r^2$  in short axis  $\lambda$ , successively enter the critical values of  $r^2$  for the short-axis peak profile fitting of the diffraction peaks. If the  $r^2$  value is below the input threshold, it is deemed that the diffraction peak has not been successfully fitted, and it will not be used for calculating dislocation density.
  - iii. To the right of  $\Delta$ , successively enter the critical values of the angular difference between the actual long-axis direction of the diffraction peaks and the theoretical elongation direction of the slip system. If the angular difference for all slip systems is above the input threshold, it is deemed that the diffraction peak has not been successfully matched to a slip system, and it will not be used for calculating dislocation density.
10. In From, To, and Step, enter the start number, end number, and step length for calculations.
11. After completing all the above settings, click the Export button to start the calculation.
12. After completing the calculation, select different parameters and numbers of different diffraction peaks to draw their relationship graphs through two dropdown menus. The different parameters include the slip system, long-axis peak width, short-axis peak width, X-ray penetration, GND dislocation density, and total dislocation density.
13. Select different diffraction peaks in turn and click Save List to save the calculated dislocation density data, with saved files being ASCII-encoded .txt files, including numbers, Bragg angles, long-axis peak width of diffraction peaks, short-axis peak width of diffraction peaks, X-ray penetration, GND dislocation density, and total dislocation density data. Click the Save Curve button to save the pictures drawn below the dropdown menu. Here, each diffraction peak needs to be selected in turn, and data should be saved for each one.

## 7.4 Subpeak Analysis

For the one-dimensional peak shape distribution data obtained in the reconstruction and automatic analysis of reciprocal space intensity, this feature offers the functionality to conduct more precise analysis using methods like the Voigt multi-peak fitting. The specific operations are as follows:

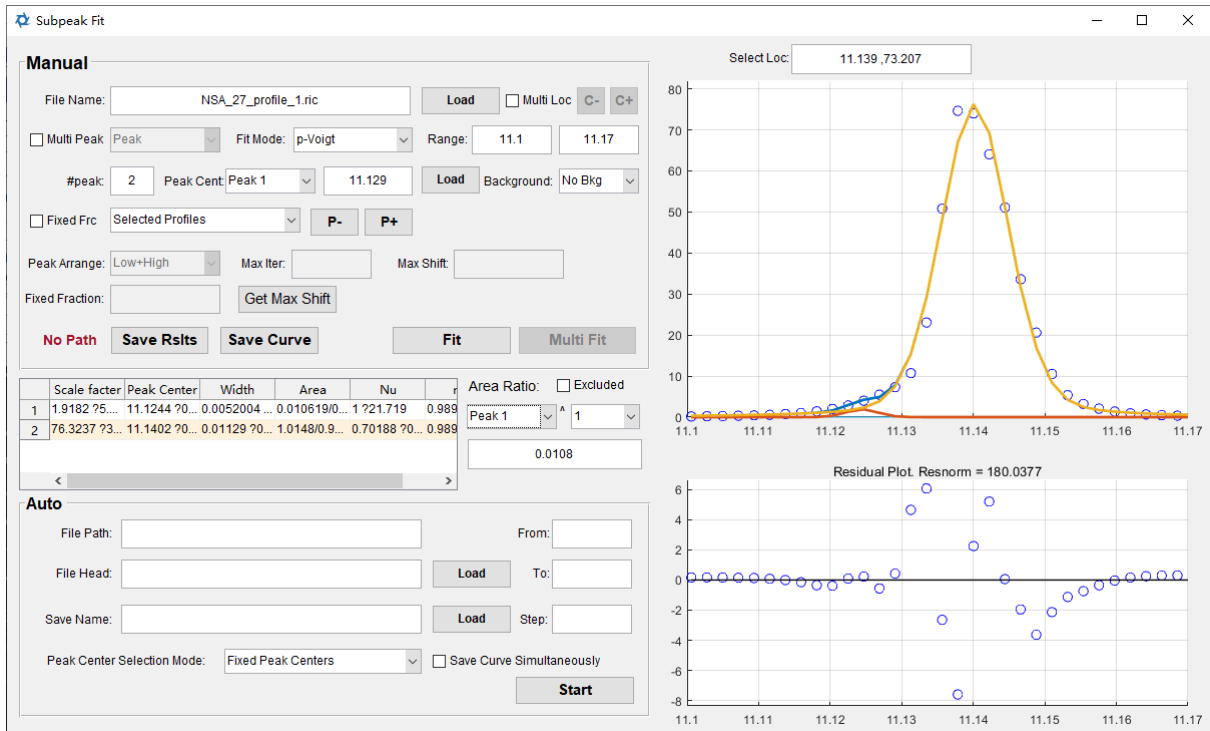




The specific method for manual sub-peak analysis is as follows:

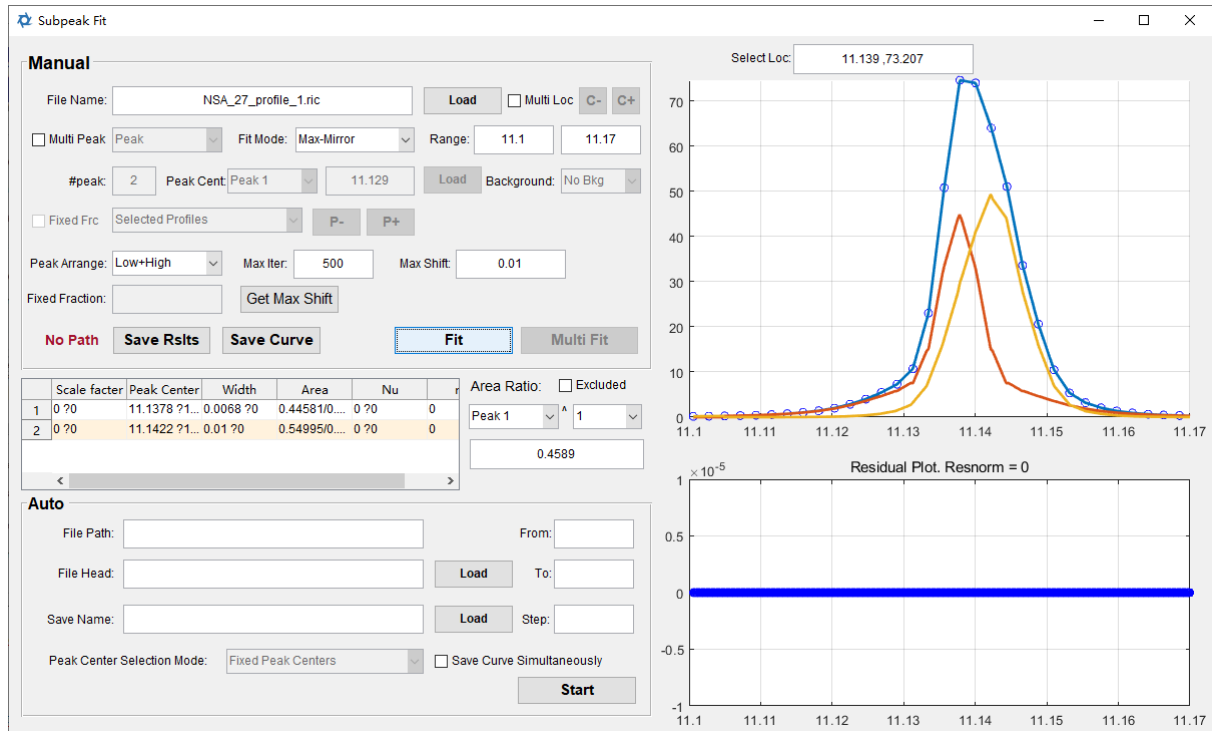
1. In the Manual panel, click the Load button at the top to import the .ric file storing the one-dimensional peak profile. The one-dimensional peak profile will be displayed in the coordinate axis in the upper right. If the obtained .ric file is automatically analyzed and batch obtained in the interface of reciprocal space reconstruction and automatic analysis, the naming of the .ric file will include its corresponding location number. If multiple diffraction subpeaks have been recognized and analyzed in automatic analysis, its number will also include the number of the corresponding subpeak. If these numbers are present in the file, you can light up the Multi Loc and Multi Peak buttons and then switch the .ric files located in the front and back positions by the "C-" and "C+" buttons. The same location different subpeaks will appear in the drop-down menu after Multi Peak, and can be selected through this drop-down menu.
2. The software provides two peak separation methods. Here we first introduce the method of multi-peak fitting using the pseudo-Voigt distribution. To use this method, select p-Voigt in the Fit Mode drop-down menu.

3. Enter the number of sub-peaks in #peak. After entering, press the Enter key, and you can select the corresponding subpeak in the drop-down menu after Peak Centers.
4. Click the approximate position of the subpeak in the coordinate axis in the upper right. The coordinate point clicked will be displayed above the coordinate axis. Select the corresponding subpeak through the drop-down menu after Peak Centers, enter the abscissa of the clicked coordinates behind it, and click the Load button on its right to enter the approximate position of the subpeak. Record the approximate positions of all sub-peaks through the obtained coordinates and the drop-down menu.
5. Enter the abscissa range for subpeak fitting analysis in Range. If not entered, the software will fit the entire curve.
6. Choose the way to remove the background from the drop-down menu after Background.
7. Click the Fit button to perform subpeak analysis. The fitting analysis results will be displayed in the table below, the fitting results will be displayed in the coordinate axis in the upper right, and the error distribution will be displayed in the coordinate axis in the lower right. At the same time, the software will display the proportion of the selected diffraction peak area to the total area in the Area Ratio column, and you can select the diffraction peak occupying the area ratio through the drop-down menu on the left. By using the drop-down menu on the right, you can choose the power of this ratio. If you need to calculate the proportion of other diffraction peak areas except for the selected diffraction peaks, light up the Excluded button.
8. After the fitting is complete, click Save Fit Results, and the software will store the fitting results in a .txt file. If it is the first time saving and the storage path of this .txt file has not been set, clicking this button will prompt the software to set the storage path of this .txt file. After the setting is complete, as shown below, the words Path Defined will be displayed, indicating that the storage path has been set, and the fitting results will be directly stored in this .txt file.



