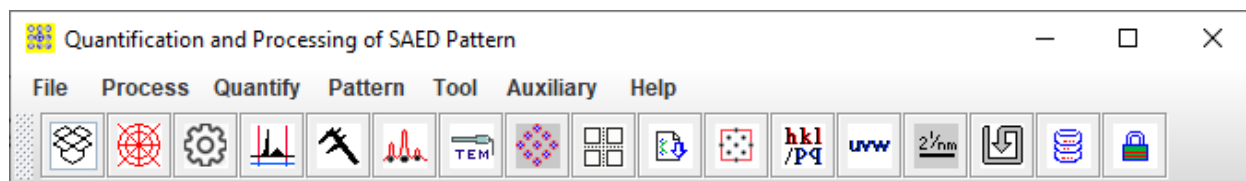


# **User Manual**

Quantification and Processing of SAED Patterns

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## 1. Introduction

Selected area electron diffraction (SAED) analysis is widely utilized in materials science for tasks such as phase identification, interpretation of twins, and analysis of coexisting phases. Electron diffraction patterns from single crystal grains and polycrystalline samples share a common essence but differ significantly in many aspects. Therefore, we approach these two cases separately to quantify and process electron diffraction patterns.

QPCED (Quantitative Polycrystalline Electron Diffraction) has been specifically developed for SAED patterns obtained from polycrystalline samples (Li, 2011, 2012, 2024). This method focuses on analyzing patterns where multiple crystal orientations contribute to the observed diffraction spots.

QSAED (Quantitative Single-Crystal Electron Diffraction), on the other hand, has been tailored for SAED patterns from single-crystal samples (Li, 2006, 2014). It is designed to analyze diffraction patterns originating from a single crystal grain, ensuring precise characterization of that crystal's properties.

These developments in SAED methodologies enable detailed and accurate analysis of electron diffraction patterns, enhancing our understanding and application in materials science and related fields.

### *1.1 Version history*

The initial version of QSAED was developed between 2003 and 2006 and was integrated into the JECF package (Li, 2006). Subsequent improvements were implemented in the following version between 2014 and 2015, which were presented at the Microscopy & Microanalysis meeting in Hartford, CT (August 3-7, 2014) (Li, 2014).

In version 5, significant updates were introduced, including enhancements to the original functions such as image processing operations and the addition of new features. Notably, the capability to process experimental images directly into publication-ready figures was incorporated.

The current iteration, QSAED version 6, includes further advancements such as histogram processing for both grayscale 8-bit and 16-bit images. Handling of the TIFF format is supported in the openJDK21 system, ensuring compatibility and robust functionality for image processing tasks within QSAED.

### *1.2 Design features*

QSAED was coded in Java and compiled using openJDK21. The main interface of QSAED, illustrated in Figure 1, comprises:

1. A window frame featuring a drop-down/graphical menu and a panel. Users can adjust the size of both the frame and the panel.
2. Processing operations and parameter inputs are managed through corresponding dialog windows.

3. SAED patterns can be swiftly loaded via drag-and-drop functionality or through the standard Windows file system.
4. Image processing capabilities include enhancing the display of 8-bit and 16-bit grayscale images.
5. Both processed data and images can be saved to files.

These features collectively enhance the usability and functionality of QSAED for analyzing and processing electron diffraction patterns efficiently.

