LANDYNE 蓝带软件

User Manual

Quantification and Processing of PolyCrystalline

Electron Diffraction Pattern

Quantification and Processing of PCED Pattern

File   Process   Pattern   Quantify   Profile   Auxiliary   Help

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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). 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 QPCED was developed between 2003 and 2006 and was integrated into the JECP package (Li, 2006). Subsequent improvements were implemented in the following version between 2010 and 2012, which was published in the Journal of Applied Crystallography (Li, 2012).

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 figures suitable for publication was incorporated.

The current version 6, includes further advancements such as updating the code for TIFF image processing and recompiling it under openJDK21. These updates ensure compatibility and improved functionality, enhancing the usability and performance of QPCED for electron diffraction pattern analysis and publication-ready figure preparation.

1.2 Design features

QPCED is written in Java (openJDK21) and has undergone further code optimization, including obfuscation, for the compiled class files. The size of the frame, including display panel, can be adjusted by users. The main interface of QPCED, shown in Figure 1, includes:

1. A frame with a drop-down/graphical menu and a panel.
2. Processing operations and parameter inputs managed through corresponding dialog windows.
3. Quick loading of input PCED patterns using the drag-and-drop functionality and the standard MS-Windows file system.

4. Image processing functions, including contrast inversion, resizing, rotation, and centering.
5. The ability to load previously saved polycrystalline diffraction profiles for further quantification.
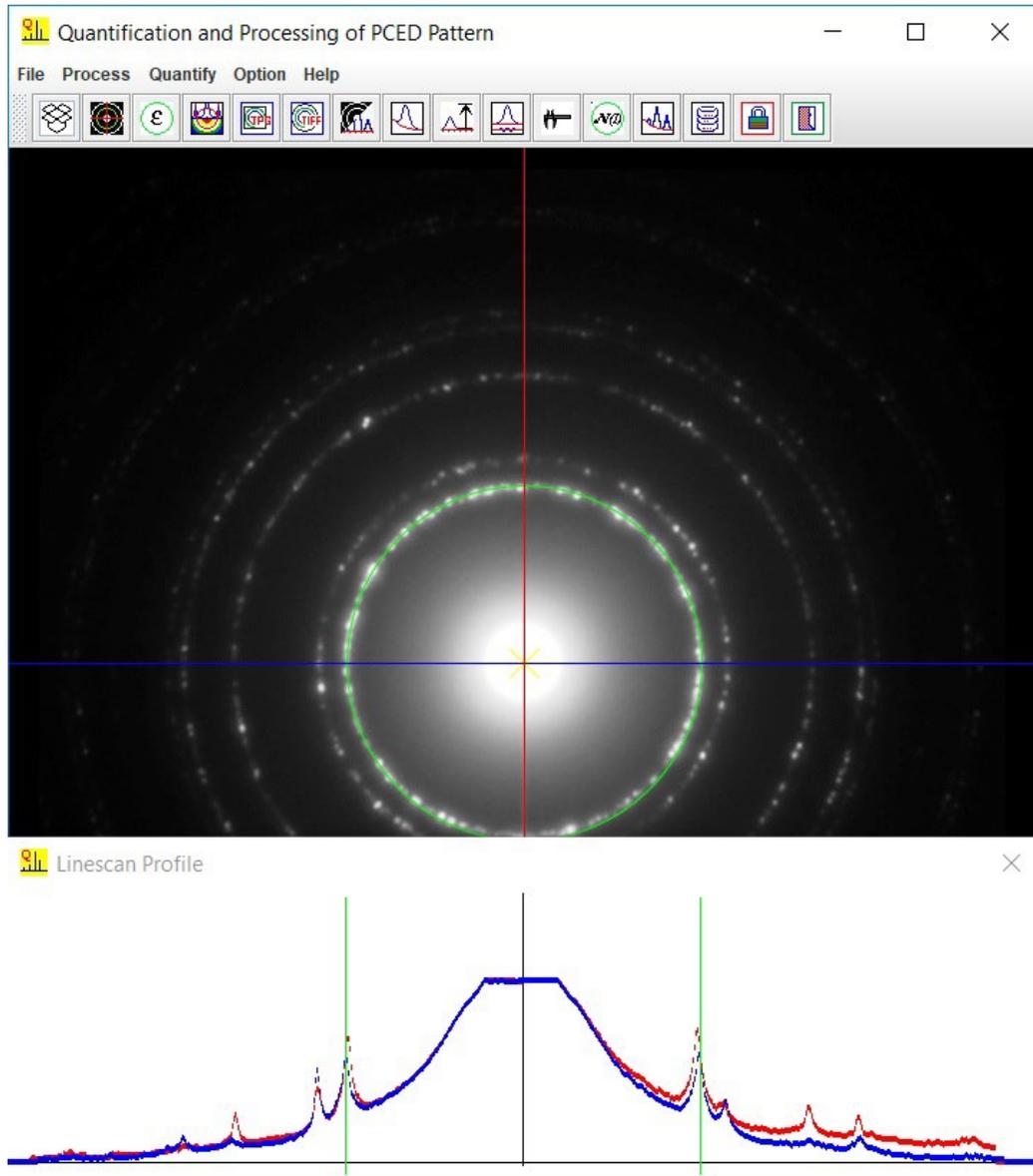6. The option to save both processed data and images to files.