- Click the Save Curve button, and the software will save the fitted curve. This curve will be stored in the storage path of the txt file mentioned in the previous step, and it will be named the same as the currently imported ric file.

If you choose the maximum value mirror method for peak separation, select Max-Mirror in the Fit Mode drop-down menu, then Peak Arrange, Max Iter, and Max Shift will be highlighted. In this mode, only dual peaks can be separated. In the Peak Arrange drop-down menu, select the layout of the two peaks. Low+High means the left side is the lower peak and the right side is the higher peak, High+Low means the left side is the higher peak and the right side is the lower peak. Max Iter represents the number of mirror iterations; if not entered, the software will iterate until it converges. Max Shift represents the offset between the initial mirror point and the highest point of the curve, where a positive number is offset to the right, and a negative number is offset to the left. More details on the maximum value mirror method can be found in the reference "*Quantification of local dislocation density using 3D synchrotron monochromatic X-ray microdiffraction*".

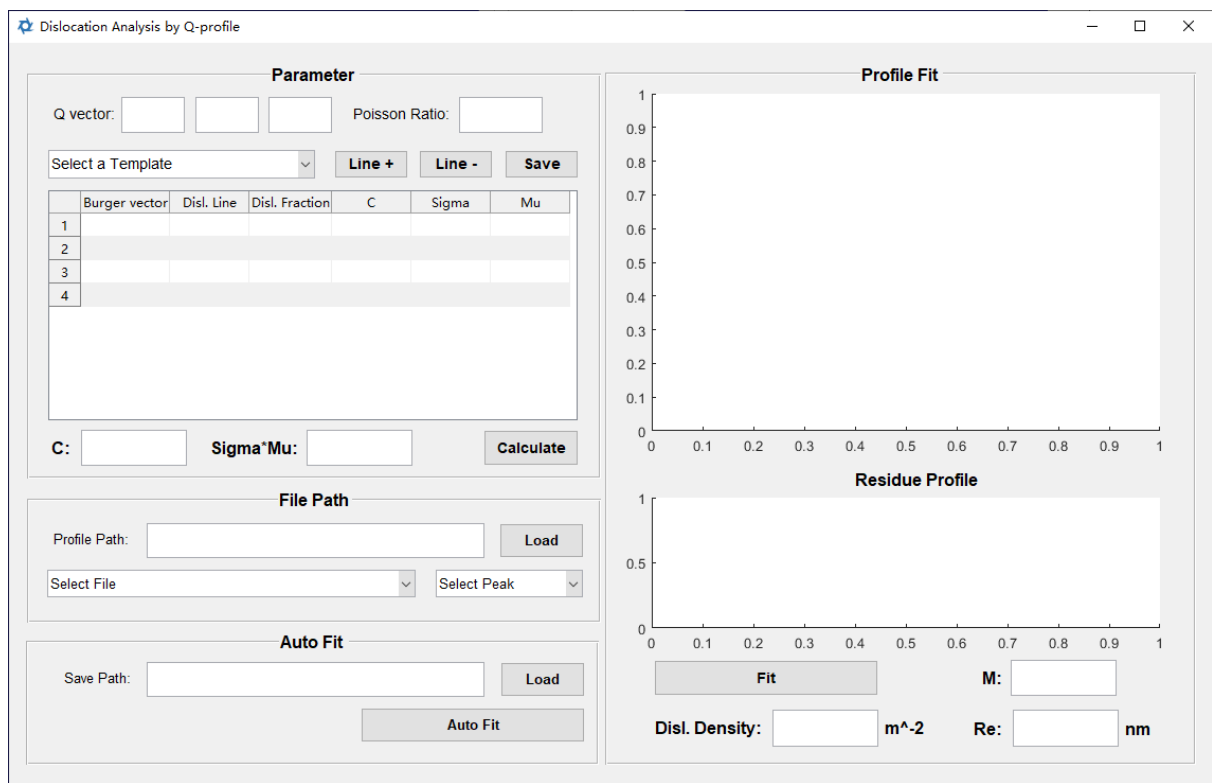
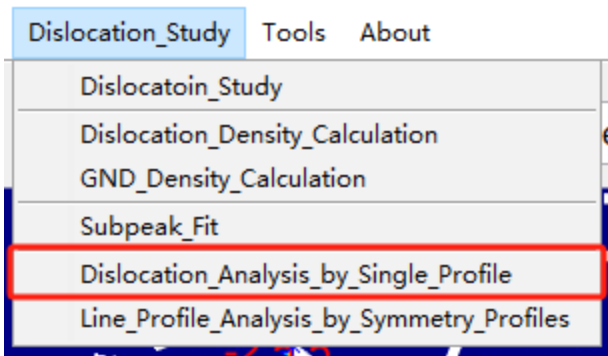


The specific method for automatic subpeak analysis is as follows, it is noted that the automatic subpeak analysis is executed on p-Voigt method.

1. Click the Load button at the top in the Auto panel to import the path and filename prefix of the one-dimensional peak profile file, the .ric file.
2. Click the Load button below to set the file path for storing the results.
3. Enter the start and end file numbers and step length in From, To, and Step.
4. In the Peak Center Selection Mode drop-down menu, select the method for selecting the approximate sub-peak position coordinates. The software provides two selection methods: Fixed Peak Centers, using this method, the software will fit and analyze all .ric files using the approximate subpeak positions entered in manual analysis; Previous Results, using this method, the software will use the approximate subpeak positions entered in manual analysis in the analysis of the first .ric file. For the subsequent .ric files, the analysis results of the previous .ric file will be used as the approximate subpeak positions for the current .ric file's fit analysis.
5. Click the Start button to start the automatic sub-peak fitting analysis; if you need to save the obtained curves simultaneously, light up the Save Curve Simultaneously button.

## 7.5 Dislocation Analysis with Q-profile

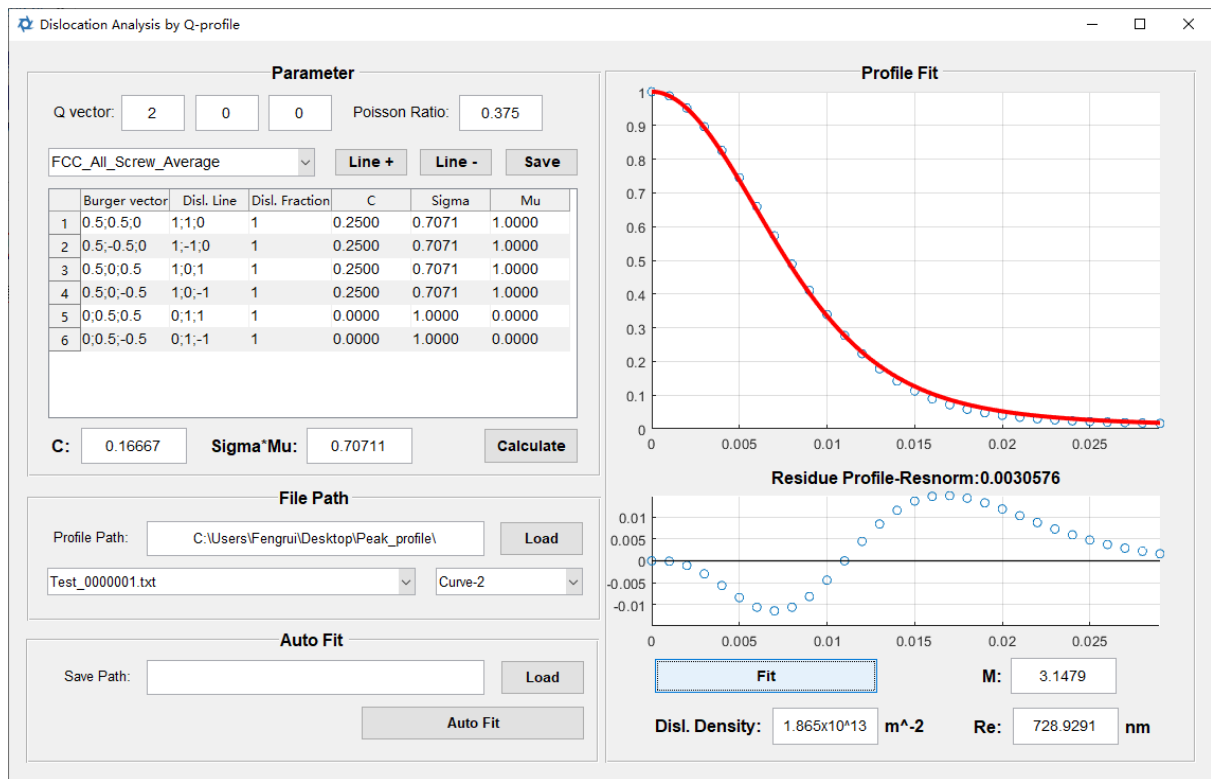
Based on the diffraction peak profile in the  $q//$  direction obtained by energy scanning (stored in the ric file, see Section 6.3) or the fitted diffraction peak shape in the  $q//$  direction saved in the subpeak analysis (stored in the txt file, see Section 7.4), dislocation analysis can be performed. The analysis algorithm is the calculation method of the strictly random distribution dislocation model proposed by M. Wilkens. The specific method is as follows:



1. In the Parameter panel, enter the Miller index of the diffraction peak to be analyzed in Q-vector, and enter the material's Poisson ratio in Poisson Ratio.
2. Enter the Burgers vector and the direction of the dislocation line of all existing slip systems in the material and the fractions of dislocations with different slip systems in the list. Click the Calculate button, and the software will compute the parameter supplement list and calculate the average structure factor C and the average  $s^*m$  value for each slip system. When entering the slip system, click the Line+ and Line- buttons to add or delete rows in the list. After entering, click the Save button to save the list content; the software will prompt to save it in the dislocation\_template folder in the software root directory. When opening this interface again, select the saved list content in the

dislocation\_template folder from the drop-down menu. All screw dislocation systems of FCC crystal is available, and could be selected by the drop-down menu.