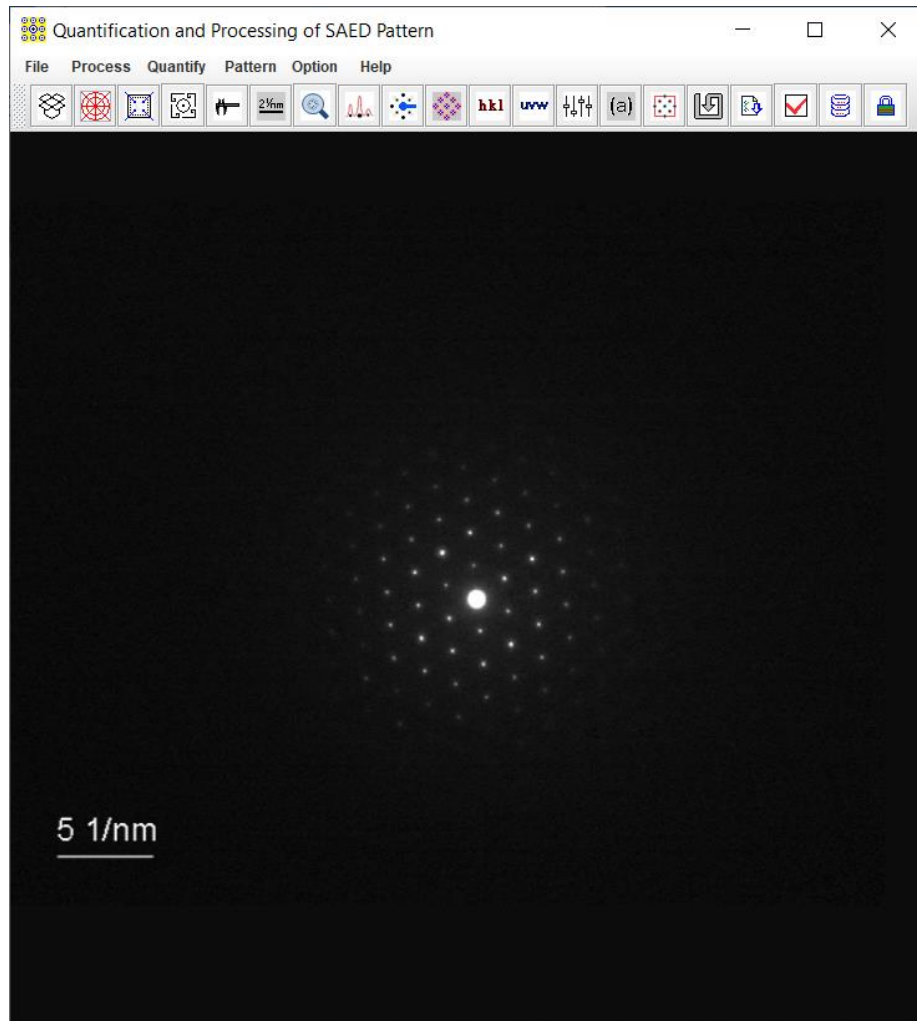


Figure 1. Main GUI of QSAED.

### 1.3 Purposes

In preparing an experimental SAED pattern for publication, several processing steps are typically required such as resize, rotate, invert, and square operations. QSAED simplifies this process significantly, providing tools to facilitate the creation of SAED pattern images suitable for publication. Key functionalities include:

1. **Processing Tools:** QSAED offers tools for resizing, rotating, inverting, and squaring SAED patterns, ensuring they meet publication standards.

2. Enhancement Tools: Tools are available to add essential elements to figures, including:
  - Scale bar to indicate size in the processed image.
  - Histogram and enhancement of 8 bits and 16 bits grayscale images.
  - Indices to denote specific features or orientations.
  - Zone axis labels in various fonts, enhancing clarity and understanding.
3. Reciprocal Lattice Spacing Measurement: QSAED allows precise measurement of reciprocal lattice spacing in pixels, with conversion to nanometers facilitated after measuring the scaling bar. The accuracy is better than 1 pixel.
4. Intensity Analysis: SAED patterns can be analyzed both as 1D intensity profiles along user-defined lines and as 2D intensity distributions:
  - Background intensity distribution is first identified.
  - Intensities of all diffraction spots are extracted and quantified.
5. Reflection Intensity Processing: Reflection intensities can be processed according to assigned symmetry or replaced by the maximum intensity. Measured intensities can also be visualized on the SAED pattern as circles with varying radii.
6. Integration with Analysis Tools: Measured intensities can be directly utilized in advanced analysis tools like ESPOT and EMIPA within Landyne+ for comprehensive electron crystallography analysis.

These capabilities make QSAED a powerful tool for preparing, analyzing, and enhancing SAED patterns, supporting detailed structural analysis and facilitating publication-quality figure preparation in electron crystallography studies.

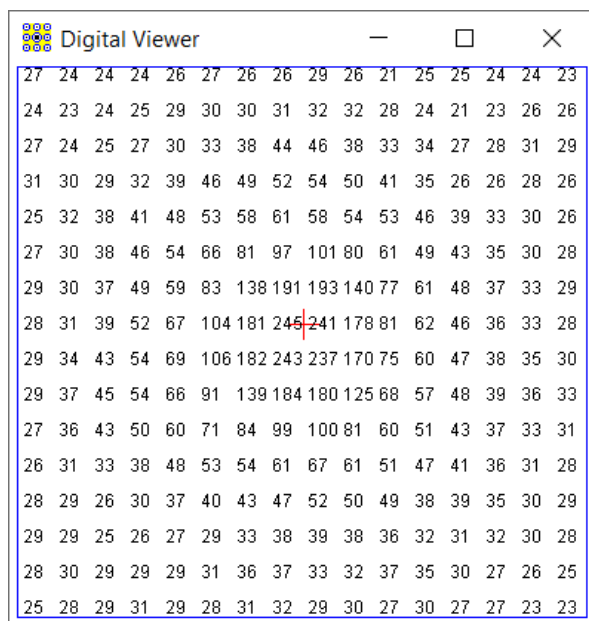


Figure 2. Digital viewer.

