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1. Introduction

1.1 Landyne suite

Landyne suite is a software package developed by Dr. X.Z. Li for electron diffraction simulation and crystallography analysis since 2010. The software package can be used as research tools as well as teaching aids. The current version includes ten stand-alone software components [1]. Each of them was designed for one topic of application in simulation, analysis, or data processing. A launcher is available for the software suite, a tool to conveniently access all software components. The executable codes, user manuals, and a set of crystal structural data are available on the author’s webpage https://www.unl.edu/ncmn-enif/xzli/computer-programs.

The software components were introduced in several published papers, such as SVAT4 [2]. It provides a 3D visualization of crystal structures. SAED5 [3] is used to simulate electron diffraction patterns on a single-phase, twining and coexisted multiple phases. It has an extension for the projected atomic potential map. PCED5, as an updated version of PCED [4], is for simulation of electron diffraction patterns from polycrystalline phase and phase identification. SAKI5 is used for simulation and analysis of Kikuchi patterns and simulation of double diffraction effect. A function is added recently for the precise determination of crystal orientation using an electron diffraction pattern with three Kikuchi pairs [5]. SPICA3 [6] is for stereographic projection with an application for specimen orientation adjustment using TEM holders. HOLZ3, as an upgraded version of JECP/HOLZ [7], is an interactive program for simulation of the higher-order Laue zone (HOLZ) lines using kinematical approximation and a first-order dynamic correction. QSAED5, as an updated version of JECP/QSAED [8], is used to quantitative retrieve/display the intensities of reflections on the electron diffraction patterns and to measure line profiles on the electron diffraction pattern. QSAED5 has an extension for the projected atomic potential difference map. QPCED5, as an updated version of QPCED [9], is for digitization and quantification of polycrystalline electron diffraction patterns. TEMUC3 [10] is a program to determine the unit cell of a crystalline phase in TEM using both the reciprocal unit cell reconstruction approach and the reduced cell approach.

1.2 Landyne plus SIMPA

Landyne plus is a collection of multipurpose software beyond the Landyne suite. Structural IMage Processing and Analysis (SIMPA) is the first product in the Landyne+ collection. SIMPA adopts crystallographic image processing (CIP), a technique used to aid in the structure determination. The method has been first applied to periodic organic complexes imaged with high-resolution transmission electron microscopy, subsequently been utilized for TEM images of inorganic crystals, scanning TEM images, and even scanning probe microscope (SPM) images of two-dimensional periodic arrays.

The necessary steps are described succinctly in the following quote by Nobel Prize winner and CIP pioneer Sir Aaron Klug [11]: “The essence of image processing of this type is that it is a two-step procedure after the first image has been obtained. First the Fourier transform of the raw image is produced. Next, Fourier coefficients are manipulated, or otherwise corrected, and then transformed back again to reproduce the reconstructed image.” Although with the common
purpose on the enhancement of electron microscopy images, SIMPA has its unique design and features in comparison with the CIP computer software in public domains or commercially available, *i.e.*, CRISP [12], EDM [13], VEC [14], T4SC [15].

<table>
<thead>
<tr>
<th>Timeline</th>
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<tr>
<td>2000</td>
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<td>2010</td>
<td>Landyne suite (version 1-4)</td>
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### 2. Design and features

#### 2.1 Graphic design

SIMPA graphic user interface (GUI) was written in Java Swing. Figure 1 shows the main panel with a drop-down menu and a graphic toolbar menu. The menu includes i) load (load image, clear image, and exit), ii) image (image operation, area for FFT and line profile), iii) FFT (FFT, Mask, Quantification, and Inverse FFT); iv) Quantify (Image quantification, CIP, Prepare the contour map and Display the contour map); v) Output (ROI and PPI, Scale bar); vi) Option (Auxiliary, Hide the toolbar and Look and feel); vii) Help (Current drive, SN, and version). The toolbar menu includes the most frequent operations for the dropdown menu.

The second panel is for the FFT pattern and the inverse FFT image. Figure 2 shows the FFT/IFFT panel with an example pattern that overlays an aperture-like circular filter. The third panel is for contour maps of the 1x1, 2x2, and 3x3 unit cells of the crystal structure. Figure 3 shows the contour map of a unit cell of the crystal structure. Various dialogues are provided for input, output, and operations. We will illustrate the usage of these dialogues in the next section.

