LANDYNE 蓝带软件

User Manual

Quantification and Processing of SAED Patterns

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Contents

1. Introduction 3
1.1 Version history *3*
1.2 Design features *3*
1.3 Purposes *3*
2. Image processing of SAED patterns 4
2.1 Digital viewer *4*
2.2 Image adjustment *5*
2.3 Preparation of SAED patterns for publication *5*
3. Analysis and quantification of SAED pattern 5
3.1 Calibration using the scaling bar *5*
3.2 A 1D line profile *5*
3.3 Measurement of the basis vectors and intensity *6*
3.4 Preparation of (hkl) intensity list *6*
4. Tools 6
4.1 Angle calculator for a TEM holder *6*
4.2 Merging multiple SAED patterns with the same zone axis *7*
5. Usage of QSAED 7
5.1 Step by step *7*
5.2 Save the data of the retrieved intensities *10*
5.3 Save the SAED pattern with the retrieved intensities *10*
6.1 Installation *16*
6.2 QSAED in the Landyne suite *16*
6.3 License *16*

1. Introduction

Selected area electron diffraction analysis has been extensively used in materials science for phase identification, interpretation of twins, and coexisted multiple phases, *et cetera*. Electron diffraction patterns from a single crystal grain and a polycrystalline sample are common in essence but different in many aspects, so we treat the two cases separately to quantify and process electron diffraction patterns. QPCED has been developed for selected-area electron diffraction patterns of polycrystalline samples (Li, 2011, 2012). QSAED has been developed for selected-area electron diffraction patterns of single-crystal samples (Li, 2006, 2014).

1.1 Version history

The first version of QSAED was developed during 2003~2006, which was included in the JECP package (Li, 2006). Improvements were made in the following version during 2014~2015, which was reported in Microscopy & Microanalysis meeting in Hartford, CT (August 3-7, 2014) (Li, 2014). The current QSAED is version 5x. The original functions have been updated, e.g., the image processing operations and new functions have been added, especially, the experimental images may be processed to figures ready for publication.

1.2 Design features

QSAED has been written in Java SE8. Further code optimization (including obfuscation) is carried out for the compiled class files. Java Runtime Environment (JRE) and Java Advanced Imaging (JAI) are required to run QSAED. The installation of JRE and JAI is given in section 6.

The main interface of QSAED is shown in Figure 1. It includes:

1. a window frame with a drop-down/graphical menu and a panel.
2. the processing operation and parameters input are carried out in corresponding dialog windows.
3. an input SAED pattern can be quickly loaded using the drag-drop-box or the standard Windows file system.
4. Both of the processed data and images can be saved to files.

1.3 Purposes

An experimental SAED pattern is usually needed to go through resize | rotate | invert | square processing before it is used in the manuscript for publication. QSAED simplifies the process for getting the images of the SAED pattern. Tools are available for adding i) the scale bar in the processed image, ii) the indices, iii) the zone axis in various fonts to the figures ready for publication.

The reciprocal lattice spacing can be precisely measured in QSAED. The spacing is measured in pixels and can be converted to nm after the scaling bar is measured. The accuracy is better than 1 pixel.

The SAED pattern can be analyzed as a 1D intensity profile along a line defined by the user. The SAED pattern can be quantified and processed as 2D intensity distribution. The background intensity distribution is searched first, and then the intensities of all diffraction spots are retrieved.

The reflection intensities can be processed according to the assigned symmetry or replaced by the maximum one. The measured intensities can be displayed on the SAED pattern as circles with different radiuses. The measured intensities can be used in the structure-related analysis, ESPOT, and EMIPA in Landyne+ for electron crystallography analysis.