## 2. Image processing of SAED patterns

### 2.1 Digital viewer

The Digital Viewer in Figure 2 can be used to view 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.

### 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 using Image Tools in Figure 3: invert | overexposure | resize | rotation | edge paint | in gray contrast. The guidelines and circles can be displayed for rotation and alignment. A histogram is available for contrast adjustment. For very weak diffraction patterns, overexposure can be used to reveal the weak intensity of diffraction spots.

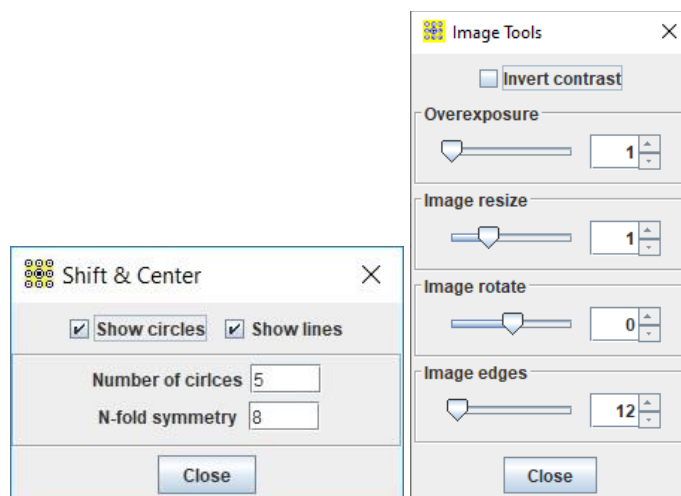


Figure 3. Tools for image adjustment, including alignment, invert, overexposure, resize, rotation and edge paint with a grayscale.

### 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.

## 3. 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 like 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 4 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  $\varphi$  is the main tilt angle of the holder (double tilt holder or rotation holder), angle  $\theta$  is the second tilt angle of the double tilt holder, angle  $\omega$  is the rotation angle of rotation holder.

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

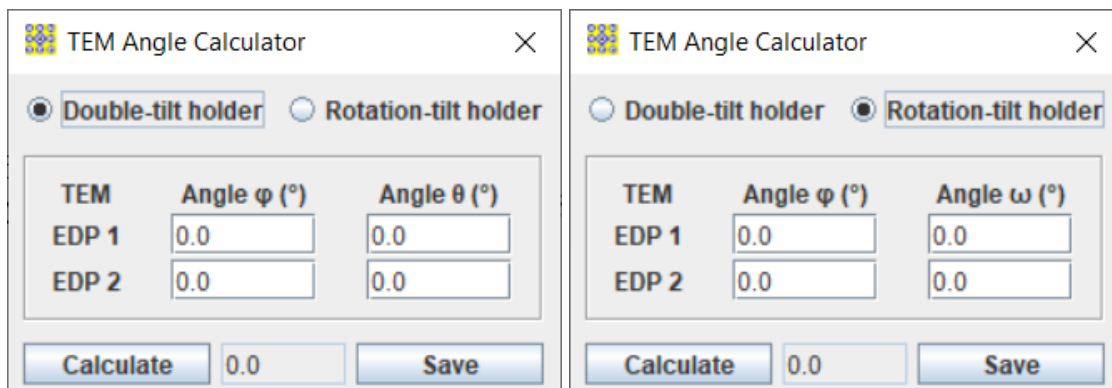


Figure 4. (a) angle calculators for double tilt holder and (b) for rotation holder.

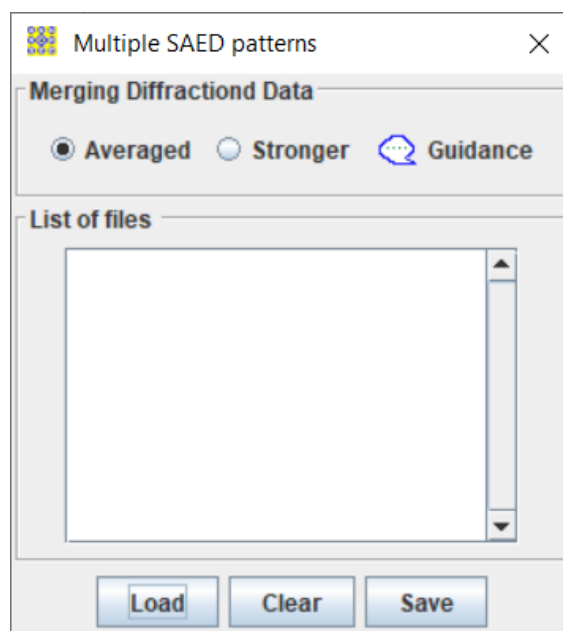


Figure 5. A merging tool for the data from multiple SAED patterns.