#### 2.2 Function features

SIMPA provides a simplification of the procedure to prepare the EM images for publication. The contrast of the image can be inverted. A selected spot in the image can be easily shifted into the center of the panel. The image can be resized and rotated while the selected spot is kept in the panel center. The scale bar in the original image can be measured, and the length of a new scale bar can be reset and repositioned to the selected area of the image. The image can be saved to a file in the TIFF format. SIMPA also provides a tool to generate a series of intensity profiles. The profiles can be used for comparison of the spacing in the various areas of the image and also for the measurement to the spacing.

SIMPA provides the FFT transformation of electron microscopy images. A square-area with the various power-of-2 edge length or a circular area within the squares can be selected. After calibrating the scale bar in the original image and the scale-bar can be added to the FFT patterns. The FFT patterns can be saved to a file in TIFF format. Compared with the square areas, the circular areas will reduce the streak lines on the FFT patterns [16]. The circular areas for the FFT patterns are especially suitable to the electron microscopy images of the nanoparticles.
Figure 1. The GUI of SIMPA with a dropdown menu and a toolbar menu. The panel shows an electron microscopy image as an example.

Figure 2. The FFT and IFFT panel with an example pattern and an aperture-like circular filter.
SIMPA provides inverted-FFT transformation with various filters. The filters include an aperture-like inside-circle, an outside-circle, a circular band, a strip passing the incident beam, a pair of disks in mirror symmetry, an array of disks. The inverted-FFT image can be shown in pseudo-color and posted back to the original image. The aperture-like inside-circle filter is similar to the objective aperture in microscopy, which controls the images’ resolution. The strip filter is good to show if there is any mismatch in the lattice image. The array-of-disks filter can be used to quantify the FFT pattern and calculate the lattice parameters.

SIMPA provides quantification of the unit-cell in contour maps. After defining the two basic vectors for the array-of-disks filter, a unit cell of the structure will appear in the inverted-FFT image, and the diffraction data, amplitude, and phase can be saved. The amplitudes can be replaced by the FFT data or corresponding SAED data. The contour map of the unit cell can be further calculated and displayed using the diffraction data.

A subroutine of the CIP in the SIMPA can force the selected symmetry from one of the 17 planar symmetric groups. For simplification and consistency in the program design and analysis in SIMPA, the 17 planar groups have been expanded to 21 to distinguish the same symmetry on the two basic vectors. A centered unit cell is also transformed into a primitive unit cell. The crystallographic phases in the diffraction data depend on the unit cell's original coordinates, which can be adjusted on the contour maps. Three figure-of-merit, R-values, resident phase, and extinction ratio are also available for evaluating if the symmetric data represents better the diffraction data.
The design and features of SIMPA have been summarized in a flow chart, as showed in Figure 4.

3. Usage specification

For an unlicensed user, the license file dialogue will show in Figure 5. User may go ahead to click Explore or Volveré (I will be back in Spanish).

3.1 Load an EM image and calibration the scale-bar

Two ways are provided to load the image file. If the image is not in the experiments folder, it is convenient to load the image with the drag-and-drop function (dragging the image to the drop-box on the menu bar). If the image is in the experiments folder, users may use the window-like file system to load the image (clicking on the drop-box on the menu bar or the drop-down menu and following up).
Figure 6. The image operation dialogue.

Figure 6 shows the image operation dialogue for inverted contrast, resize, and rotation of an image. The image's shift operation can be done by pointing to a selected spot on the image and then using the mouse right-button while holding down the Alt key. The resize and rotate operations will keep the center of the image unchanged.

Figure 7. (a) The line profile analysis tool and (b) a profile analysis on the scalebar.

Figure 7 shows the line profile analysis tool. Besides the display and measure of the image features, the tool should be used to measure the scale bar and used for calibration (see ROI and scale bar).

3.2 A series of intensity profiles

A series of intensity profiles of an image can be compared or measured. Figure 8 (a) shows three lines in blue, green and red, (b) the corresponding line-scan profiles.

Figure 8. (a) The line profile analysis on an image and (b) the line-scan profile.
3.3 FFT and IFFT processing

Figure 9 shows the area selection dialogue. The square area with its edge length in the power of 2 will be used for FFT transformation. The length can be determined by holding the mouse left button and dragging the mouse pointer. The location of the area can be replaced by click the mouse left button. A circular area within the square area is an option for FFT transformation. Compared with the square areas, the circular areas will reduce the FFT patterns' streak lines [16]. The circular areas for the FFT patterns are especially suitable to the electron microscopy images of the nanoparticles.