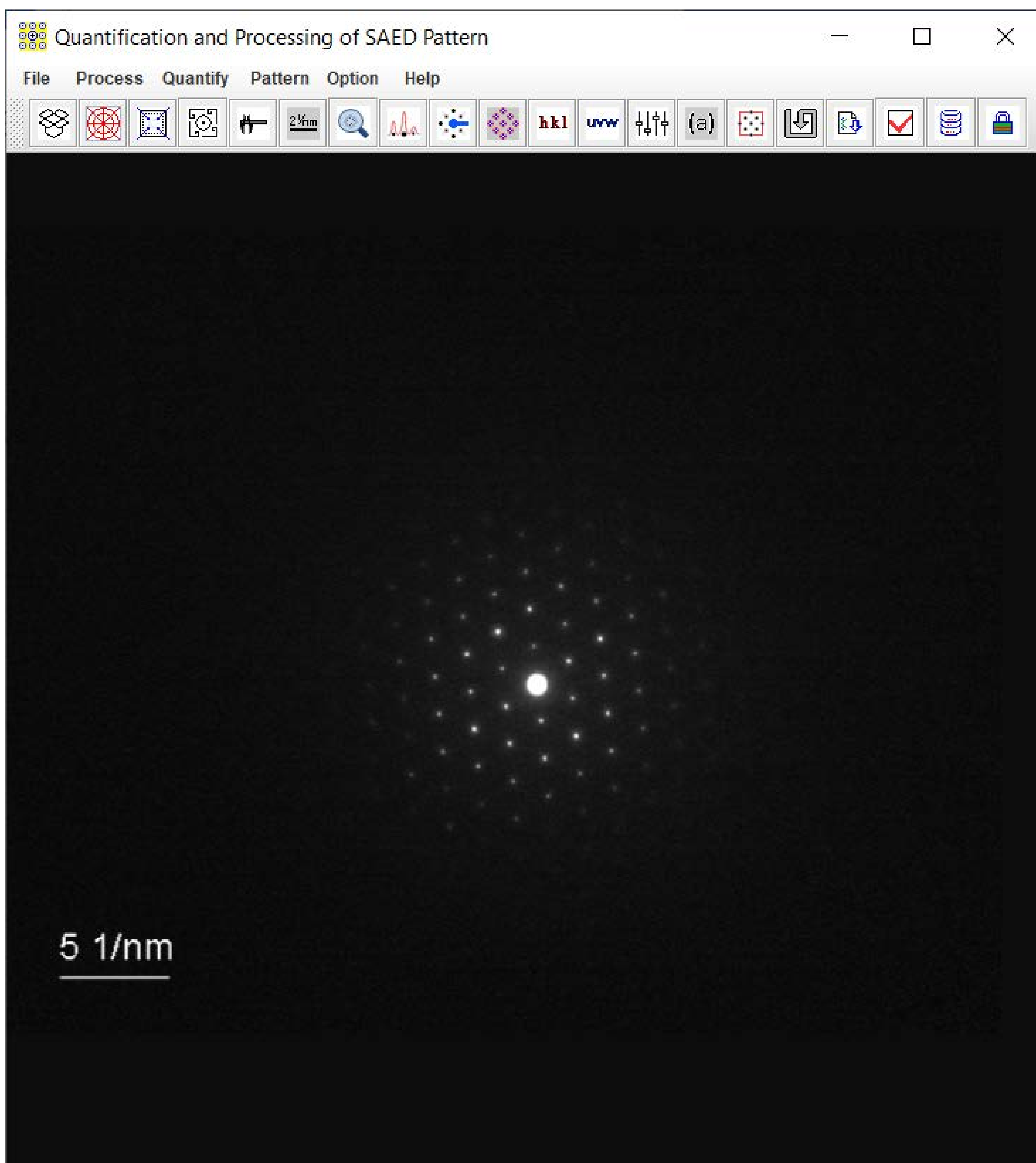


Figure 1. Main GUI of QSAED.

1. Image processing of SAED patterns

2.1 Digital viewer

The Digital Viewer in Figure 2 can be used to view the digital data in a popup window when a mouse pointer is moving in the loaded SAED image. It is a useful tool, e.g., to check if a peak is saturated in the center part; to select the location of a diffraction spot.

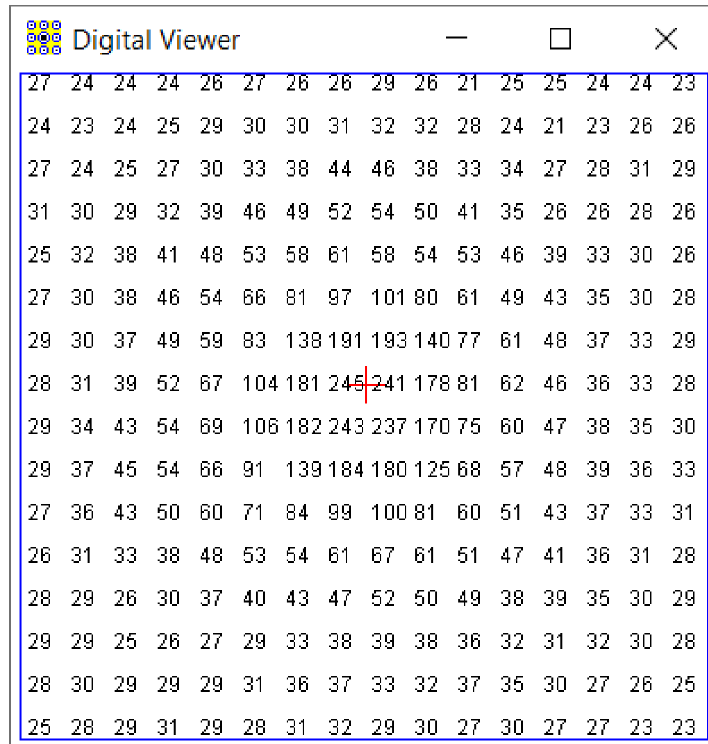


Figure 2. Digital viewer.

2.2 Image adjustment

The SAED pattern image will appear square after it is loaded in; even the original image is rectangular. The pattern can be adjusted by the following operations: histogram and contrast adjustment | resize | rotation | center | invert in gray contrast. The guidelines and circles can be displayed for rotation and alignment.

2.3 Preparation of SAED patterns for publication

The region of interest (ROI) size and pixel per inch (PPI) of the output image can be customized. The ROI can be further added to the scale bar, the indices, and the zone axis in various fonts. The image, the retrieved intensity, or their combination can be saved in the output file.

2. Analysis and quantification of SAED pattern

3.1 Calibration using the scaling bar

The scaling bar on the SAED pattern can be measured and saved for later use, e.g., the new scale bar in ROI and the basic reciprocal vectors are measure in pixel and then changed to 1/nm.

3.2 A 1D line profile

The line profile tool provides a quick and rough way to estimate the diffraction intensity profile by drawing the line on the SAED pattern. The 1D line profile is especially useful for SAED patterns from aperiodic structure or the second phase.

3.3 Measurement of the basis vectors and intensity

After the refinement of the basis vectors against many selected diffraction spots, the basis vectors' lengths and the angle between them can be precisely measured down to 0.1 pixels. With the data of the scaling bar measured before, the basis vectors can be accurately determined.

The background intensity can be determined and checked as a profile of intensity vs. the radius. After removing the background intensity for each pixel, the diffraction spot's intensity can be measured by using direct integration/sum or using the Gaussian bell function. The second method is useful for the diffraction spot with saturated pixels.