#### 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 5.

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 6 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 7 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 Figure 8.

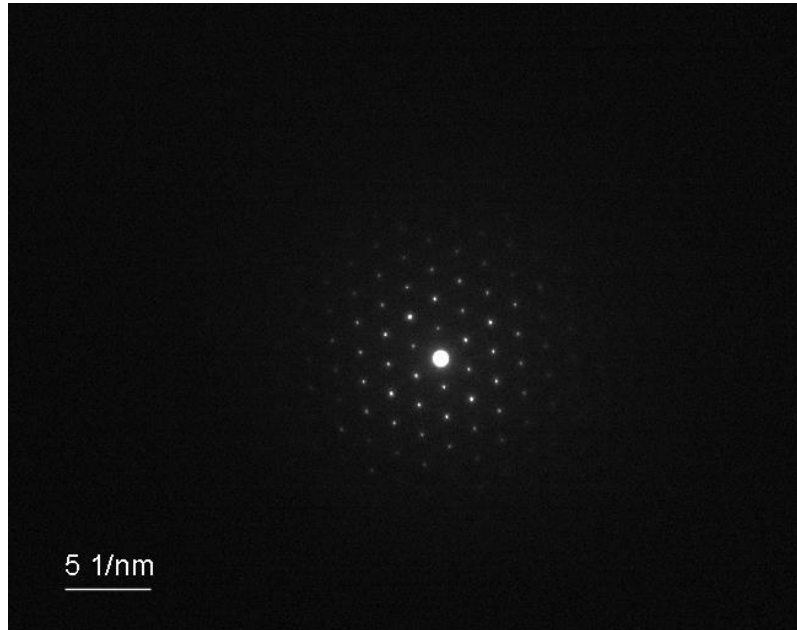


Figure 6. Image of the demo\_qsaed.tif.

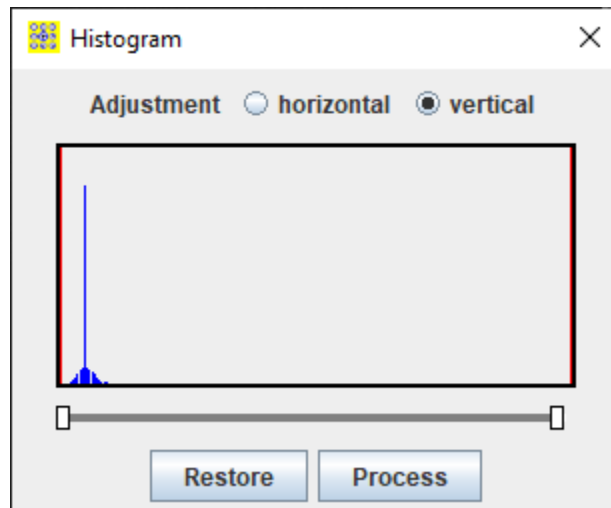


Figure 7. Histogram and image contrast adjustment.