![Area Selection Dialogue](image)

**Figure 9. The area selection dialogue.**

Figure 10 shows the FFT and IFFT dialogue. The autocorrelation, inverted contrast, and replacement are implemented on the FFT panel; the unit-cell display, pseudocolor, and replacement are implemented on the IFFT panel. The zoom, brightness, and gamma adjustment operation on both of the FFT and IFFT panels. The FFT operation has to be carried out before the

![FFT/IFFT Dialogue](image)

**Figure 10. The FFT and IFFT dialogue. The adjustment operations are available.**
IFFT operation. The FFT operation can also be re-executed after the IFFT operation has been executed. The selected area is on the original image even though a replacement is shown.

Figure 11. The FFT masks for the IFFT operation.

The IFFT operation needs an FFT mask after the FFT operation. Six FFT masks are shown in Figure 11. The sizes or positions of the marks can be defined with the mouse pointer. Their sizes can be adjusted with the mouse wheel or the arrow keys. The band type mask is formed by the inside-aperture-like mask and the outside-aperture-like masks, so the band type's size is set by the first two masks. The array mask can be chosen as a 1-dimensional array or a 2-dimensional array, as shown in Figure 12. Two basic vectors can be more accurately defined by enlarging the FFT panel and using the reflections' positions with higher indexes. The FFT pattern reflections' quantitative intensities can be saved and used to construct the contour map of the unit cell.

Figure 12. The array mask for the IFFT operation and quantitative analysis.

Figure 13. The Region of Interest dialogues for image and FFT/IFFT panels.
3.4 Output of the processed images

Figure 13 shows the image's region-of-interest (ROI), used for output as TIFF or JPEG images. The point-per-inch (PPI) is for the TIFF format. Users may define the size and location of the ROI. Two special cases are given as FFT and Full areas. The FFT pattern and IFFT image can be saved when duplicated to the image using the replacement button in Figure 8. At the same time, the scale bar can be put on the FFT pattern.

Before adding the scale bar on the image or the FFT pattern in the ROI for output, the original image's scale bar must be measured and fill the info in Figure 14. Two pre-selected positions are available, which can be further adjusted, so are the font-size, thickness, and color of the bar. In the default setting, the scale bar is hidden.

Figure 15. Image quantification of a unit cell.
3.5 Quantification of a unit cell

A unit cell must be selected on the IFFT image to generate the data for the contour map of an image. User can choose the origin of the unit cell by the mouse pointer and fine-tune later on the contour map. Figure 15 shows the image quantification of a unit cell. Users may view the result as an option to load and merge the FFT data or SAED data and save the unit cell's crystallographic data for a contour map.

Figure 16 shows the dialogue for the preparation of the contour map. After loading the crystallographic data generated above, the filename will appear on the top line. Users may use the default or customized parameters to build the contour map. After displaying the contour map, the shift (x, y) parameters of the origin can be obtained, as shown below. The shift parameter can be used for resetting the unit cell origin in Figure 15. The updated crystallographic data can be saved for crystallographic image processing, as shown later.

Figure 17 shows the dialogue for the contour display. Once the show button is clicked, it shows the contour map. An example is given in Figure 3. The options are available to show the unit cell's frame, the coordinate of any point in the unit cell, the user-defined grids, and the maximum and minimum densities. A contour map display may vary with the Bezier curve parameter, the number of layers, noise filter in percentage, zoom, and shift parameters. It can display 1x1, 2x2, or 3x3 unit cells. The coordinate of any point in the unit cell can be precisely measured using the mouse pointer.

3.6 Crystallographic image processing

Figure 18 shows the dialogue for crystallographic image processing. The essence of image processing of this type is a two-step procedure after the first image has been obtained. First, the Fourier transform of the raw image is produced. Next, Fourier coefficients are manipulated, or otherwise corrected, and then transformed back again to reproduce the reconstructed image.

User may evaluate the possible symmetry of the original image or its contour map and compare the 17 planar space groups [17], which extend to 21 choices due to some of the planar space groups
are given in two different a and b axes. The symmetries in the selected planar space group will be applied to a unit cell's crystallographic data. Three figures of merit parameters can be used to evaluate the relation between the original data to the processed data. The enhanced data can be viewed and analyzed using the contour map display tool.

Figure 17. The dialogue for contour map display.

Figure 18. The dialogue for crystallographic image processing.
4. Examples

4.1 Selected area of an EM image

In this example, we plan to choose an area in the SIMPA_demo.tif in Figure 19(d) and save it as a TIFF file. The following steps are needed, 1) calibrate the scale bar, 2) set the ROI using the mouse coordinates on the menu bar, as shown in Figure 19(a), 3) add the new scale bar and adjust the position, as shown in Figure 19(b), 4) output the image in a TIFF file, as shown in Figure 19(c).