Figure 1. Main GUI of QPCED.

1.3 Purposes

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

The display of a PCED pattern can be enhanced with pseudo-color, and the weak rings can be traced with the relatively intense spot in the ring.

The 2D PCED pattern can be converted into a 1D profile from the whole pattern or along a selected ring. The 1D profile from the whole pattern can be further analyzed by removing the background and automatically fitting into peak curves with parameters. Thus, the intensities and reciprocal lattice spacing can be precisely measured in QPCED. 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 measured intensities can be used in structure-related analysis, especially in electron crystallography.

2. Image processing of PCED pattern

2.1 Image alignment of the PCED pattern

After loading the PCED pattern, the incident beam should be moved to the center by clicking the mouse right button. Adjustment of the PCED pattern on resizing and rotation. The key arrows may provide fine adjustment of the center (Make sure the panel was clicked by mouse pointer and keep the mouse pointer within the panel). The vertical and horizontal line profiles may be used as a reference for the adjustment. The Adjustment dialogue is shown in Figure 2.

2.2 The measurement and correction of elliptical rings on the PCED pattern

The possible residual stigmatic optical error in the diffraction experiment may cause elliptical rings instead of perfect circular rings in the PCED pattern. The detection of the ellipticity and correction can be done with the PCED. Align the PCED pattern regarding the adjustable ring in green; the horizontal and vertical scanned profiles are displayed in the Line-Scan-Profile dialog. If the peak pair from two profiles are not in the same position, the ellipticity exists. The horizontal and vertical lines can be tilted to find the maximum difference between the two profiles from perpendicular scanned lines. The long axis can be rotated along the horizontal line; the long axis and short axis are measured, the PCED pattern can be corrected and undo if needed.
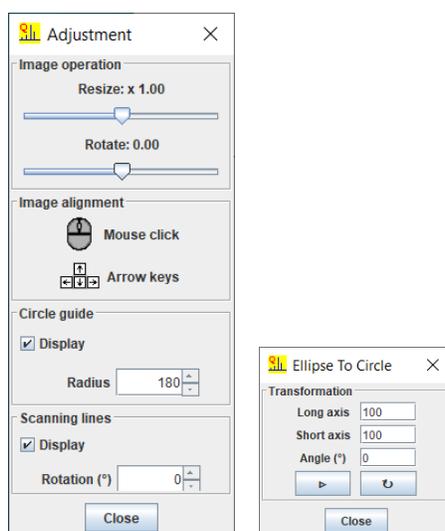

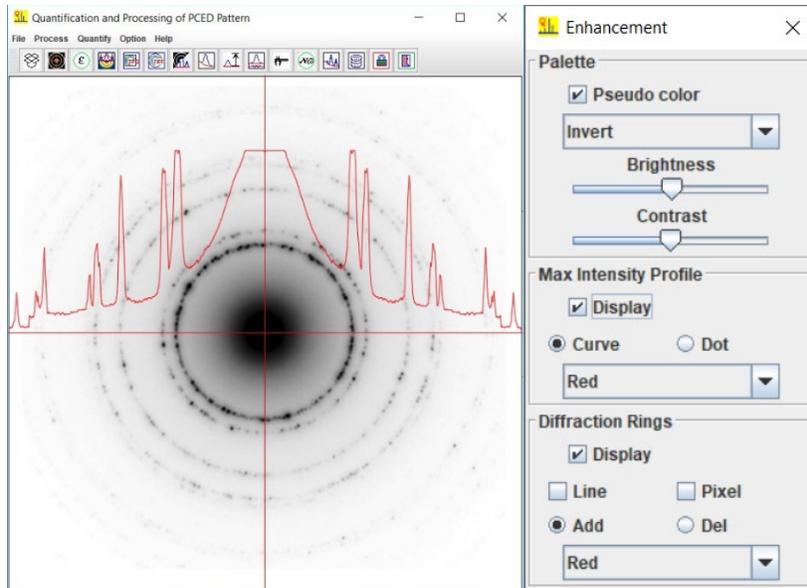Figure 2. (a) The adjustment dialog and (b) the ellipticity dialog.