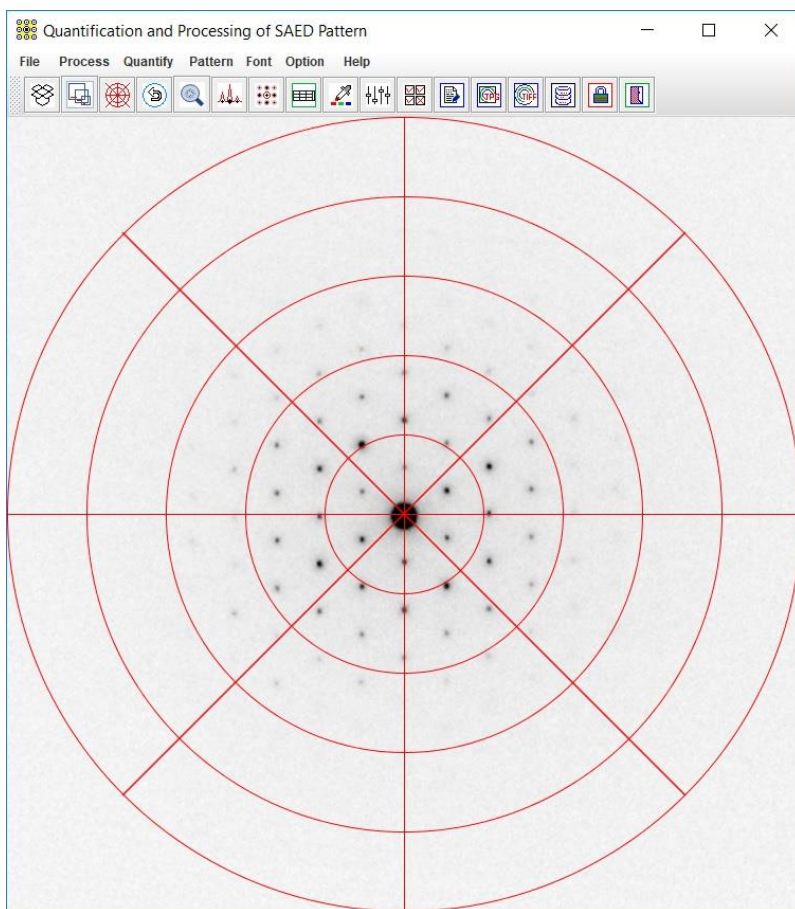


Figure 8. Guidelines for resize, rotation, center, invert operations on the SAED pattern

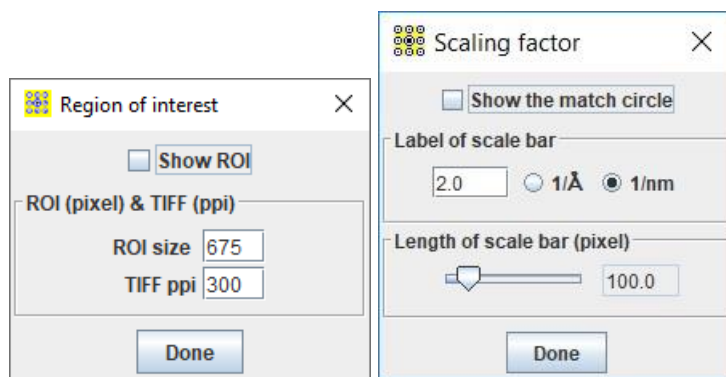


Figure 9. Region of interest and Scaling factor

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.

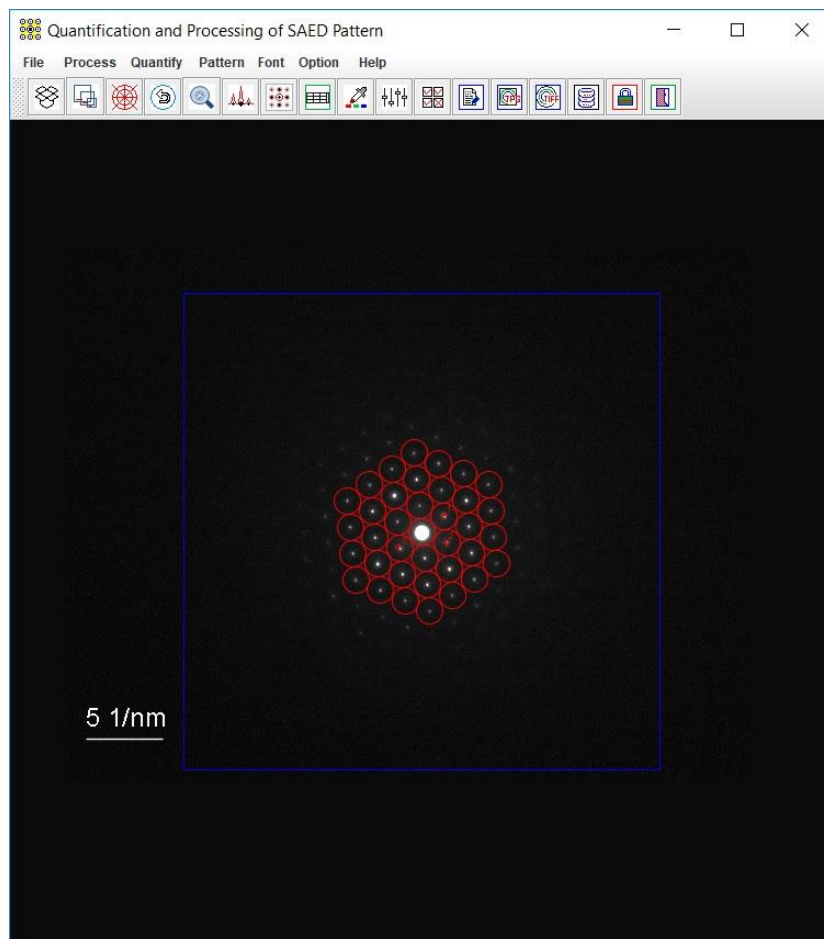


Figure 10. Lattice refinement

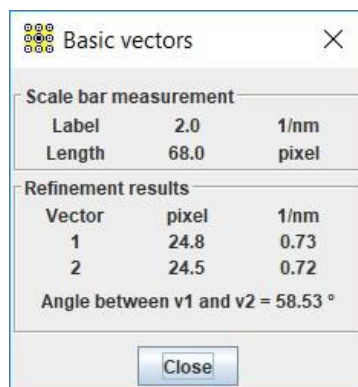


Figure 11. Basis vectors.