3. In the File Path panel, click the Load button to import ric files or txt files that have the peak profiles saved. After importing, the drop-down menu below will display all the same type of files in the same storage path. If a txt file is imported, multiple peak profiles possibly contained in the txt can be selected through the drop-down menu on the right. After selecting the peak profile, it will be plotted as a scatter plot in the Profile Fit panel on the right, only displaying the right half of the peak shape due to its left-right symmetry, and its vertical axis is normalized to its highest.
4. Click the Fit button in the Profile Fit panel to fit the peak shape. The fitting result is displayed in red, the distribution of residuals after fitting is displayed below, and the average of residuals is displayed in the title of the residual distribution graph. The dislocation screening factor  $M$ , dislocation density, and the effective outer cut-off radius  $R_e$  are displayed below. After completing all the above operations, the interface is as shown in the figure.



5. For automatic fitting, after completing all the above settings, click the Load button in the Auto Fit panel to set the save path for the fitting results. The fitting results will be saved in csv format, including the filename of the peak profile, dislocation screening factor  $M$ , dislocation density, the effective outer cut-off radius  $R_e$ , and the average fitting residuals, etc.

6. Click the Auto Fit button in the Auto Fit panel, and the software will fit all peak shapes saved in all peak profile files in the drop-down menu in File Path.

## 7.6 Dislocation Analysis with multi-profiles

This method is based on the modified Williamson-Hall method and the modified Warren-Averbach method. It analyzes the peak profiles of multiple diffraction peaks to assess the fractions of various types of dislocations in the material, the dislocation density, and the effective outer cut-off radius.

This method is under testing and will be published in subsequent versions of PYXIS.

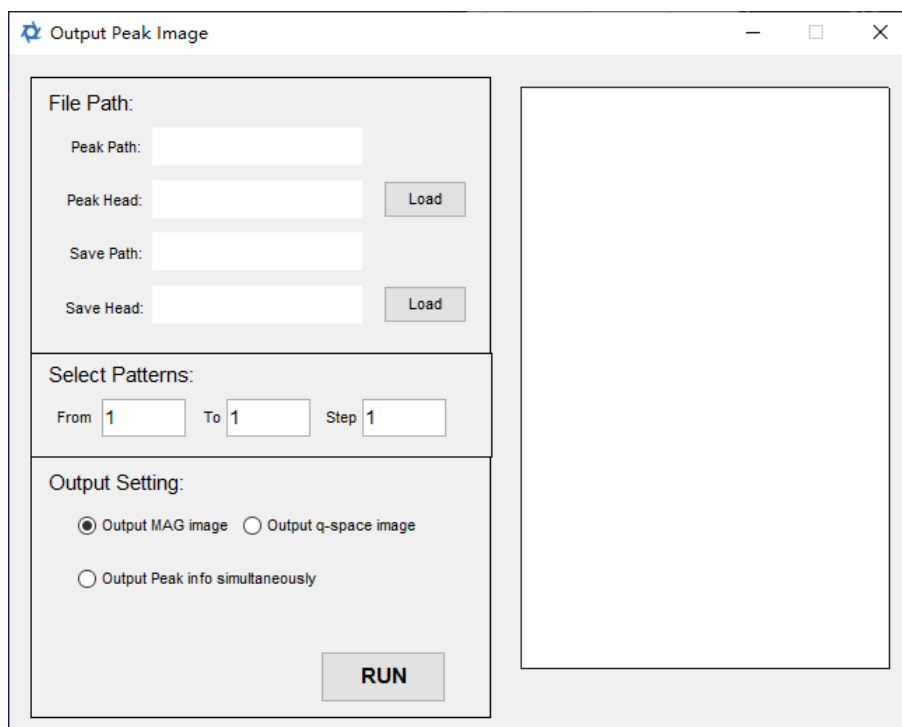
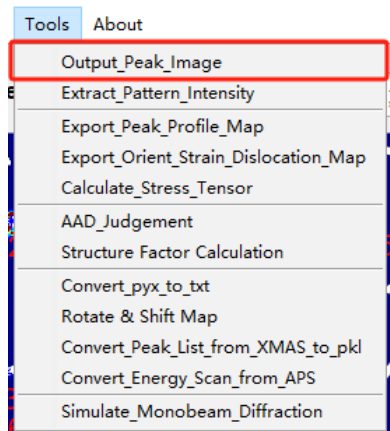
## Other Tools



## 8 Other Tools

### 8.1 Batch Export of Laue Peak Profile

After entering the experimental geometric parameters and experimental scanned area parameters (see Section 2.1) and confirming the Peak Mag local magnification position on the main interface, the output of diffraction peak profile images can be performed. The specific method is as follows:

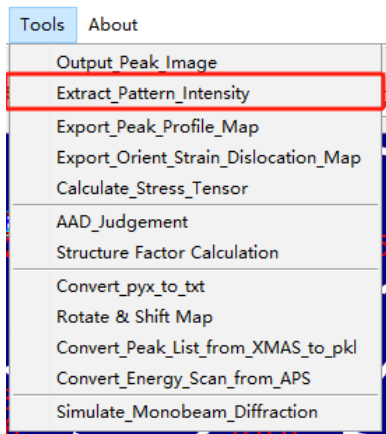


1. Click the Load button next to Peak Head in File Path to import the file path and filename prefix of the .pkl file that saves the diffraction peak information.
2. Click the Load button next to Save Head in File Path to set the path and filename prefix for saving the diffraction peak images.

3. Enter the starting number, ending number, and step size in From, To, and Step.
4. By selecting the Output MAG image or Output q-space image button, you can switch between exporting the magnified image of the diffraction patterns or the diffraction peak intensity distribution map in q-space.
5. If you light up the Output Peak info simultaneously button, you can synchronously output the diffraction peak information extracted from the .pkl file.
6. Click RUN to start the output. After starting the output, the right side of the interface will sequentially display the exported images.

## 8.2 Export Peak Profile Map

This function is used to calculate and plot the peak profile features obtained from the diffraction peak profile fitting. The specific operation is as follows:



1. In the File Path area, click the Load button to import the file path and filename prefix of the .pkl file storing diffraction peak information. When generating this .pkl file, the peak fitting must be performed on all diffraction peaks, that is, the Fit All Peaks button needs to be clicked when generating, and the method is detailed in Section 4.1.
2. In the Select Peak area, choose the way to filter diffraction peaks from the dropdown menu. The software provides three filtering methods:
  - i. Select by location: After selecting this method, switch to the main window, click on the location where the diffraction peak appears in the diffraction pattern, and check in the Peak Mag on its left whether the selected area includes the area where the diffraction peak appears. After selecting the diffraction peak in this way, the software will output the peak profile features of the diffraction peak found by the automatic peak search located in the Peak Mag area currently displayed in each diffraction pattern.

- ii. Select by HKL: After selecting this method, the software will automatically output the peak profile features of the diffraction peak of a certain Miller indices. After selecting this method, the idx file input box and the Load button in this area will be activated. After clicking, you need to import the file path and filename prefix of the corresponding .pkc, .idx, or .ind files produced by XMAS software. Enter the HKL value of the diffraction peak that needs to be outputted in Miller indices. After lighting up the involve the missing reflection button, it will automatically find the diffraction peaks near the missing reflection and treat them as indexed diffraction peaks.
  - iii. Select by intensity order: After selecting this method, the software will activate various filtering functions. Light up Intensity Order and enter the intensity ranking of the selected diffraction peak to its right, i.e., filter the diffraction peaks within the ranking range and output their average. Light up Range of  $R^2$  of 2D fit and enter the range of the  $R^2$  value of the two-dimensional Gaussian fit to its right, i.e., simultaneously filter the diffraction peaks that meet the conditions. Similarly, light up the range of  $r^2$  in long axis and range of  $r^2$  in short axis and enter the corresponding ranges to filter the diffraction peaks that meet the conditions.
3. If you need to output a one-dimensional distribution, enter the starting and ending pkl file numbers and step size in From, To, and Step in the Select Patterns area. If a two-dimensional distribution is needed, light up the Select by region button in the Select Patterns area and enter the coordinates of the lower left and upper right corners of the selected area in Start and End.
4. Click the Export button in Select Peak area to start reading data for calculations.
5. After the calculation is completed, select the parameters for plotting from the dropdown menu. The parameters that can be plotted include
  - i. FWHM\_L: Full Width at Half Maximum of the long axis of the diffraction peak
  - ii. FWHM\_S: Full Width at Half Maximum of the short axis of the diffraction peak
  - iii. PB\_L: Equivalent peak width of the long axis of the diffraction peak
  - iv. PB\_S: Equivalent peak width of the short axis of the diffraction peak
6. Click the Save Map button in Peak Select area to save the data used for plotting in a list form, and click Save Figure to save the plotted image.