Figure 3. (a) An inverted grey PCED pattern with enhanced peak positions and (b) the enhancement dialog.
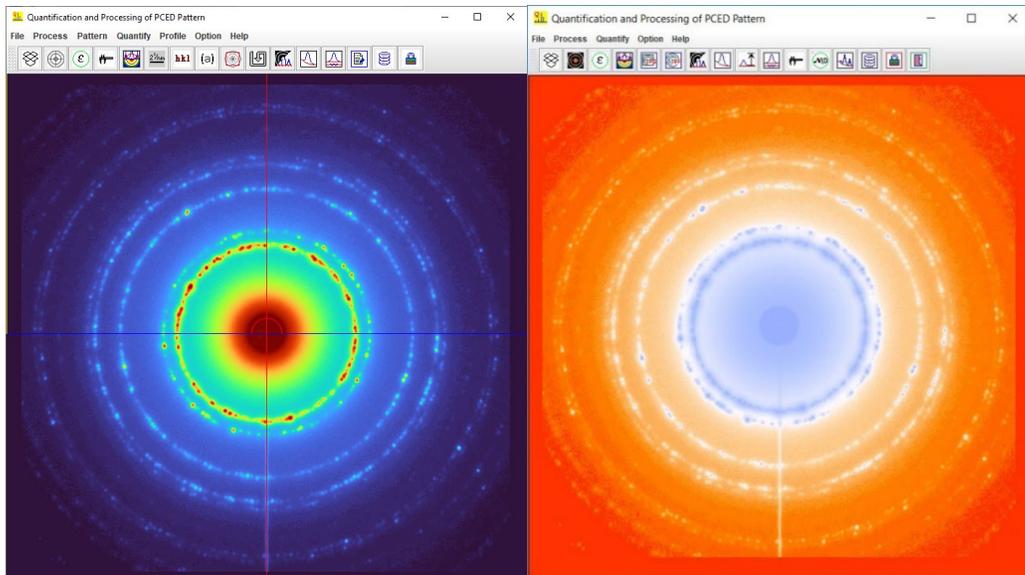

Figure 4. Pseudo color PCED pattern in a palette of (a) turbo and (b) blackbody.
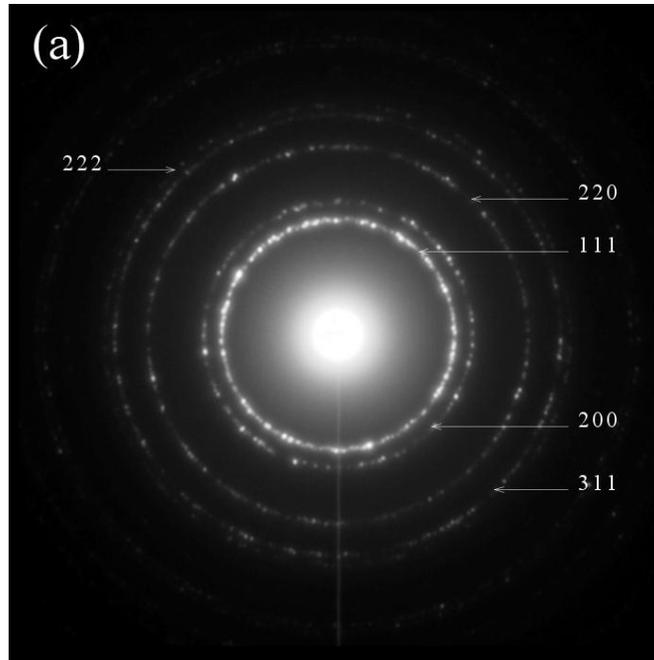
Figure 5. Preparation of a figure for publication.

2.3 Pattern enhancement

The enhancement can be done by image process with brightness and contrast, pseudo-color palette (invert, turbo, blackbody, rainbow), max intensity spot for a ring, marking the ring position. Figure 3 shows (a) the inverted gray PCED pattern and (b) the enhancement dialog, and Figure 4 shows the pseudo-color PCED pattern in a palette of (a) blackbody and (b) rainbow.

2.4 Preparation of SAED patterns for publication

An enhanced image can be saved as output files in TIFF and JPEG format. The output size can be selected through the region of interest (ROI) and the point per inch (PPI). 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, as shown in Figure 5.