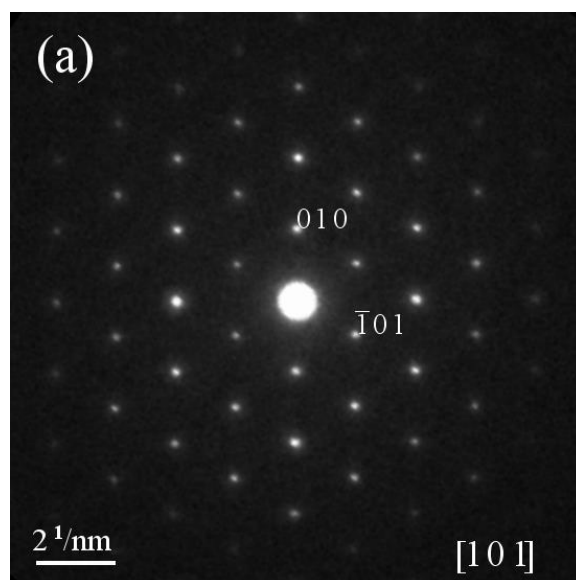


Figure 12. SAED pattern is prepared for publication.

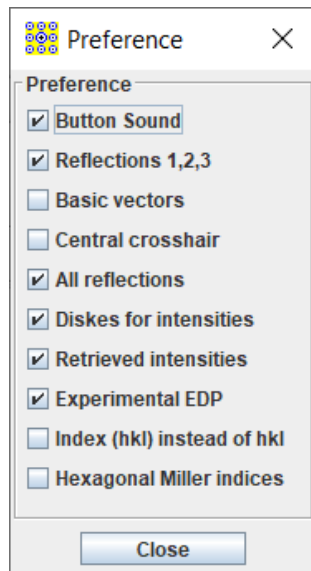


Figure 13. The preference dialogs.