QSAED provides two methods to improve the SAED pattern. In case that a beam stopper was used in a SAED pattern, the diffraction spot (h, k, l) under the shadow of the beam stopper can be replaced by the opposite spot (-h, -k, -l), so a complete pattern can be displayed.

In case the SAED pattern was taken slightly away from the accurate zone axis, the averaged intensities can be used according to the pattern symmetry, so a SAED pattern similar to the accurate zone axis can be restored.

3.4 Preparation of (hkl) intensity list

Initially, the SAED pattern is analyzed by using two basis vectors, which should be indexed with (H, K). When the zone axis of the SAED pattern under study is known, the two basis vectors can be labeled as the Bravais indices; thus, the transformation from (H, K) to (h, k, l) can be done.

4. Tools

4.1 Angle calculator for a TEM holder

Angle calculator in Figure 3 is a tool for user to calculate the tilt angles in SAED experiment conveniently. It can be applied to the double tilt holder and the rotation holder. The tilt angle is calculated and automatically stored in a list. The list can be saved in a txt file.

The formulas were recorded in the literature.
For double tilt holder (Li, 2024),

$$\cos(\varphi,\theta) = \cos(\varphi_j - \varphi_i)\cos\theta_i\cos\theta_j + \sin\theta_i\sin\theta_j$$

and for rotation holder (Kelly *et al*. 1994),

$$\cos(\varphi,\omega) = \cos(\omega_j - \omega_i)\sin\varphi_i\sin\varphi_j + \cos\varphi_i\cos\varphi_j$$

Here, the angle φ is the main tilt angle of the holder (double tilt holder or rotation holder), angle ϑ is the second tilt angle of the double tilt holder, angle ϖ is the rotation angle of rotation holder.

The usage is the calculator is straightforward, single click the icon on QSAED toolbar to start the dialog. Input φ and ϑ (or ϖ), to get the answer. Once all data is calculated, the calculation history is stored and can be saved to a text file.

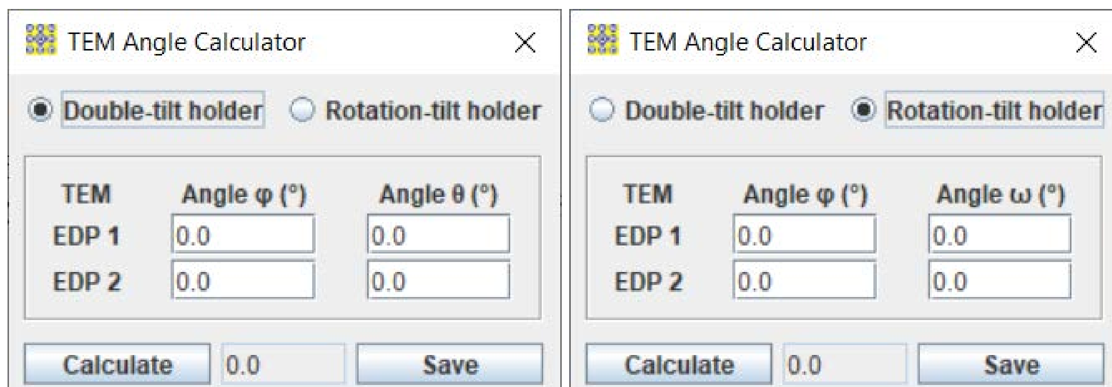


Figure 3. (a) angle calculators for double tilt holder and (b) for rotation holder.

4.2 Merging multiple SAED patterns with the same zone axis

When multiple SAED patterns at the same zone axis were recorded and processed to data files, the diffraction data can be merged into a file with either the averaged amplitudes or the stronger amplitudes for all reflections, as shown in Figure 4.

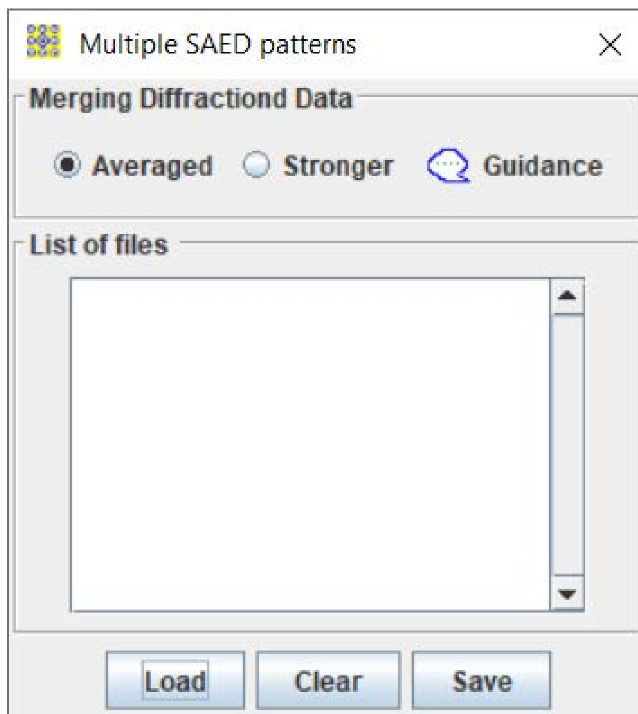


Figure 4. Merging tool for the data from multiple SAED patterns.

Be sure that the data files are for the same zone axis. Load to the list of files and select the averaged mode or the stronger mode, then save a file which is in the same format as the original files.

5. Usage of QSAED

5.1 Step by step

The usage of QSAED is easy and straightforward. A step-by-step guide is presented here. In demo mode, QSAED is fully functional, but only the demo_qsaed.tif in Figure 5 is allowed to be loaded.