3. Analysis and quantification of PCED pattern

3.1 Conversion from a ring to 1D profile

The intensity variation on the ring is obtained by conversion from a selected ring to a 1D profile. One of the application examples is to detect the in-plane texture of a thin film sample.

After a PCED pattern is aligned to the center and the correction for its ellipticity is done, select the integral profile method: Ring in the conversion dialog. Set radius and width, then click convert to display the profile in the viewer panel. Figure 6 shows an example.
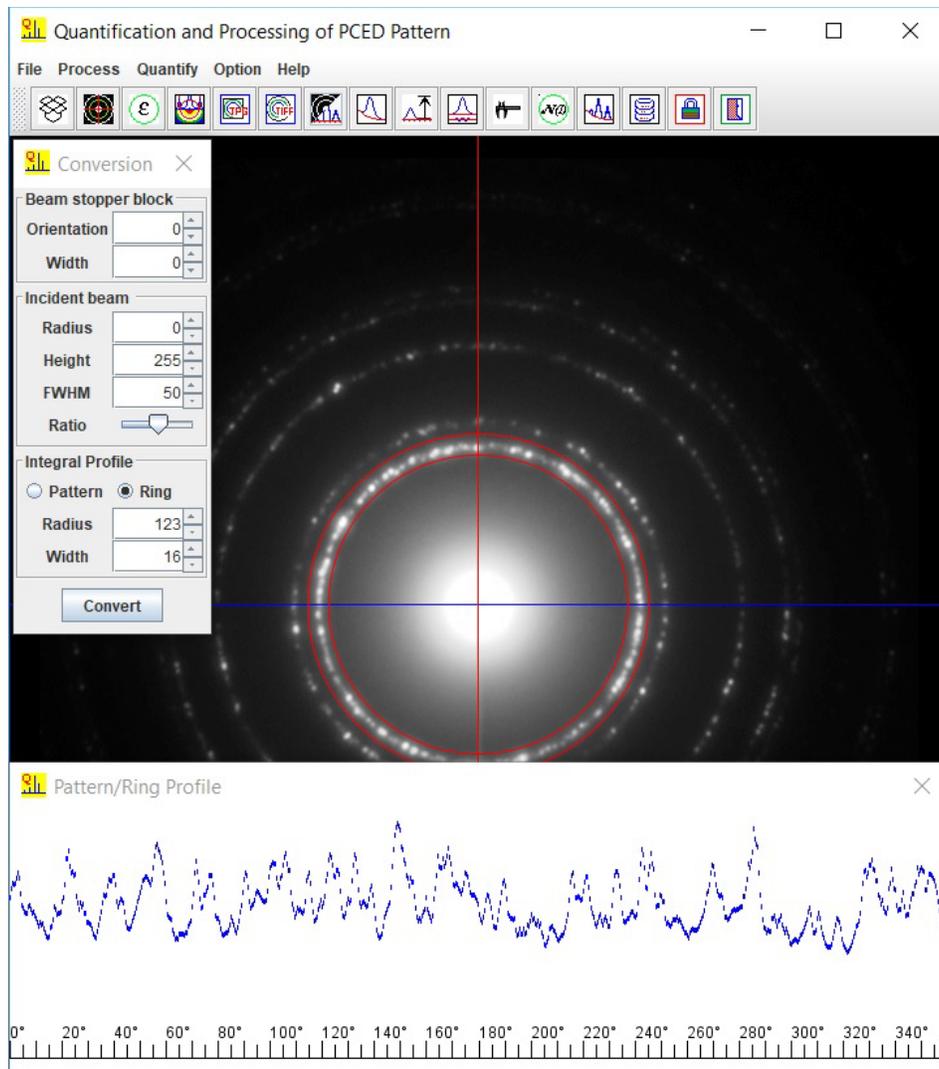
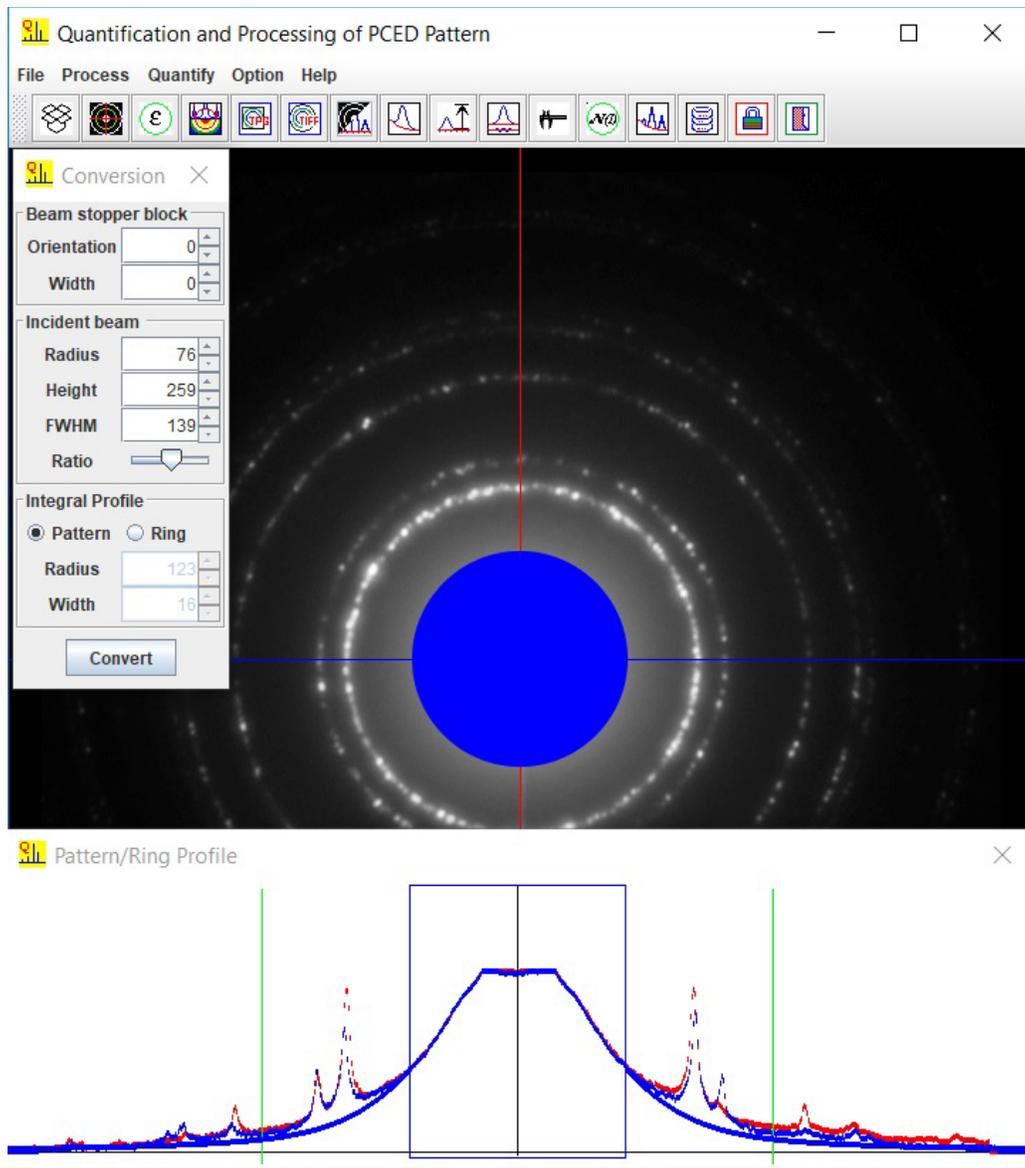Figure 6. An example of the conversion from a ring to 1D profile.