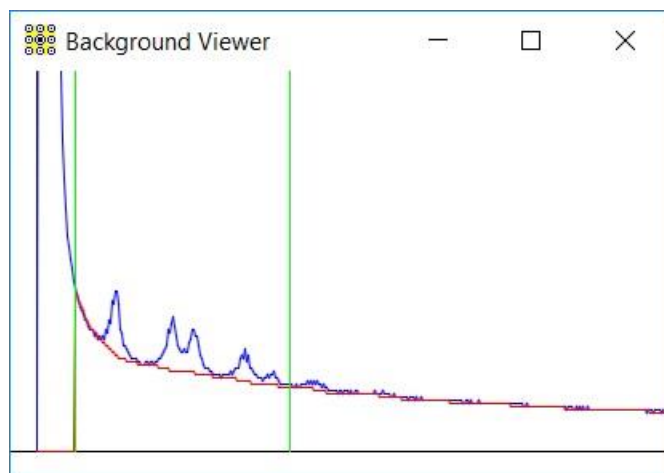


Figure 14. Background intensity

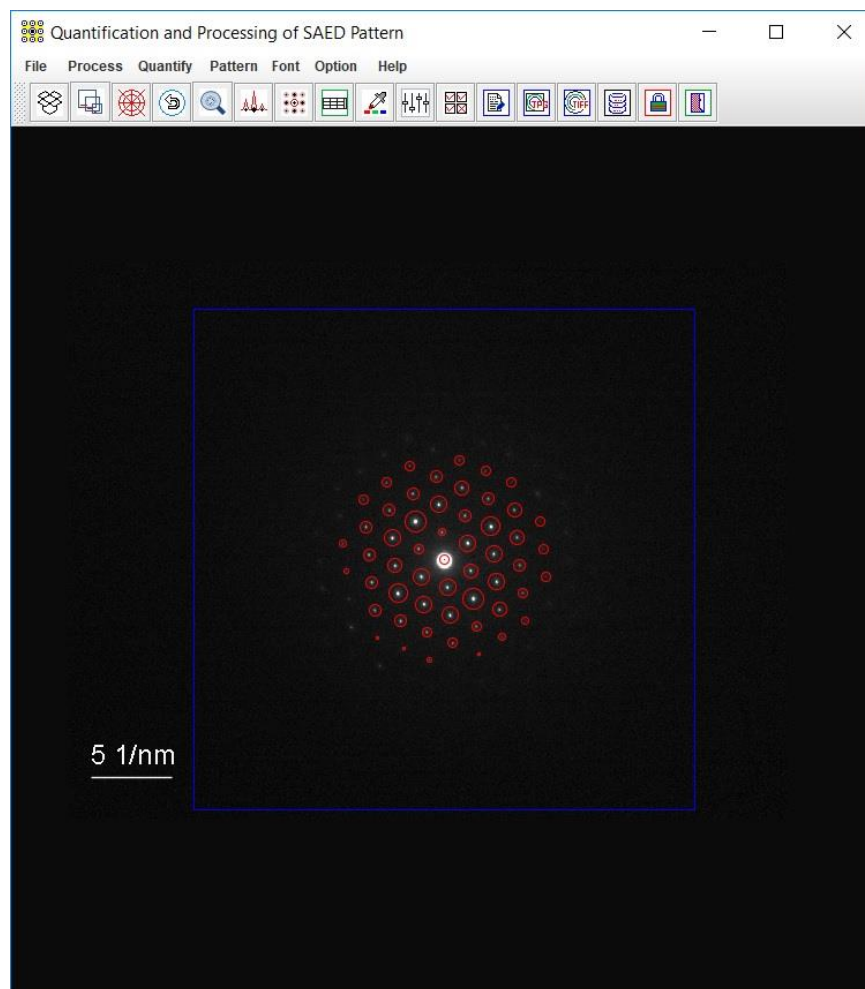


Figure 15. The SAED pattern with extracted intensities.

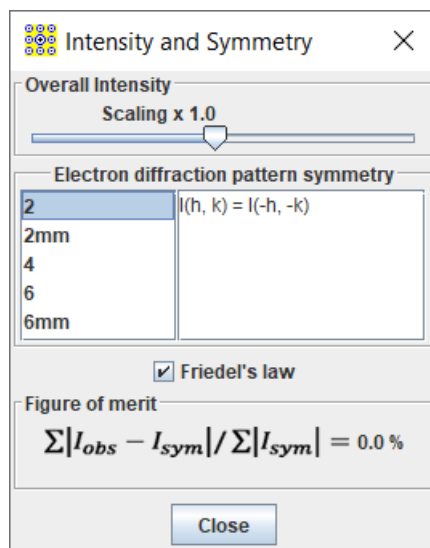


Figure 16. Adjustment of the retrieved intensities.

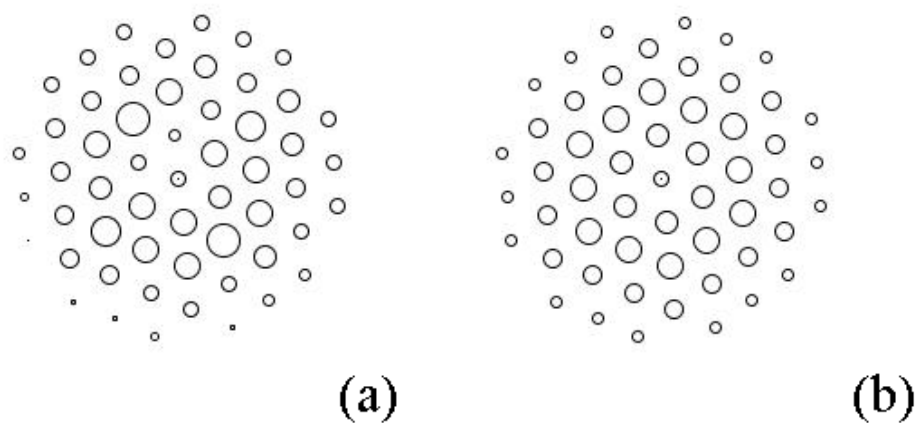


Figure 17. (a) Retrieved intensities and (b) adjusted intensities.