1. Experimental SAED pattern in .tif or .jpg format can be loaded in two methods. Drag-and-drop method: the mouse points on the SAED pattern, hold the left mouse button and drag the image to the drag-drop box on the graphic menu bar, and release the mouse button. MS-Windows file system: click the drag-and-drop box, find and load the SAED pattern.
2. If diffraction intensities in the image are very weak, a histogram can be used to adjust the contrast of the diffraction pattern. Figure 6 shows the histogram interface.
3. Turn on the digital viewer.
4. In the Process drop-down menu, there is a resize and rotation panel. The SAED pattern can center by mouse right-click operations, as shown in Figures 7 and 8.

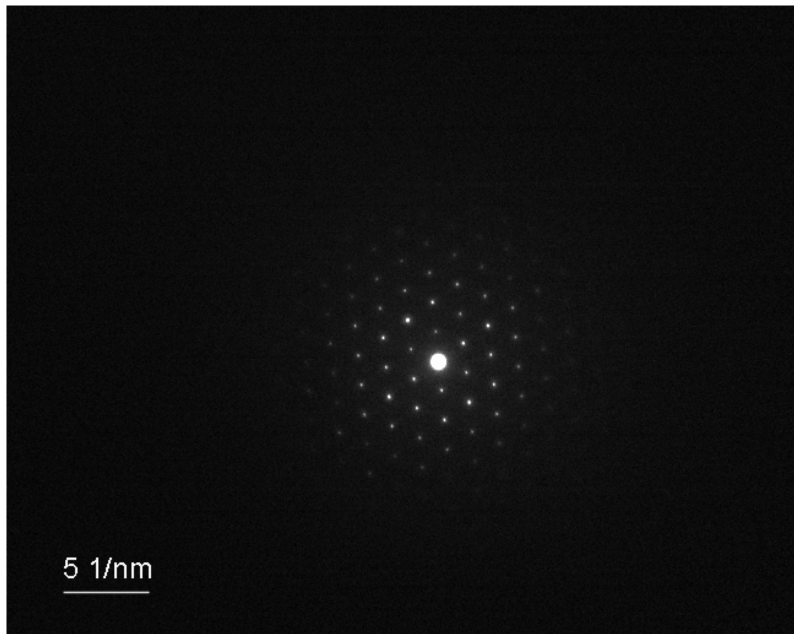


Figure 5. Image of the demo_qsaed.tif.

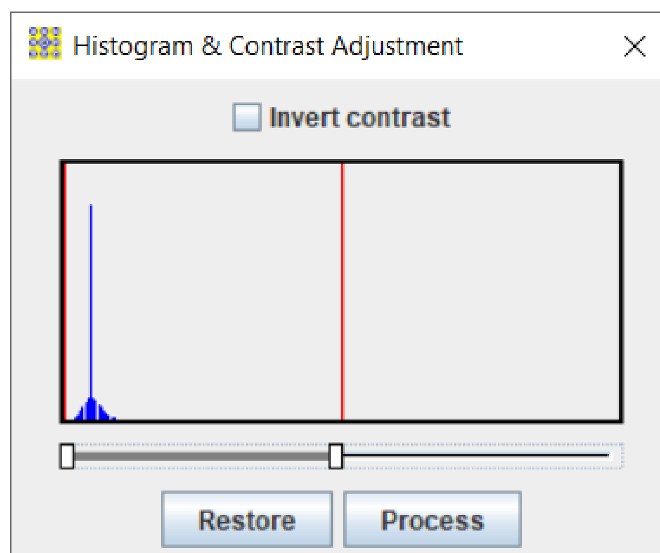


Figure 6. Histogram and image contrast adjustment.

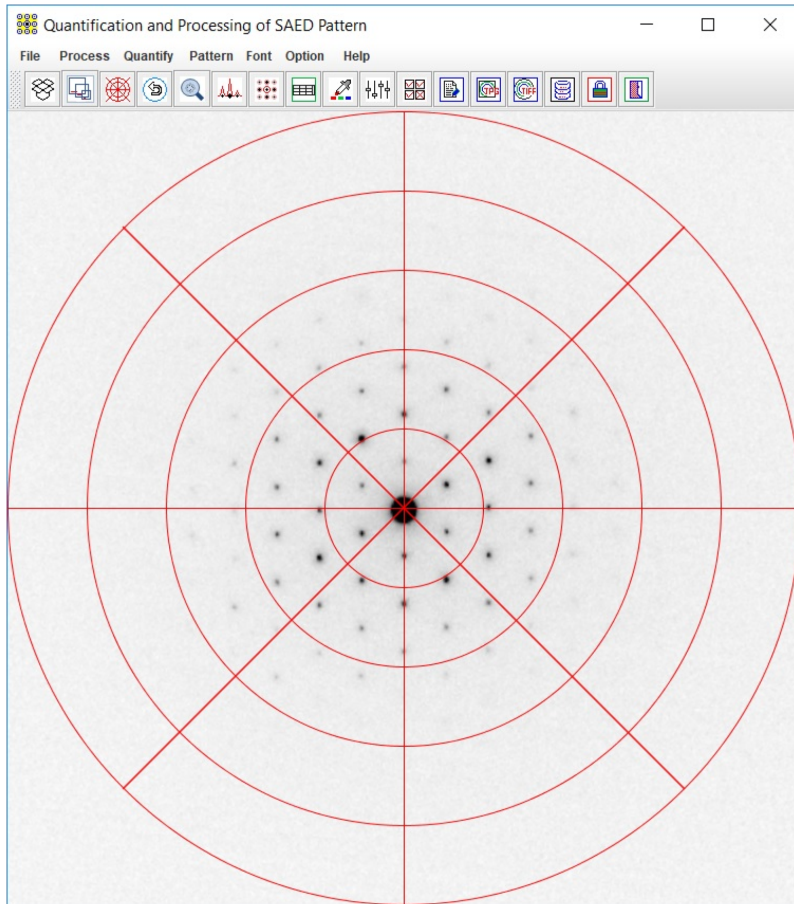
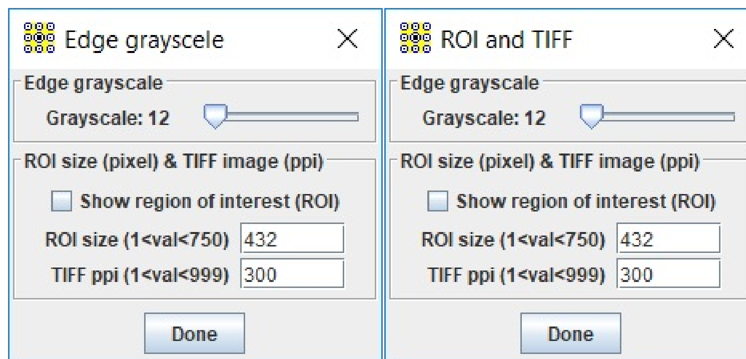