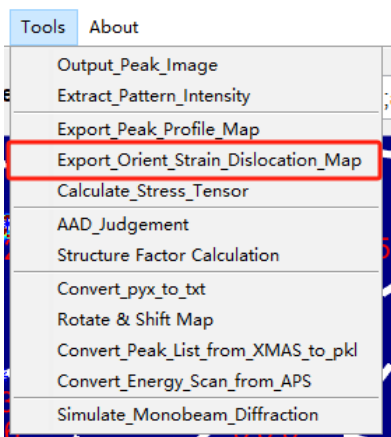
### 8.3 Export Orientation/Strain or Dislocation Map

In the automatic indexation, corresponding .idx and .stn files, or .mid and .mst files, for each diffraction pattern are generated. It is needed to read each .idx file and .stn file and summarize the information in them to form a indexation result file for mapping orientation/strain distribution, namely a .pyx file. The software-generated pyx file can currently be opened and plotted using the XTALcamp software (XTALcamp can be found from [XtalCAMP-CAMP NANO 微纳尺度材料行为研究中心 \(xjtu.edu.cn\)](http://XtalCAMP-CAMP NANO 微纳尺度材料行为研究中心 (xjtu.edu.cn))). If you want to read the indexation results with other software, PYXIS can convert pyx to ASCII encoded txt format, see details in Section 9.7.

Since the results calculated through different diffraction peaks during the dislocation density calculation are all saved separately, and the calculated data only correspond to the

diffraction pattern number, it is impossible to draw a two-dimensional distribution map. The software provides the function to read the results calculated from different diffraction peaks and summarize them to include two-dimensional coordinates to draw a two-dimensional distribution map.

The specific operation is as follows:



To generate and output .pyx files, perform the following steps:

1. Light up the Create Orient/Strain Map button.
2. Click the Load button for Phase I and select the rpl file of the crystal structure of the analyzed material; the software will automatically read the material entered for the indexation parameters. Detailed methods in setting indexation parameters are found in Section 2.3. If using PPC automatic indexation, you can light up the Phase II button and click the Load button to import the rpl file of the crystal structure of the second phase and the phase map output in PPC automatic indexation.
3. If you are importing single grain idx and stn files, choose Mono-grain from the drop-down menu and click the Load button in the activated box below to import idx files. To import stn files, light up the Include Strain Tensor button and click the Load button.
4. For importing multiple subgrain mid and mst files, select Multi-grain from the drop-down menu and import mid files by clicking the Load button in the activated box below. To import mst files, light up the Include Strain Tensor button and click the Load button.

5. If you need to output the fit results of experimental geometric parameters simultaneously, light up the Include geometry setup refinement button and click Load to import the gsr file storing the fit results of experimental geometric data. Detailed methods to generate gsr file are found in Section 5.4.
6. Click the Load button in the Output area, set the save path and file name for the output file. Enter the scan area and scan step size in the x and y directions in Scan Scale and Step Size in the Output area. Choose whether the experiment is first scanned along the X-axis or the Y-axis by clicking the along X and along Y buttons. The software will automatically import the data in the experimental geometry parameter setting window. Enter the coordinates of the lower left and upper right corners of the output area in Start and End. The software will automatically select the entire scanning area.
7. Click the Start button in this area to read, summarize, and output. The information contained in the outputted .pyx is detailed in Section 9.12.

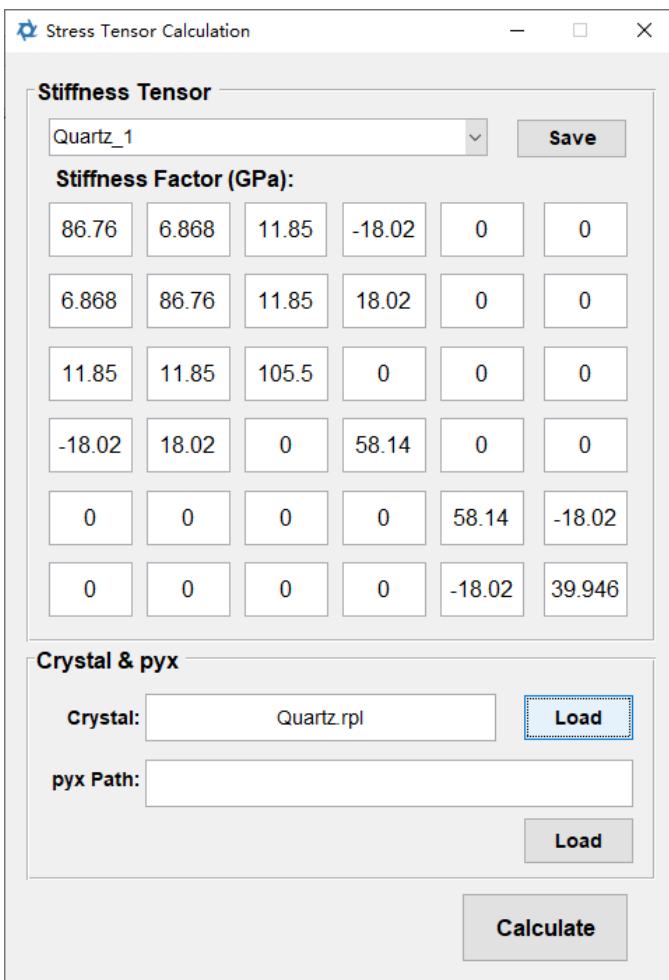
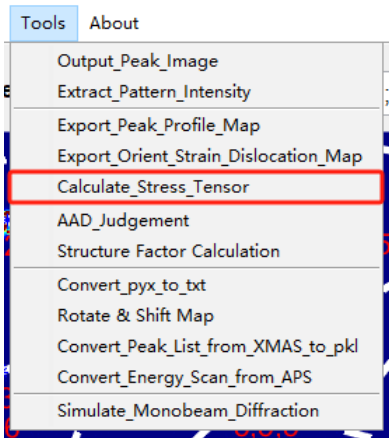
To generate and output dislocation density distribution data, perform the following steps:

1. Light up the Create Total Density Map button if summarizing a total dislocation density file (see Section 7.2 for the generation of this file); if summarizing GND density and total dislocation density files (see Section 7.3 for the generation of this file), light up the Create GND Density Map button.
2. This function can summarize up to 5 dislocation density files of diffraction peaks. Light up the buttons in front of Peak I to Peak V, choose how many dislocation density files of diffraction peaks need to be inputted, and click the Load button to the right to import the corresponding dislocation density files.
3. If you need to calculate the average dislocation density of each peak, open the Calculate Average button.
4. The remaining operations are the same as steps 6 to 7 for generating and outputting .pyx files. The summarized dislocation density is written in txt file encoded by ASCII codes.

## 8.4 Calculate Stress Tensor

The indexation process allows for the output of stn or mst files, which contain strain tensor information, and this strain tensor information can be consolidated and output to .pyx files. By using this feature, you can read the strain tensor information saved in the .pyx file, calculate the stress tensor based on this and then save it in the .pyx file.

The specific operations are as follows:



1. Enter the elastic modulus tensor in the Stiffness Tensor panel. After entering, click Save, the software will prompt you to enter the name of this elastic modulus, and it will save this elastic modulus. When you need to use it, you can select the previously saved elastic modulus from the drop-down menu above.



2. In the Crystal & pyx panel, click the Load button after Crystal to select the crystal's rpl file.
3. In the Crystal & pyx panel, click the Load button after pyx Path to import the .pyx file that has the strain tensor saved.
4. After completing the above settings, click the Calculate button. The software will read the .pyx file, calculate the stress tensor and output it to the .pyx file.

## 8.5 Check Indexation Results

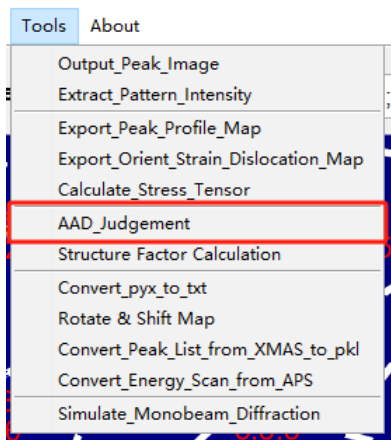
This function checks for excessively deviating diffraction peaks in the indexation results through the deviation in relative angles.

The verification process is based on two assumptions:

- The offset between the indexed diffraction peak and its theoretical position caused by strain and peak-searching errors is much smaller than the position offset caused by mis-indexation of the diffraction peak.
- Only a few diffraction peaks are misidentified during the indexation process.

Hence, this method is only applicable when there are a large number of indexed diffraction peaks (typically more than 50) and the material exhibits poor plasticity (with no significant elongation of the diffraction peaks).

The specific operation is as follows:



The screenshot shows the 'AAD Judgement' software window. It is divided into two main sections: 'Deviation Map' and 'Import File Path'.