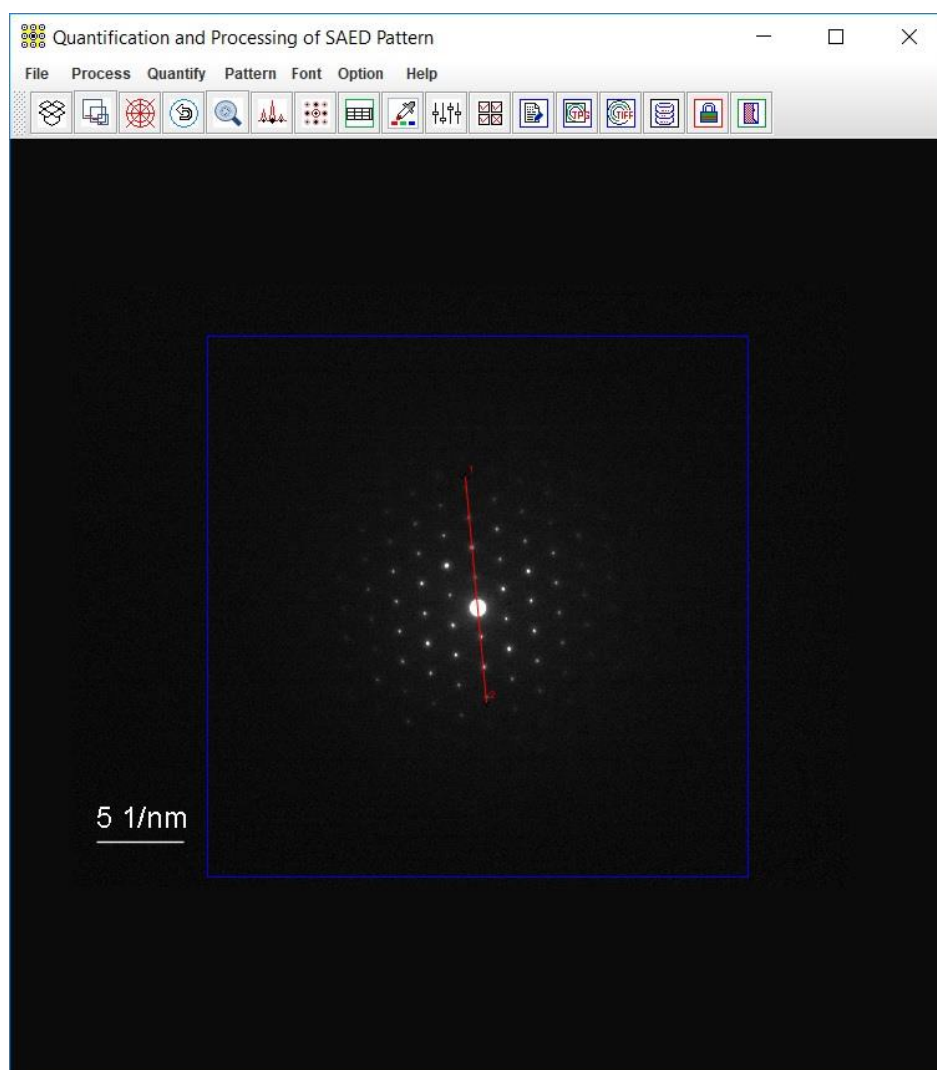


Figure 18. Selection of a line for intensity profile.



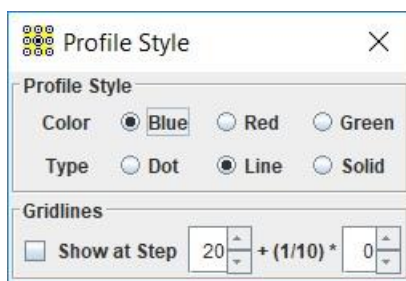


Figure 19. Profile style.

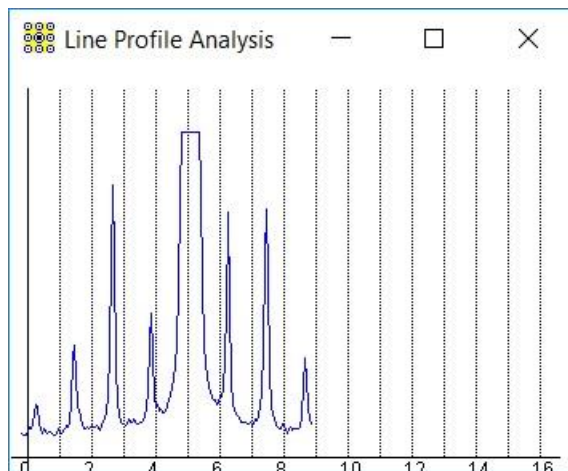


Figure 20. The intensity profile.

## 6. Installation of QSAED

### 6.1 Installation

Download and install the openJDK21 or higher version from the internet. Download (<https://landyne.com>) and decompress the Landyne6 package. Copy the license to the programs\ subfolder. Click the QSAED in the Landyne launcher to start the software.

### 6.2 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-qsad.tif. A license is available from LANDYNE computer software.

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