Figure 7. Resize, rotate, center, invert operations on the SAED pattern



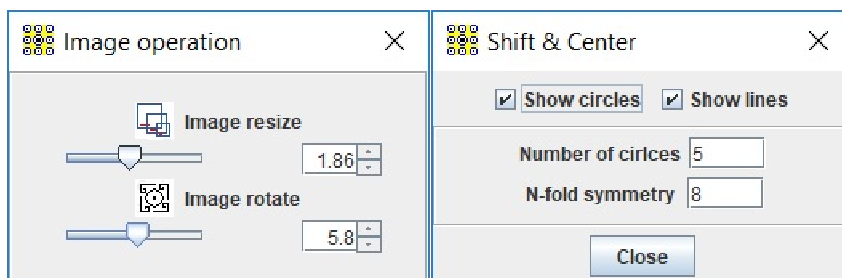


Figure 8. Edge grayscale dialog, resize and rotate dialog, and the shift & center dialog.

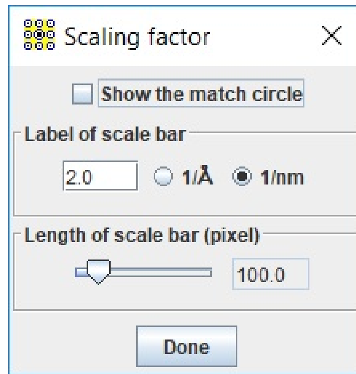


Figure 9. Scaling factor

5. Calibrate the scaling bar in Figure 9: turn on the shift & center dialog, hold the mouse left button to drag the image, and release. Measure the scaling bar and click the Done button.
6. Quantification of 2D lattice: the experimental image is better in the TIFF format. Define the beam blocker area if it is necessary. Click three spots on the SAED pattern to define the two basis vectors. With the help of the digital viewer, the positions can be roughly located. Refine a few times until the basis vectors are acceptable, as shown in Figure 10. Click the basis vector button to get the info of the two basis vectors, as shown in Figure 11.
7. A function of ROI is provided for output. The scale bar, indices, zone axis, and figure label can be added, as shown in Figure 12.
8. The preference panel provides a list of display options, as shown in Figure 13.
9. After the lattice was refined, the 2D pattern should be further quantified by defining the resolution-range and the background intensity, as shown in Figure 14. Select the intensity extracting option and get the intensities, as shown in Figure 15.
10. The retrieved intensities may be adjusted according to the SAED pattern's plane symmetry, as shown in Figures 16 and 17.
11. Analysis of the 1D profile: draw a line by defining the beginning point and the endpoint, as shown in Figure 18. Select the gridlines step. The profile is movable by holding the mouse left button, as shown in Figures 19 and 20.
12. To get the serial number (SN), click Help/current driver.

5.2 Save the data of the retrieved intensities

The retrieved intensities with indices can be saved in the MS-Windows file menu.

5.3 Save the SAED pattern with the retrieved intensities

The image of SAED pattern with/without the retrieved intensities can be saved in the MS-Windows file menu.