**Deviation Map Section:**

- A dropdown menu is set to 'Uniform Peak Distribution'.
- 'Deviation Size' is set to 2.
- 'Horizontal Peak Num' is 9.
- 'Vertical Peak Num' is 9.
- 'Total Peak Num' is 81.
- 'HKL to XYZ Matrix' contains the following values:
 

```
1,0,0
0,1,0
0,0,1
```
- A 'Generate Devation Map' button is present.
- Below it is a 'Deviation Map:' text box and a 'Load' button.

**Import File Path Section:**

- 'Strain File Path:' is an empty text box.
- 'Strain File Head:' is an empty text box with a 'Load' button to its right.
- 'From:' is 1, 'To:' is 1, and 'Step:' is 1.
- There is a radio button labeled 'Select a region'.
- 'Start:' and 'End:' are empty text boxes.
- 'Saving Path:' is an empty text box with a 'Load' button to its right.
- A large 'Start' button is located at the bottom center of the window.

This function verifies by comparing the indexation results with a Deviation Map. The Deviation Map can be obtained in two ways:

1. If the area scan contains only one grain, i.e., the orientation is similar, use the "Orientation Determined Distribution" mode. In this mode, select "Orientation Determined Distribution" from the drop-down menu in the Deviation Map panel, and input the HKL to XYZ orientation matrix of the grain contained in the area scan in the HKL to XYZ Matrix box.

This is a close-up view of the 'Deviation Map' section from the software interface.

- The dropdown menu is now set to 'Orientation Determined Distribution'.
- 'Deviation Size' remains 2.
- 'Horizontal Peak Num' is 9.
- 'Vertical Peak Num' is 9.
- 'Total Peak Num' is 81.
- 'HKL to XYZ Matrix' contains the same values:
 

```
1,0,0
0,1,0
0,0,1
```
- The 'Generate Devation Map' button is visible.
- The 'Deviation Map:' text box and 'Load' button are also visible.

- If the area scan contains multiple grains, the software assumes that the diffraction peaks are uniformly distributed. After selecting "Uniform Peak Distribution", input the number of diffraction peaks in the horizontal and vertical directions in "Horizontal Peak Num" and "Vertical Peak Num", respectively. The entered number should roughly match the actual number in the pattern.

**Deviation Map**

Uniform Peak Distribution  Deviation Size:

Horizontal Peak Num:  HKL to XYZ Matrix:

Vertical Peak Num:  1,0,0  
0,1,0  
0,0,1

Total Peak Num:

Deviation Map:

After setting the above two modes, input the diffraction peak offset possibly caused by strain and peak-searching errors in "Deviation Size", with the unit being pixels. Then click "Generate Deviation Map", and the software will calculate the deviation map and prompt to save it upon completion.

The saved Deviation Map can be used directly later by selecting "Load Deviation Map" from the dropdown menu and clicking the Load button to import the previously saved Deviation Map.

**Deviation Map**

Load Deviation Map  Deviation Size:

Horizontal Peak Num:  HKL to XYZ Matrix:

Vertical Peak Num:  1,0,0  
0,1,0  
0,0,1

Total Peak Num:

Deviation Map:

After calculating or importing the Deviation Map, you need to import the indexation results. The indexation results used here are stn or mst files that retain strain information. XMAS-produced str files can also be imported. Then input the starting number, ending number, and step in "From", "To", and "Step", respectively. If you need to import files from a specific region, select the "Select a region" button, and input the coordinates of the bottom-left and top-right corners in "Start" and "End". Then, click the Load button after

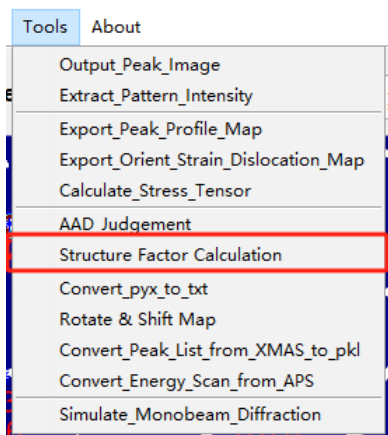
"Saving Path" to set the result save path. After that, click the Start button to begin verification. The verification results are saved in ASCII-encoded txt format.

The results include:

- i. X, Y, Num: File coordinates and number;
- ii. diff\_mean: Average deviation of all diffraction peaks;
- iii. diff\_std: Average of the theoretical maximum deviation of all diffraction peaks;
- iv. index\_num: Number of indexed diffraction peaks;
- v. over\_thres\_ratio: Fraction of diffraction peaks exceeding the theoretical maximum deviation. Those exceeding the maximum theoretical deviation are verified as mis-indexed diffraction peaks;
- vi. mean\_over\_diff: Average value of the part exceeding the theoretical maximum deviation; average\_intensity\_(k): Average intensity of the diffraction peak.

## 8.6 Calculate Structure Factor

This feature can calculate the material's structure factor. The specific method is as follows:



By selecting a crystal with the same space group as the measured crystal in the "Select Crystal with Same Structure" panel, the space group and atomic coordinates of the chosen crystal will be displayed below.

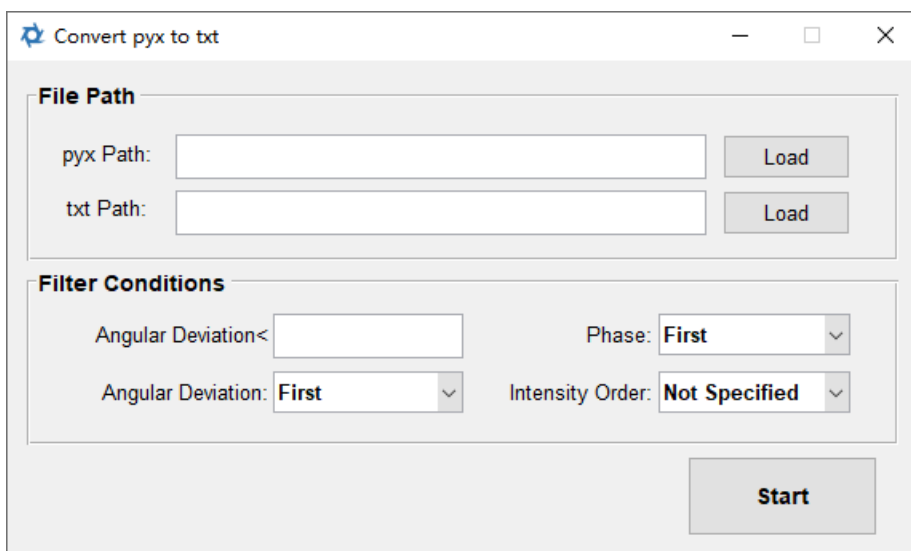
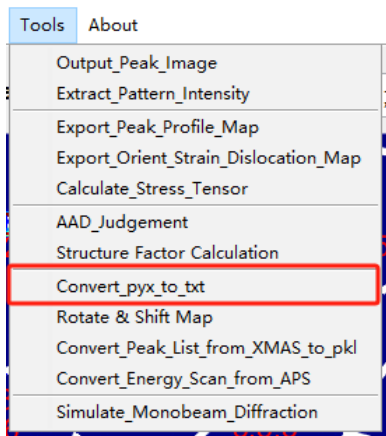
Then, in "Input Composition", add atoms and their probability of appearing at each atomic position. The specific operation is to select the atomic position from the dropdown menu, and then input the element's abbreviation and its occurrence probability into the "Element" column and "at" column of the table, respectively. If there are more atoms, you can adjust the table size using the "Line -" and "Line +" buttons. After completing all inputs, click the "Confirm" button. Once confirmed, the "Unconfirm" sign in the panel will change to "Confirmed".

Then, in the "HKL & d-spacing" panel, input the HKL values of the crystal plane to be calculated, the lattice parameters abc, and angles alpha, beta, and gamma in the "HKL", "abc", and "abg" columns, respectively.

After completing the above settings, click the "Calculate" button, and the results will be displayed in the "Structure Factor" panel.

## 8.7 Convert pyx to txt File

The software-generated pyx file can currently only be opened and plotted using the XTALcamp software (XTALcamp can be found from [XtalCAMP-CAMP NANO 微纳尺度材料行为研究中心 \(xjtu.edu.cn\)](http://XtalCAMP-CAMP NANO 微纳尺度材料行为研究中心 (xjtu.edu.cn))). If you need to plot with other software, you can use this feature to convert the pyx file into a txt file. However, in the txt file, one data point only contains results from one subgrain or grain. The specific operation method is as follows:



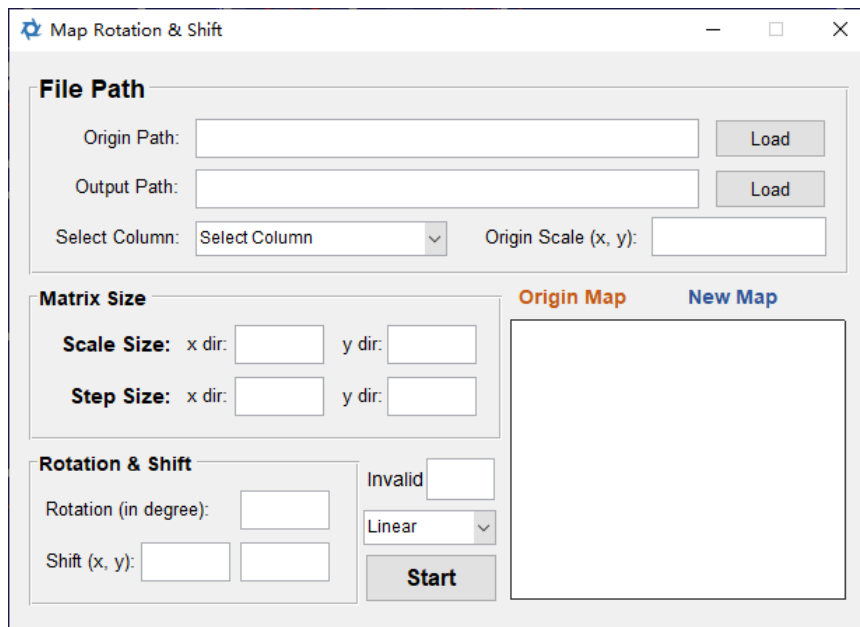
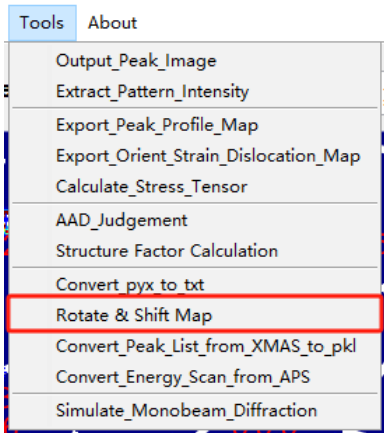
1. Click the "Load" button inside the "File Path" panel to import the pyx file and set the save path for the txt file.
2. Enter filtering criteria in "Filter Conditions" to filter the output subgrains or grains. Among them:
  - i. "Deviation<" indicates selecting subgrains with an angular deviation (the average angular difference between each diffraction peak and its theoretical position) smaller than a certain value. If "Deviation<" is not input, angular deviation filtering will not be applied.
  - ii. Choose the phase to output from the dropdown menu next to "Phase".
  - iii. Choose which subgrain to output from the subgrains sorted in ascending order of angular deviation from the dropdown menu next to "Angular Deviation". If "Not Specified" is chosen, this filtering condition won't be applied. When this condition is used, the "Intensity Order" filtering condition cannot be used.
  - iv. "Intensity Order" means choosing the subgrain that ranks a certain position in terms of the average intensity of the indexed diffraction peaks among all subgrains that meet other filtering conditions. If "Not Specified" is chosen, this filtering condition

won't be applied. When this condition is used, the "Angular Deviation" filtering condition cannot be used.

3. Click Start button to start converting pyx to text file.

## 8.8 Rotation & Shift Map

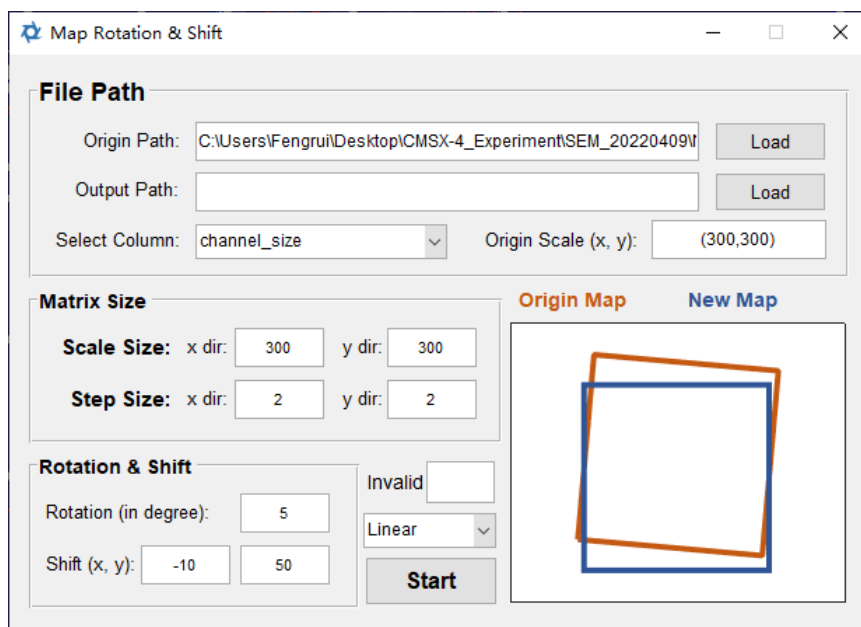
This function, through interpolation, assigns existing area distribution data to other coordinate systems. The specific operation method is as follows:



1. In the "File Path" panel, click on the "Load" button next to "Origin Path" to import the original area scanning data. The data needs to be saved in txt format as a list. The header should not exceed one line, and the first two columns should represent the x and y coordinates, respectively. Data in the same row should be separated by tabs.
2. After importing, the dropdown menu under "Select Column" will display various column information from the area scanning data. Select the information that needs to be

converted from this menu. The area size covered by the original plane scanning data will be displayed in "Origin Scale".

3. Click on the "Load" button next to "Output Path" to set the output path. The output data will be saved in txt format, containing the converted x, y coordinates, and data.
4. After completing the above settings, enter the region size and data step size in the new coordinate system in the "Matrix Size" panel's "Scale Size" and "Step Size" respectively.
5. In the "Rotation & Shift" panel, input the rotation and translation relationship between the new coordinate system and the original one. Once entered, the lower right corner will display the positional relationship of the data-covered area in the original and new coordinate systems, colored brown and blue respectively.



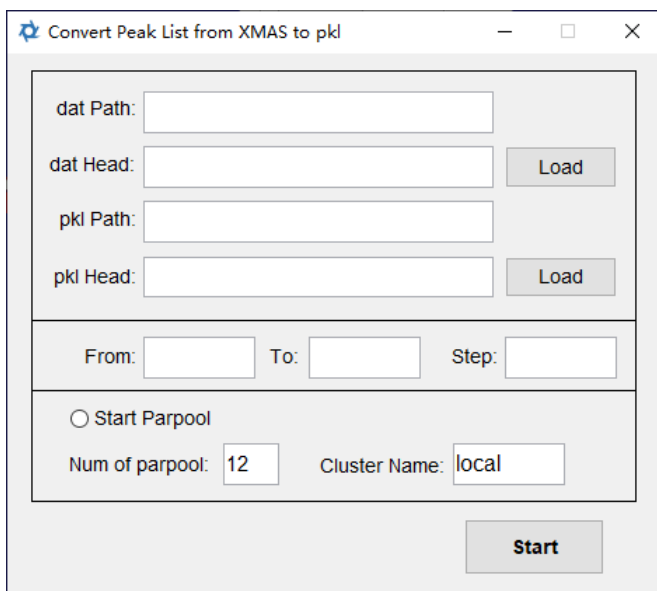
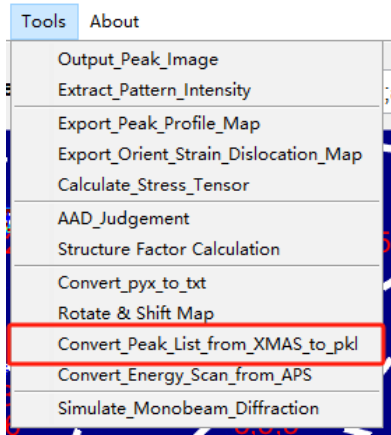
6. If certain data in the original dataset represent invalid points (e.g., 0, -1), you can fill in the data indicating invalid points in "Invalid", and these data points will be disregarded during the conversion. Choose the interpolation method from the dropdown menu, which includes:
  - i. Liner: Linear interpolation;
  - ii. Nearest Neighbor: Directly copy the nearest original data;
  - iii. Natural Neighbor: Cubic spline interpolation.
7. After completing the above settings, click the "Start" button. The converted data will be saved in the set path.

## 8.9 Convert Peak List from XMAS to pkl

The peak detection results outputted by XMAS are stored in a dat file. This file format is different from the pkl file produced by PYXIS and is not universally compatible. However, the information they contain is roughly the same. By converting the peak detection result file outputted by XMAS to a pkl file, PYXIS can be used to analyze the peak searching



results from XMAS. After correctly setting the experimental geometry parameters and peak searching parameters, the conversion can be done. The specific operation method is as follows:

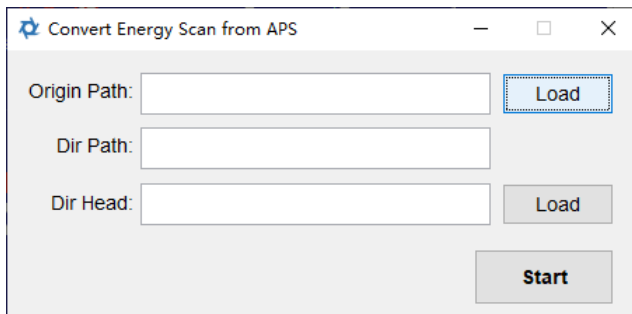
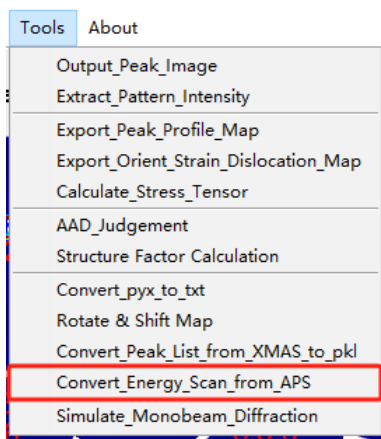


1. Click on the "Load" button after "dat Head" and the "Load" button after "pkl Head", respectively, to import the storage path and filename prefix of the dat file and the storage path and filename prefix of the generated pkl file.
2. Set the starting, ending, and interval file numbers in "From," "To," and "Step." The generated pkl file will have the same file number as the dat file.
3. If parallel computing is needed, activate the "Start Parpool" button. The "Num of Parpool" and "Cluster Name" represent the number of parallel operations and the name of the cluster where parallel computing takes place, respectively. These two settings are automatically configured by the software based on the computer's settings. If not necessary, do not modify them.