Figure 7. The beam stopper and the profile of the simulated incident beam with pseudo-Voigtian function.

3.2 Conversion from 2D pattern to a 1D profile

Integration can be done along each ring on the PCED pattern to get the intensity profile vs. radius direction. Thus the peak positions and the integrated intensity of each reflection are obtained. The steps include, i) the alignment of the pattern, ii) the setup of the beam stopper, iii) modeling incident beam, iv) the conversion from 2D pattern to 1D profile, v) background, vi) the refinement of parameters of the peak profiles, vii) the position and intensity of each reflection.

3.3 Beam stopper and the incident beam

The beam stopper is hidden since the default width of the beam stopper is 0. If the experimental PCED pattern has a beam stopper shadow, it needs to be blocked in retrieving the intensity profile. The orientation of the beam stopper can also be adjusted.

The central part of the incident beam can be blocked, and the effect of the incident beam outside the block disk can be simulated as shown in Figure 7; thus, the background can be easily modeled and removed. The pseudo-Voigtian function is used to simulate the incident beam's profile with the parameters of height, FWHM, and the ratio of Gauss and Lorentz contribution.

3.4 Background

There are two methods to search the background intensity profile in QPCED. One method is adopted from Brueckner's algorithm (Brueckner, 2000) to generate a suitable smooth curve by variant step length. The method above is a semiautomatic method to search the background intensity profile. The other method is the traditional polynomial curve fitting, in which several fitting points are defined manually. Figure 8 shows a background intensity profile defined by Brueckner's method.
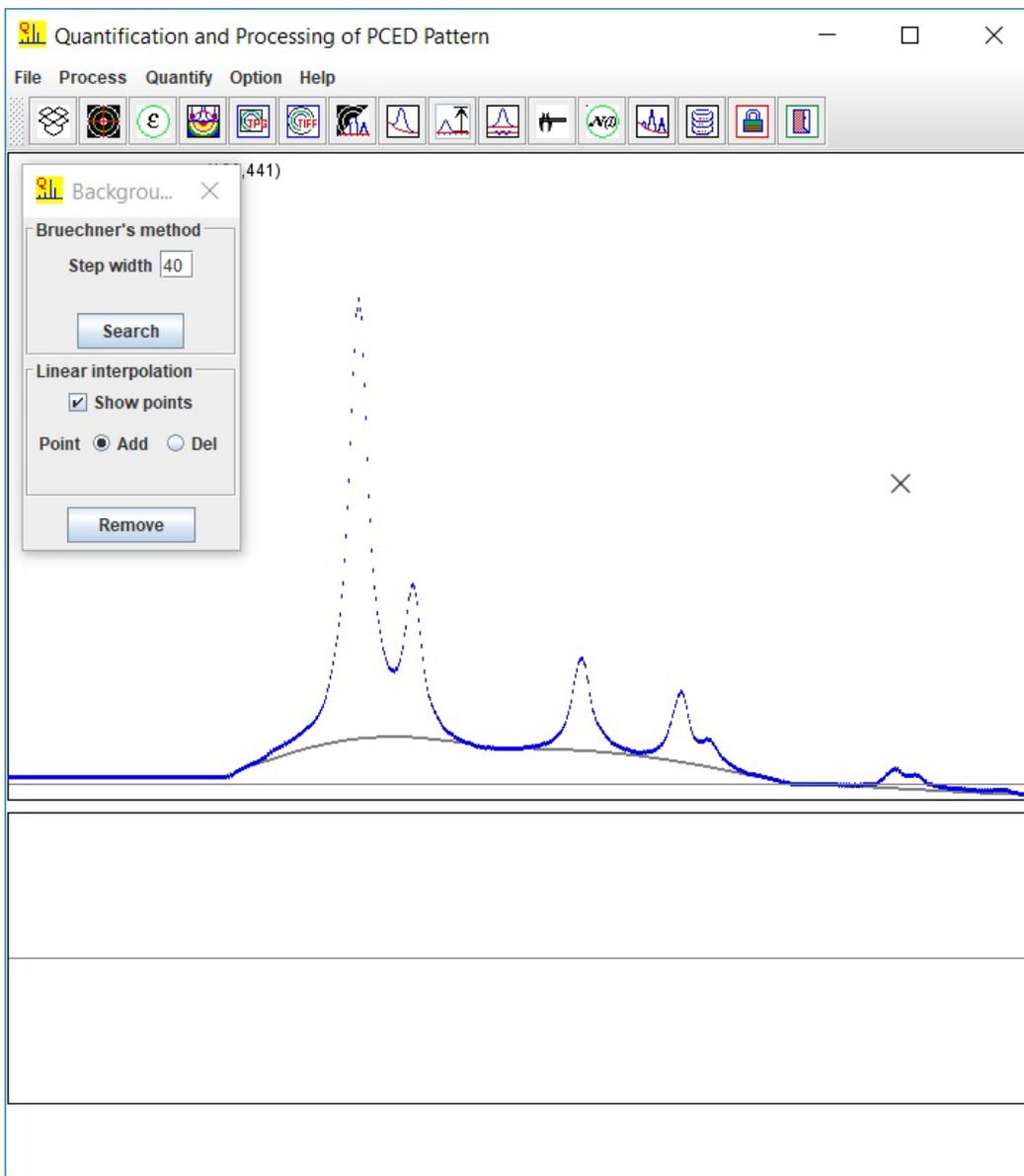

Figure 8. Background intensity profile by Brueckner's method.

3.5 From a 2D pattern to a 1D intensity profile

After removing the background, the reflection peaks can be marked with the mouse pointer with the left button click or simply searching for all possible peaks. The false peaks can be removed by peak editor or remove from the table. Figure 8 shows the peaks defined manually with the mouse pointer.