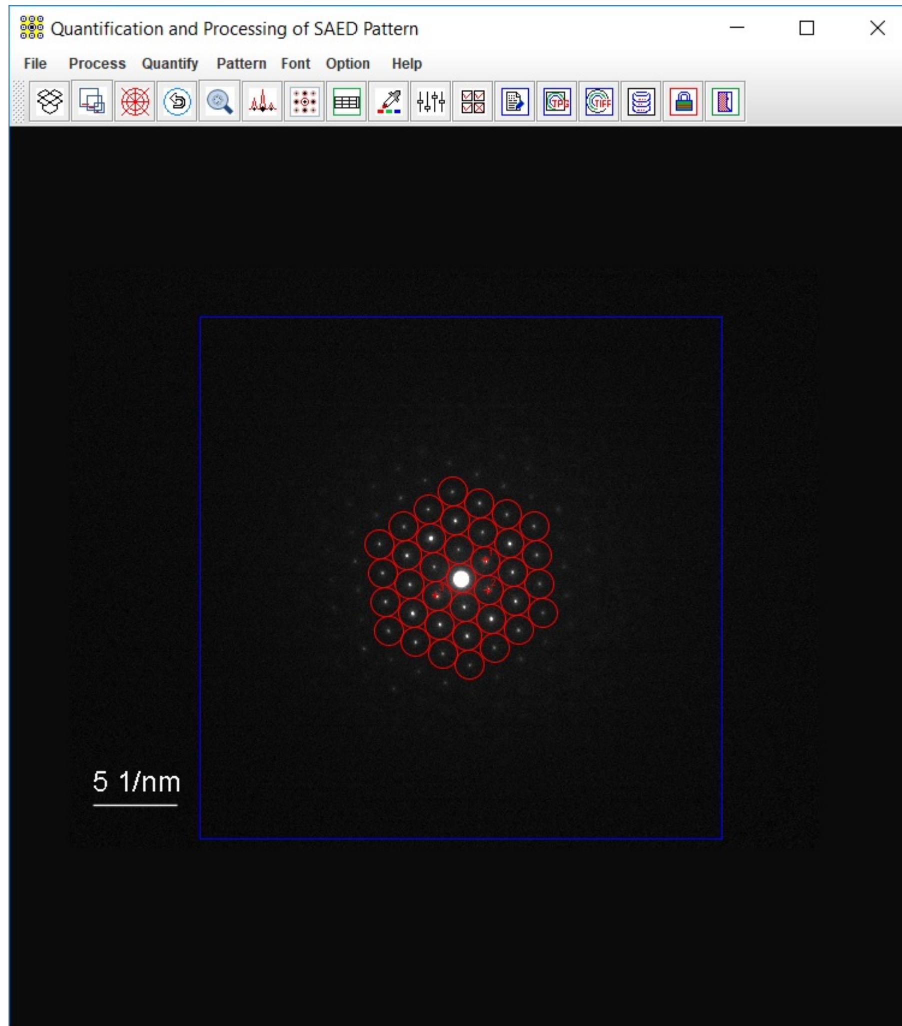


Figure 10. Lattice refinement

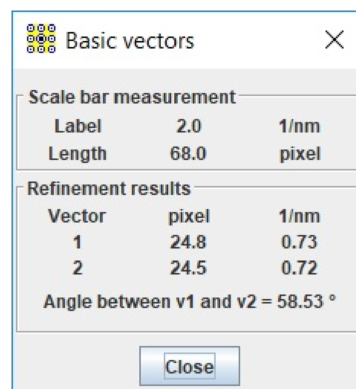


Figure 11. Basis vectors.

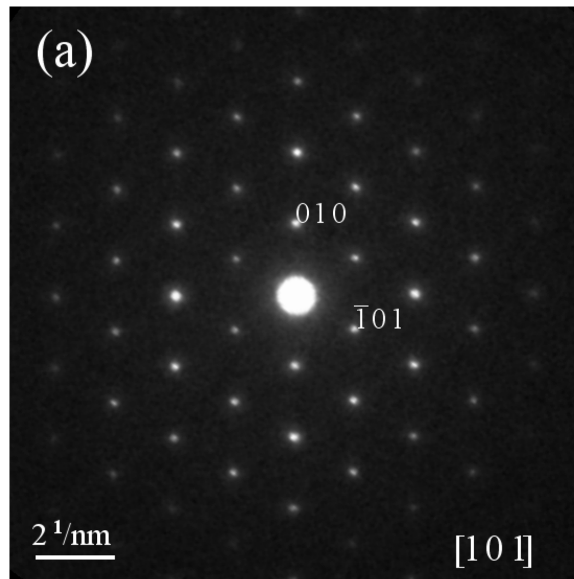


Figure 12. SAED pattern is prepared for publication.

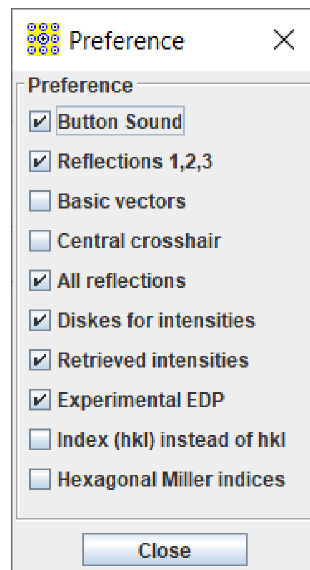


Figure 13. The preference dialogs.