4. Click the "Start" button to begin the conversion. If clustering of peaks was set in the peak searching parameters, the software would cluster the peaks outputted by XMAS. Since the peak searching results outputted by XMAS do not include the diffraction peak range, the resulting pkl file also does not contain data on the diffraction peak range or major-minor axis peak shape fitting.

## 8.10 Convert Energy Scan Data from APS

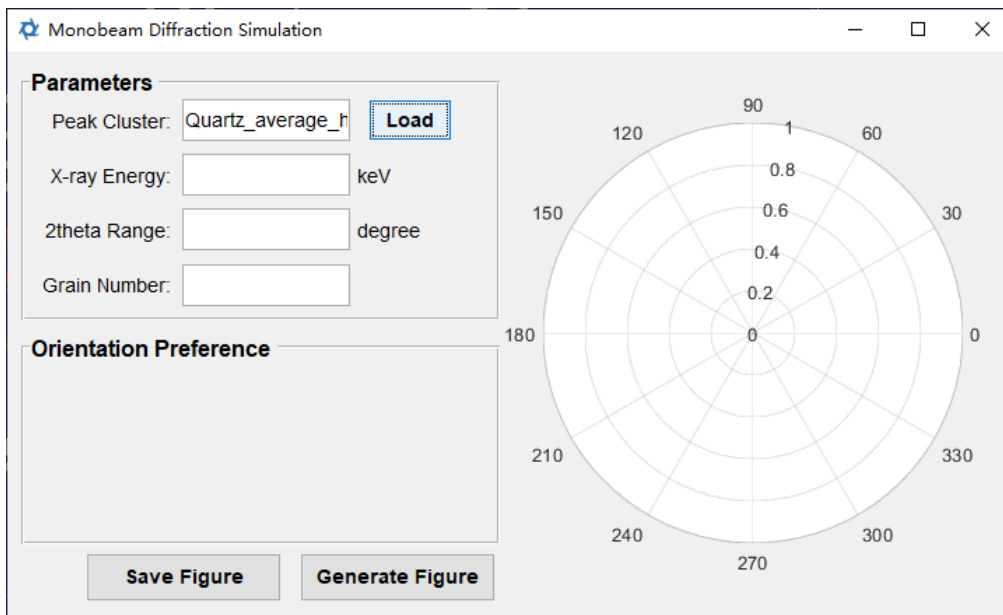
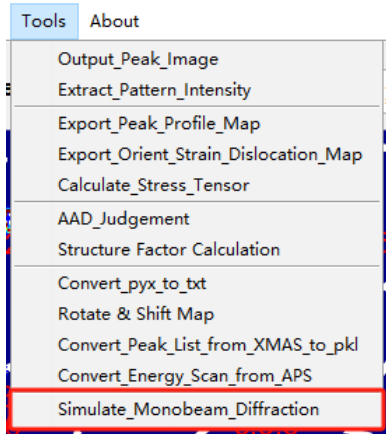
PYXIS only accepts energy scan data formats from the Taiwan Photon Source (TPS) beamline 21A. However, energy scan data from the Advanced Photon Source (APS) beamline 34-IE-D can be converted to the TPS 21A data format. The specific method is as follows:



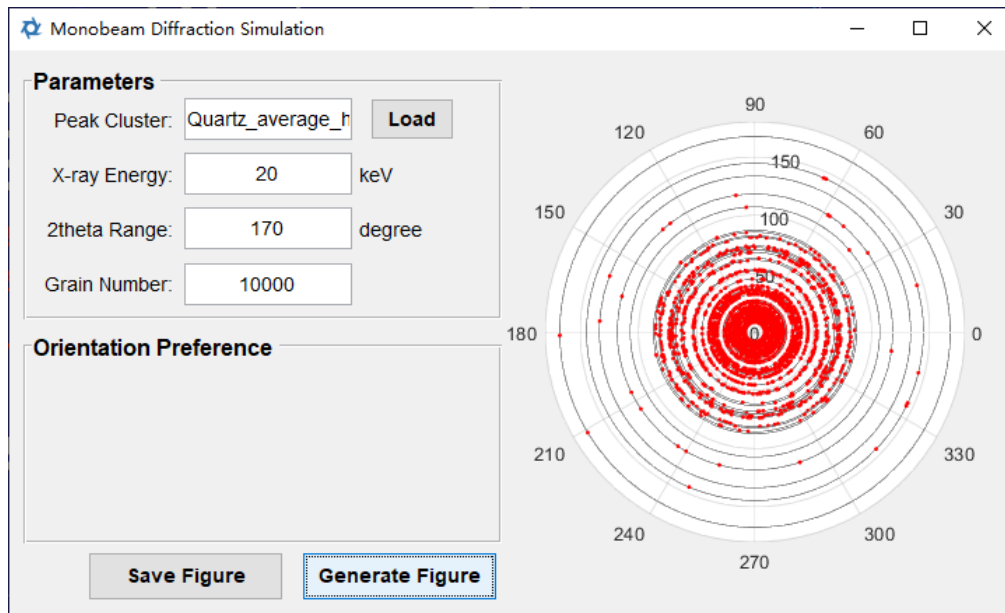
1. Click the "Load" button at the top to import the .h5 file collected by APS 34-IE-D. Then click the "Load" button at the bottom to set the export path and filename prefix.
2. Click the "Start" button to begin the export.

## 8.11 Simulate Monobeam Diffraction Pattern

This function is still under development and can only simulate monochromatic diffraction pattern of a small number (less than 10,000) of grains with a random orientation distribution. The function for simulating systems with preferential orientation is under development. The method for simulating the monochromatic diffraction pattern of a small number of randomly oriented grains is as follows:



1. Click the "Load" button in the "Parameters" panel to import the crystal information. The imported crystal information should be in .mat format. The method for generating the .mat format crystal information file can be found in Section 2.2.
2. Input the X-ray energy, the 2theta angle covered by the detector, and the number of randomly oriented grains in the system in "X-ray Energy," "2theta Range," and "Grain Number," respectively.
3. Click the "Generate Figure" button to plot the simulated diffraction pattern on the right. Click the "Save Figure" button to save this diffraction pattern.



## 8.12 Data Containing in pyx File

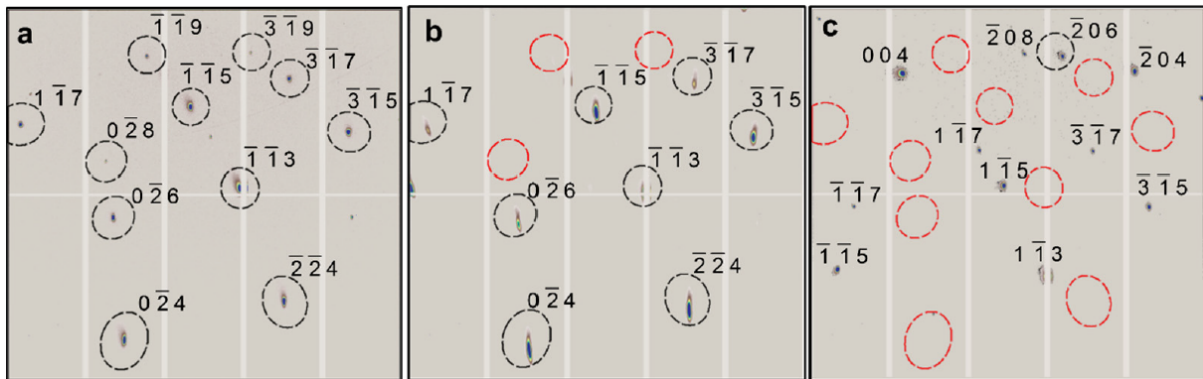
The table below contains explanations for the headers and data meanings of the pyx file. For easy comparison and understanding, the headers from the SEQ file generated by XMAS are also listed.

pyx File	seq File	Comment
X, Y	X, Y	Relative coordinates of scan spots
Pattern_number	Image_Num	Laue pattern number
Phase_type	\	PYXIS could index multi-phase simultaneously. For one phase, it is set as 1
Intensity	\	Sum of integrated intensity of all indexed peaks
dev_orient	\	Deviation of the orientation refinement
AX, AY, AZ BX, BY, BZ CX, CY, CZ	AX, AY, AZ BX, BY, BZ CX, CY, CZ	HKL to xyz orientation matrix, same as seq
dev_strain	\	Deviation of the strain refinement
XX, YY, ZZ YY, YZ YZ	Dev_EpsXX, Dev_EpsXY, Dev_EpsXZ, Dev_EpsYY, Dev_EpsYZ,	Deviatoric strain tensor in sample coordinate system, same as seq