Two peak shape functions are available, the pseudo-Voigtian and Pearson-VII. Selected the suitable one and refine the peak. Three ways show the refinement by right mouse button click: i) bar, ii) overlap-superpose, iii) overlap-compose. Figure 9 shows the overlap-superpose and overlap-composed status of the reflection peaks after refinement.
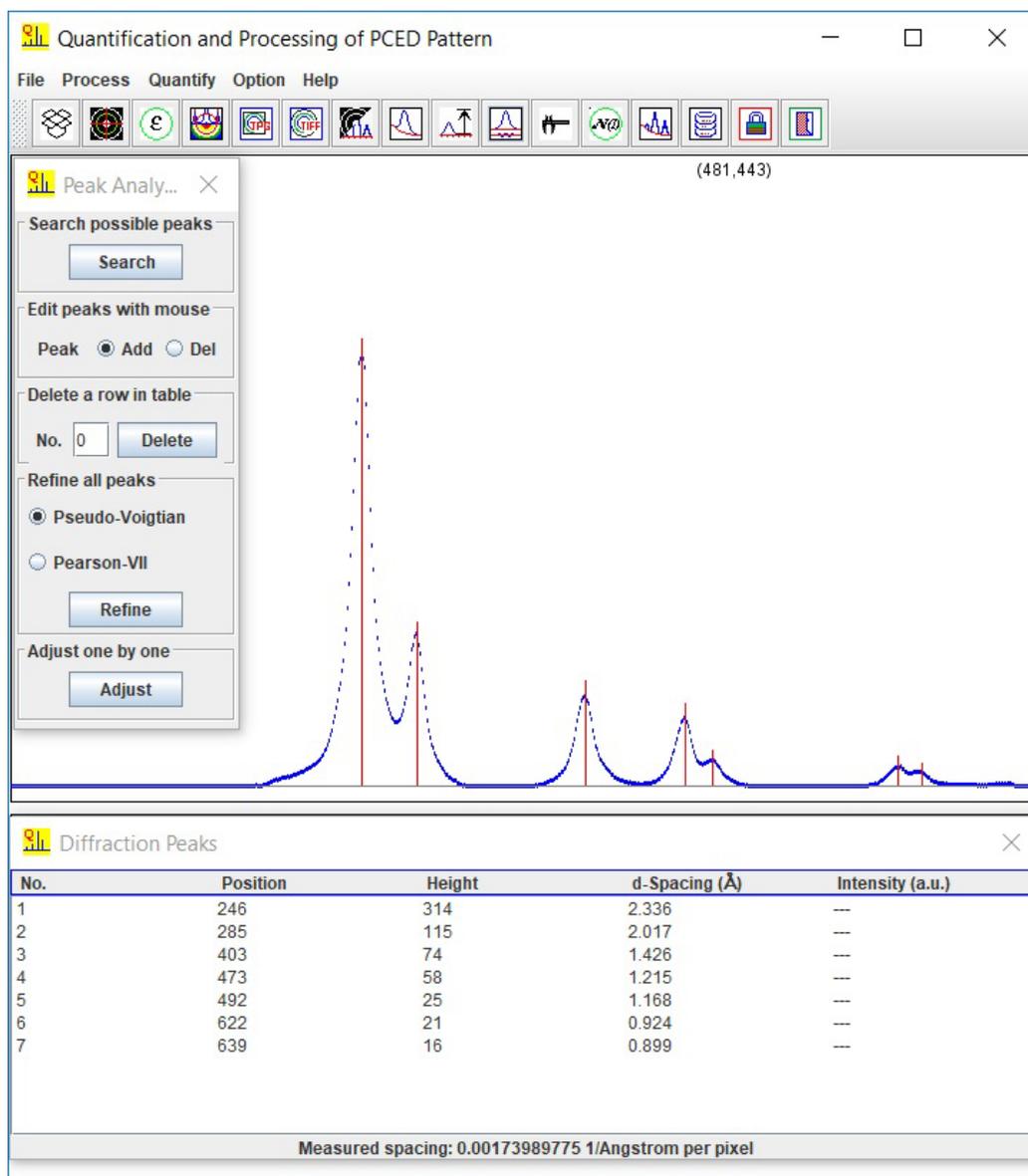