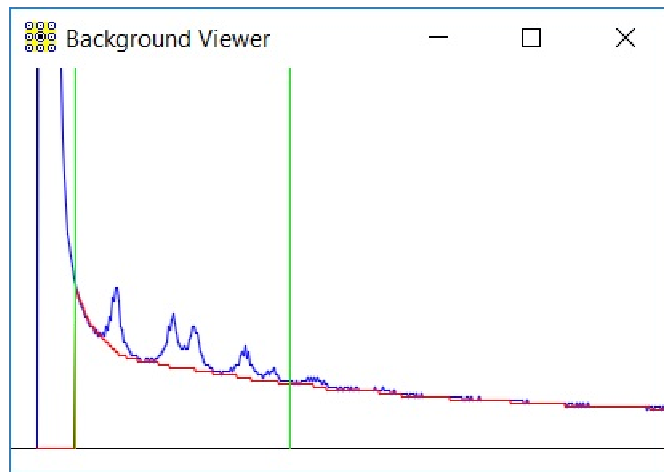


Figure 14. Background intensity

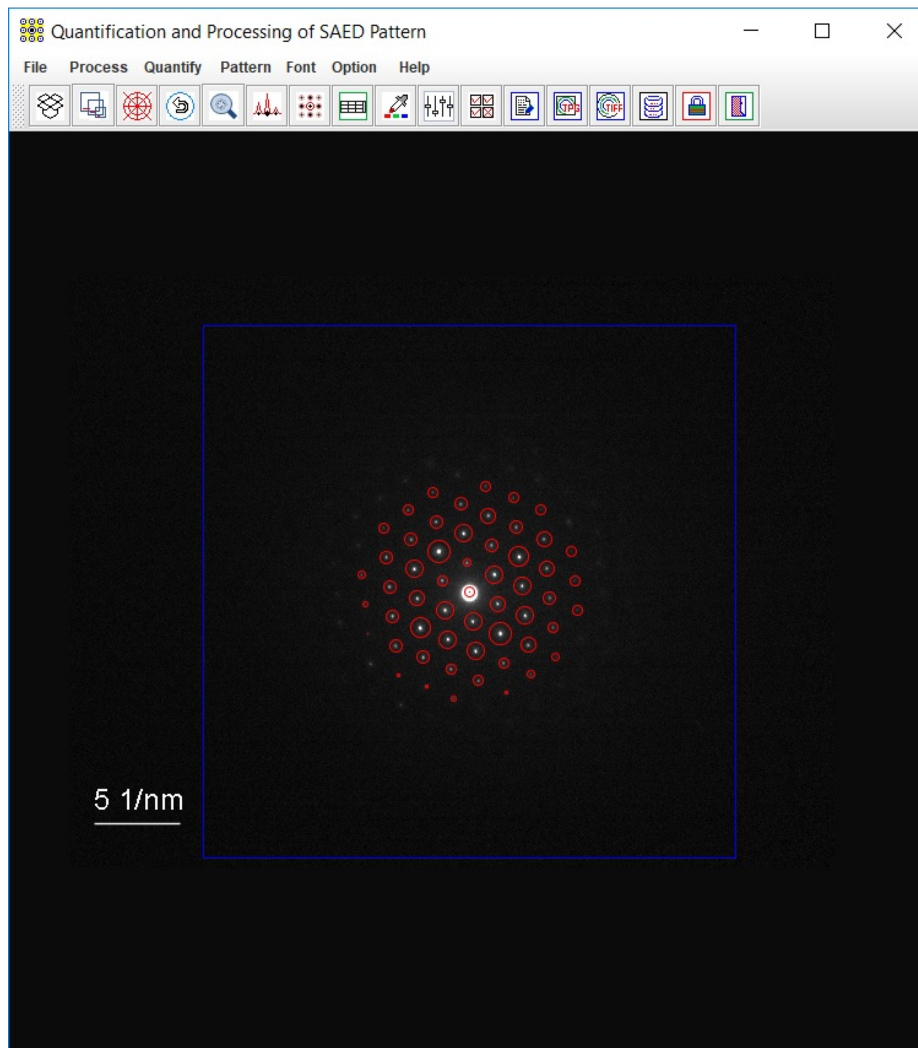


Figure 15. The SAED pattern with extracted intensities.

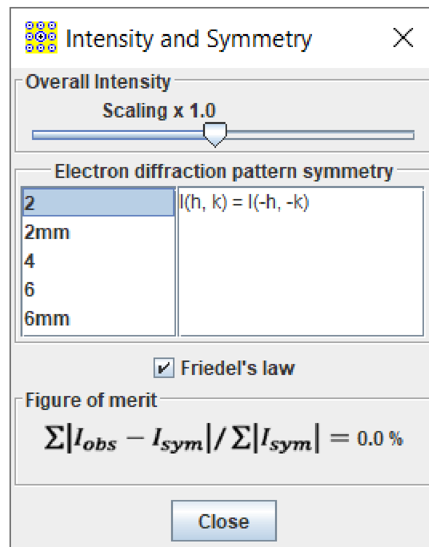


Figure 16. Adjustment of the retrieved intensities.

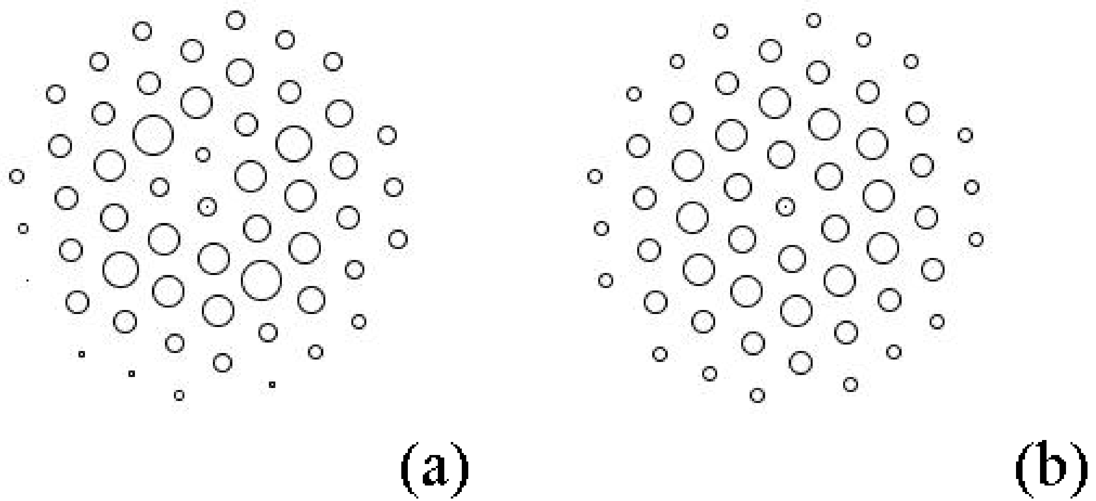


Figure 17. (a) Retrieved intensities and (b) adjusted intensities.