	Dev_EpsZZ	
11, 12, 13 22, 23 33	Dev_Eps11, Dev_Eps12, Dev_Eps13, Dev_Eps22, Dev_Eps23, Dev_Eps33	Deviatoric strain tensor in lattice coordinate system, same as seq
ASTX, ASTY, ASTZ BSTX, BSTY, BSTZ CSTX, CSTY, CSTZ	ASTX, ASTY, ASTZ BSTX, BSTY, BSTZ CSTX, CSTY, CSTZ	Coordinates of reciprocal lattice vectors $a_{star}$ , $b_{star}$ , $c_{star}$ in sample coordinates $x$ , $y$ , $z$
dd, x_center, y_center pitch, yaw	DDistance, XCent, YCent Pitch, Yaw	dd: distance from the beam focal point to the detector; x_center, y_center: pitch, yaw: coordinate of the projection of the beam focal point on the detector plane; spatial tilt of the detector; Same as seq
XR, XG, XB YR, YG, YB ZR, ZG, ZB	\	RGB color components of inverse pole figure map
ORSNR	\	Out-of-plane orientation (usually angle between the normal to the surface $z$ and the [001] direction)
reserved	\	Reserved for the future version

UASX, UASY, UASZ UBSX, UBSY, UBSZ UCSX, UCSY, UCSZ	\	coordinates of reciprocal lattice vectors $a^*$ , $b^*$ , $c^*$ in sample coordinates $x$ , $y$ , $z$ without strain refinement
QuatW, QuatX QuatY, QuatZ	\	Quaternion components
Rodr1, Rodr2, Rodr3	\	Rodrigues vector components
Rot_Angle, Rot_X, Rot_Y, Rot_Z	\	Rotation angle and the corresponding rotation axis in sample coordinates
Euler1, Euler2, Euler3	\	Bunge Euler angles $\phi_1$ , $\Phi$ , $\phi_2$ (in degree)
Bound	\	Bound = -1: intragranular spots Bound = 0: non-indexed spots Bound=1: spots located at an ordinary grain boundary
Max_Mis_Angle	\	Maximum of the Misorientation angle between four adjacent scan spots,

### 8.13 Details on PPC method



For a certain grain, the first diffraction pattern is indexed using the peak based indexation method or zone axes assisted indexation method, as shown in 'a'. Around the indexed diffraction peaks, an elliptical range with an angle of AR can be obtained (indicated by dashed lines). If the number of diffraction peaks that fall within the elliptical range in the adjacent diffraction pattern 'b' is greater than  $N_c$ , the indexation results of pattern 'a' can be copied to those peaks in 'b' that fall within the elliptical range, thereby completing the calibration of pattern 'b'. If the number of diffraction peaks within the elliptical range is less than  $N_c$ , then this pattern needs to be re-indexed using the peak based or zone axes assisted indexation method, as shown in 'c'.

With the Intensity Check feature turned on, if the number of peaks within the elliptical range is greater than  $N_c$ , but the number of peaks whose intensity ranks in the top  $N_r$  of all the diffraction peaks in that pattern is less than  $(N_c - N_s)$ , then the pattern still needs to be indexed.

If two phases are activated and both belong to the same space group, the first diffraction pattern of the grain will be indexed using both crystal structures simultaneously. When indexing with one phase, if the number of indexed peaks is greater than 'Critical' and the number of missing reflections is less than 'Missing', the indexation is considered successful; otherwise, it is unsuccessful. When successful indexation is achieved with one phase's crystal structure, it is assumed that the diffraction pattern belongs to that phase. If neither succeeds, the pattern is considered unindexable. If both are successful, the diffraction pattern is considered to belong to the first phase.

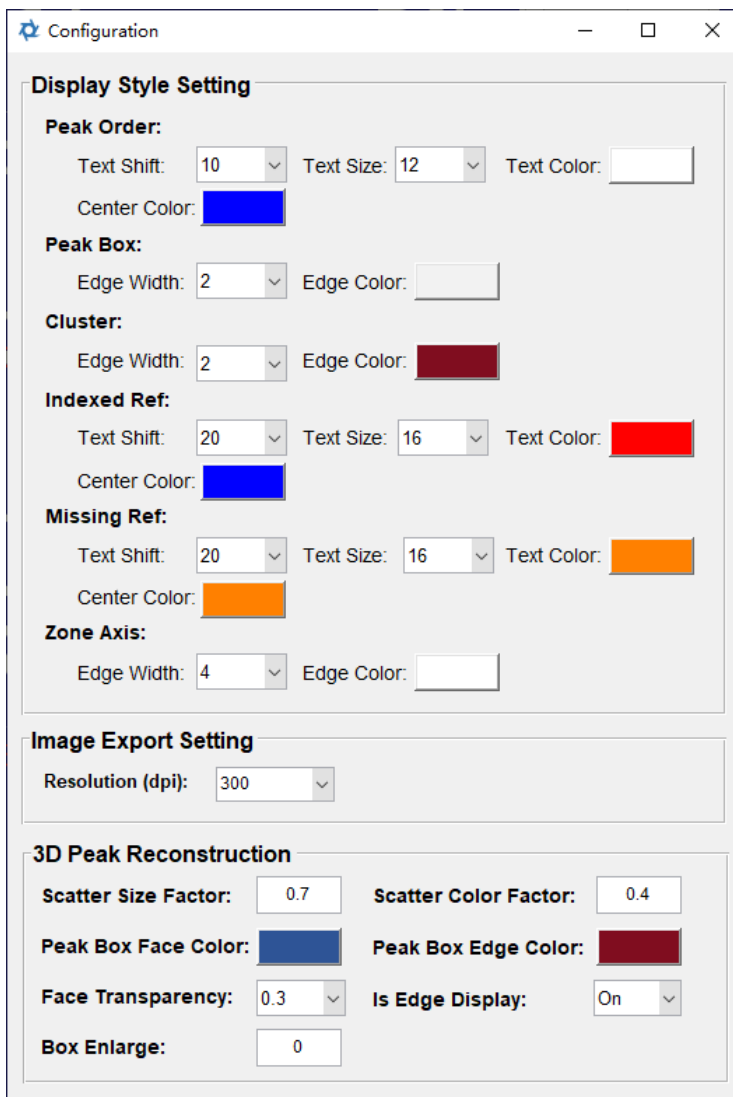
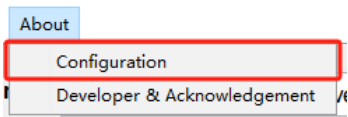
# **Configuration, Developers & Acknowledgement**



## 9 Configuration, Developers & Acknowledgement

### 9.1 Display Configuration

This feature is used to adjust the display style of diffraction peaks on the main interface, sub-peak clustering, indexed diffraction peaks, and missing reflections (Missing Reflections), the resolution of exported images, and the display method of 3D peak shape and position in the 3D peak selection interface after reciprocal reconstruction. The specific methods are as follows:



In the Display Style Setting panel:

- Peak Order:
  - Text Shift: The offset position of the intensity sequence number of the found diffraction peak from the center of the diffraction peak, measured in pixels (Pixel);
  - Text Size: Font size of the diffraction peak intensity sequence number;
  - Text Color: Font color for the diffraction peak intensity;
  - Center Color: Color of the square marker indicating the center of the diffraction peak.
- Peak Box:
  - Edge Width: The frame width of the box representing the range of the diffraction peak;
  - Edge Color: The frame color of the box representing the range of the diffraction peak.
- Cluster:
  - Edge Width: The frame width of the box representing the range of sub-peaks split from the same diffraction peak (i.e., subpeak clustering);
  - Edge Color: The frame color of the box representing the range of sub-peaks split from the same diffraction peak.
- Indexed Ref:
  - Text Shift: The offset distance between the Miller index of the indexed diffraction peak and the peak center, measured in pixels (Pixel);
  - Text Size: Font size for the Miller index;
  - Text Color: Font color for the Miller index;
  - Center Color: Color of the star marker indicating the center of the indexed diffraction peak.
- Missing Refl:
  - Text Shift: The offset distance between the Miller index of the missing reflections and the peak center, measured in pixels (Pixel);
  - Text Size: Font size for the Miller index;
  - Text Color: Font color for the Miller index;
  - Center Color: Color of the square marker indicating the center of the missing reflections.
- Zone Axis:
  - Edge Width: Width of the dashed line connecting diffraction peaks with the same zone axis;
  - Edge Color: Color of the dashed line connecting diffraction peaks with the same zone axis.

In the Image Export Setting panel:

- Resolution (dpi): Resolution of the exported image, measured in dpi.

In the 3D Peak Reconstruction panel:

- Scatter Size Factor: Controls the relative size of the scatter points used to display the 3D diffraction peak profile. The larger the value, the greater the size difference of the scatter points; Scatter Color Factor: Controls the relative color of the scatter points used to display the 3D diffraction peak profile. The larger the value, the greater the color difference of the scatter points;
- Peak Box Face Color: Color of the hexahedron surface indicating the 3D peak range;

- Peak Box Edge Color: Color of the edge of the hexahedron indicating the 3D peak range;
- Face Transparency: Transparency of the hexahedron surface indicating the 3D peak range;
- Is Edge Display: Choose whether to display the edge of the hexahedron indicating the 3D peak range;
- Box Enlarge: To clearly show the peak position, the size of the hexahedron can be slightly larger than the actual range of the peak obtained from the 3D peak-finding, and this value is the difference between the hexahedron and the actual range.

## 9.2 Developers & Acknowledgement

Developers:

Kou Jiawei, Chen Kai

Center for Advancing Materials Performance from the Nanoscale (CAMP-Nano), State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University.

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Citation Instructions:

If you use the PPC calibration method in your published work, please cite the reference: *Jiawei Kou, Kai Chen\*, Nobumichi Tamura, A peak position comparison method for high-speed quantitative Laue microdiffraction data processing, Scripta Materialia, 143, 49-53,*