Figure 9. Multiple ways for editing peak position and height mark: semiautomatic and manual methods.
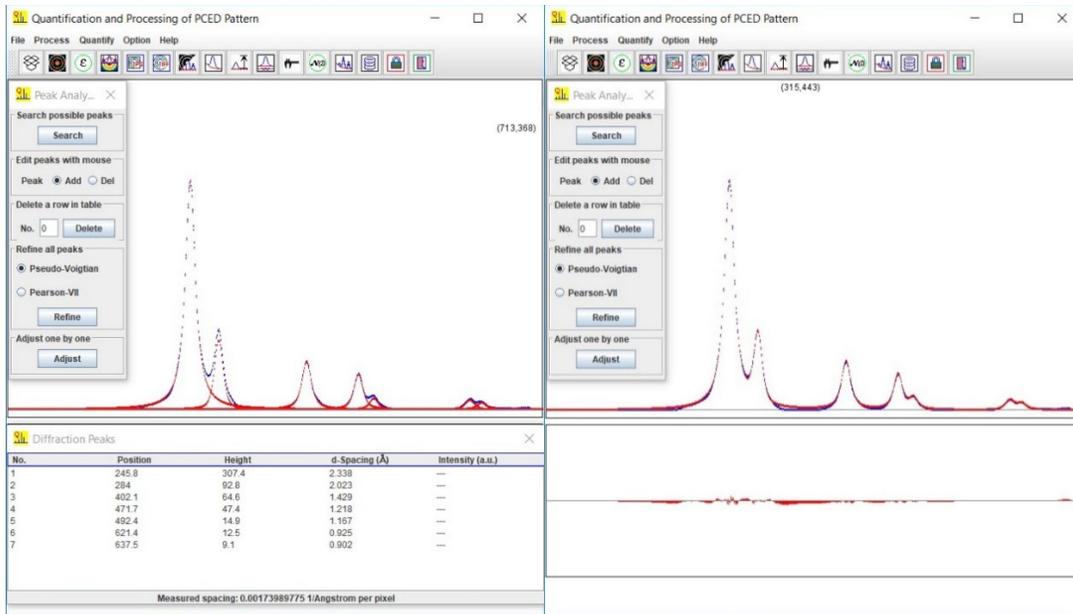
Figure 10. (a) overlap-supposed status and (b) overlap-composed status of the refined profile.

No.	Position	Height	d-Spacing (Å)	Intensity (a.u.)
1	245.8	307.4	2.338	100
2	284	92.8	2.023	21.9
3	402.1	64.6	1.429	18.5
4	471.7	47.4	1.218	12.5
5	492.4	14.9	1.167	3.7
6	621.4	12.5	0.925	3.2
7	637.5	9.1	0.902	2.6

Measured spacing: 0.0017398977464038947 1/Angstrom per pixel

Figure 11. The lattice spacings and intensities of reflections.

3.6 (hkl) position and intensity

After the refinement of the peak position and shape, the normalized intensity is easily obtained. It requests calibration of the pixel and lattice spacing from the scaling bar on diffraction pattern or a diffraction peak of a known crystal structure. As shown in Figure 10, input the pixel value and corresponding lattice spacing and click on Update. Figure 11 shows the final result of the lattice spacings and intensities of reflections.

4. Usage of QPCED

The usage of QPCED is easy and straightforward. Here we use qpced_demo_Aluminum.tif as an example, which is in the experiments folder.

1. Experimental PCED patterns in TIFF, PNG or JPEG format can be loaded in two methods. Drag-and-drop method: moving the mouse pointer on the PCED pattern, holding the left mouse button, dragging the image to the drag-drop box on the graphic menu bar, and

releasing the mouse button. Window file system: click the drag-drop box, find the PCED pattern file, and load the PCED pattern.

2. Align the pattern to the center using the mouse right button. Resize and rotate the pattern if necessary.
3. Check and correct the possible ellipticity in the experimental PCED.
4. Enhance the PCED pattern and save the result.
5. Calibrate the magnification with the scale bar.
6. Turn on the ROI and add the scale bar, indices, and figure label if needed for the publication purpose.
7. For in-plane texture PCED pattern, the measurement of the profile of the selected ring can be done.
8. For quantification of the PCED pattern, the 2D to a 1D profile can be done.
9. Adjust the beam stopper width and orientation to cover the experimental beam stopper shadow.
10. Adjust the incident beam model to remove the background.
11. Adjust the background model to remove the remaining part of the background.
12. Mark all the reflection peaks (add or remove) and then refine the peak functions.
13. Make the calibration of pixel and lattice spacing to get the final results.
14. The enhanced image generated profile and final lattice spacing and intensities can be saved in the MS-Windows file menu.

5. Installation of QPCED

5.1 Java runtime environment
Download and install the openJDK21 or later version from the internet. Download landyne6 on the web site above and decompress the package to landyne6 folder. Copy the license to the programs sub-folder. Create a shortcut of landyne.exe for the Landyne suite.

5.2 Run QPCED in the Landyne suite
Click the QPCED in the Landyne launcher to start the software.

5.3 Get a license
A license file is needed to unlock the program (QPCED6.jar) for loading experimental PCED patterns. The program runs in demo mode, which is in full functions, but limits to qpced_demo_xxx.tif. A license can be purchased from LANDYNE computer software.

6. References

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