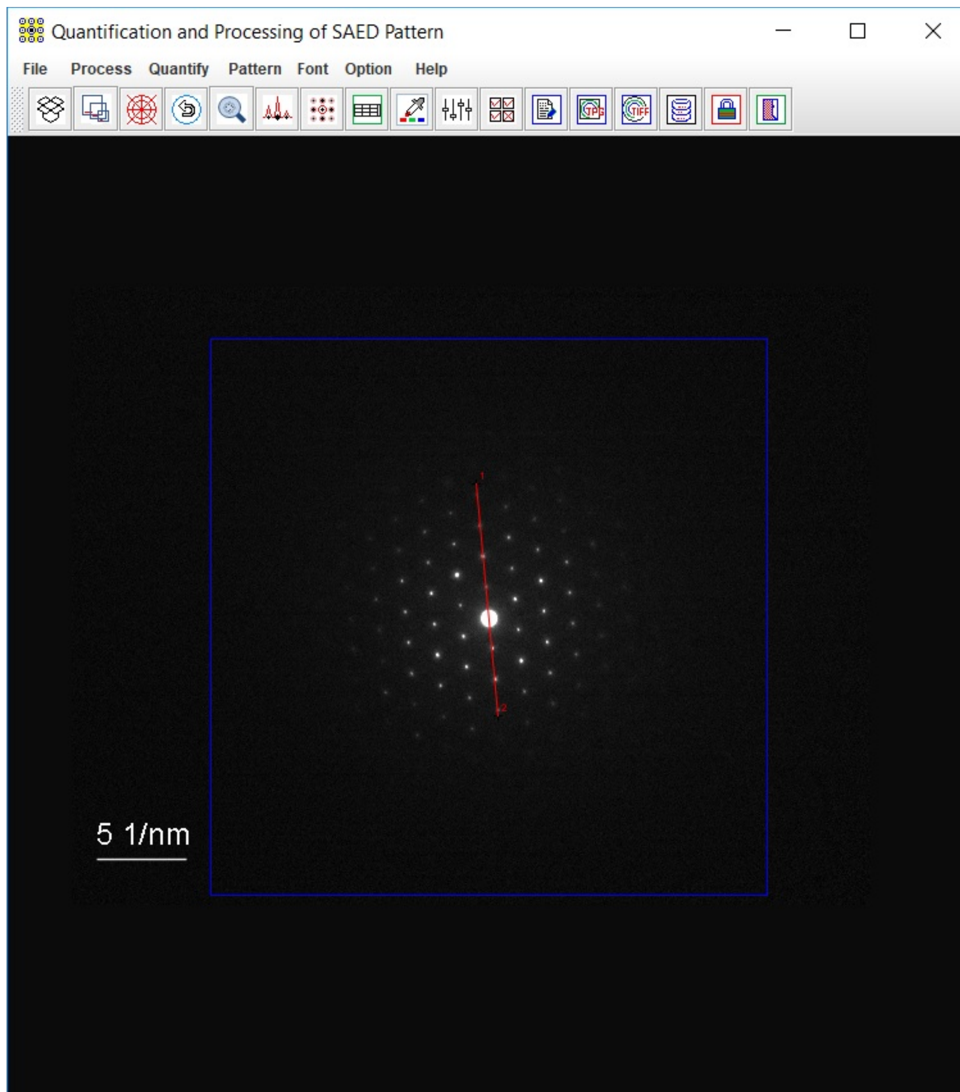


Figure 18. Selection of a line for intensity profile.

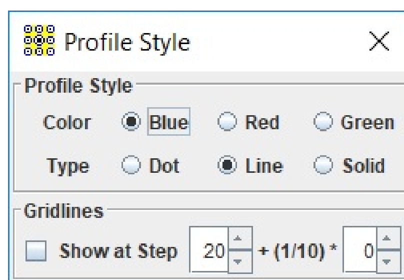


Figure 19. Profile style.

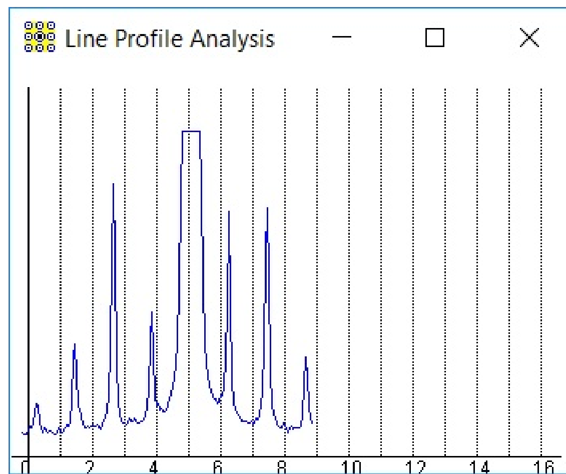


Figure 20. The intensity profile.

6. Installation of QSAED

6.1 Installation

Download and install the most recent JRE from the Java official site. Download and install the JAI, which is also available at https://www.unl.edu/ncmn-enif/xzli/download.

Download (https://landyne.com) and decompress the Landyne5 package. Copy the license to the programs\ subfolder.

6.2 QSAED in the Landyne suite

Click the QSAED in the Landyne launcher to start the software.

6.3 License

A license file is needed to unlock the program (QSAED.jar) for loading the SAED pattern. The program may run in demo mode, which works in full functions but limits to the demo-qsaed.tif. A license is available from LANDYNE computer software.

7. References

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