![Figure 19. (a-c) the procedure to prepare an image from an area in the SIMPA_demo.tif in (d).](image)

![Figure 19. (d) an area of the SIMPA_demo.tif for output.](image)
4.2 FFT and IFFT of an EM image

Figure 20. (d) an area of the SIMPA_demo.tif for output

Figure 21. The IFFT image using (a) a circular aperture mask, (b) a circular belt mask, (c) a slim rectangular mask, and (d) a reflection array mask.

Figure 20 shows the FFT patterns with (a) a square area and (b) a circular area. Multiple masks are available to reveal the various features of electron microscopy images. Figure 21 shows the
IFFT image using (a) a circular aperture mask, (b) a circular belt mask, (c) a slim rectangular mask, and (d) a reflection array mask. The reflection array mark is also used to quantify the FFT pattern. The IFFT image can be added to the scale bar, saved as a TIFF file, or replaced the original image.

4.3 Quantification of an EM image and CIP

We may use the reflection array filter on the FFT pattern and quantify the unit cell. Figure 22 shows (a) The contour map from the FFT data from a unit cell, (b) the contour map from the FFT data from the image, (c) the contour map from the CIP of data using the c1m1 symmetry, and (d) the contour map from the CIP of data using the c11m symmetry. The crystal structure is considered as a central orthorhombic lattice (in a primitive lattice description). The phase residuals' values are 15.2 for the c1m1 symmetry and 14.5 for the c11m symmetry. Figure 22 (d) is an enhanced image from Figure 22 (a) and (b). Figure 23 shows the 2x2 contour map of the unit cell after CIP using the c11m symmetry, in (a) color and (b) gray.

Figure 22. (a) The contour map from the FFT data from a unit cell, (b) the contour map from the FFT data from the image, (c) the contour map from the CIP of data using c1m1, and (d) the contour map from the CIP of data using c11m.

Figure 23. The 2x2 contour map of the unit cell after CIP using the c11m symmetry, in (a) color and (b) gray.
4.4 Study of nanoparticles

The nanoparticles were prepared by the cluster deposition method using an inert-gas condensation. In this method, which produces highly monodisperse metal and alloy nanoparticles, an atomic Fe vapor produced using direct-current plasma sputtering is condensed in a cooled inert-gas atmosphere to form nanoparticles in the gas-aggregation chamber. Carbon-coated Cu grids with low nanoparticle coverage were used for transmission electron microscopy (TEM) measurements.

Figure 24 shows a high-resolution electron microscopy (HREM) image of a Fe particle. The crystal is nearly hexagonal, and the size of the crystal is about 30 nm. The HREM image was enhanced by using SIMPA. Figure 25 shows (a) a unit cell of which the origin was arbitrarily chosen, (b) a unit cell of which the origin was reset, (c) CIP enhanced a unit cell, and (d) 9x9 unit cells which can be compared to the HREM image.

Figure 24. A high-resolution electron microscopy image of a Fe particle. The crystal is nearly hexagonal, and the size of the crystal is about 30 nm.
Figure 25. (a) a unit cell of which the origin was arbitrarily chosen, (b) a unit cell of which the origin was reset, (c) a unit cell was enhanced by CIP, and (d) 9x9 unit cells which can be compared to the HREM image.

4.5 Study of carbon fibers

Carbon fiber, the strongest commercially available structural material today, is a lightweight reinforcement used to strengthen polymer composites. Scientists seek to strengthen advanced, high-performance fibers using exceptionally strong and fatigue-resistant carbon nanotubes, sheets of one-atom-thick carbon molecules shaped into hollow cylinders.

Figure 26. The cross-sectional image of a carbon fiber along its long side.
Figure 26 shows the cross-sectional image of carbon fiber along its long side, fabricated by Prof. Dzenis’ group at the University of Nebraska, Lincoln. The distribution of the graphite sheets was studied by using SIMPA. The spacing of the graphite sheets in the carbon fiber is determined to be 0.387 nm on average. Figure 27 shows an FFT pattern and an IFFT image of the experimental image in Figure 25.

Figure 27. An FFT pattern and an IFFT image of the experimental image in Figure 26.

5. Installation

5.1 Computer requirement

Java virtual machine, i.e., J2RE, must be installed for running SIMPA. Java Advance Image is needed for TIFF file, copy jai_codec.jar and jai_core.jar to, e.g., java\jre\lib\ext\ folder.

5.2 Software installation

The executable bytecodes, together with the data files for testing and this specification file are available in compressed form (landyne_plus.zip) http://www.unl.edu/ncmn-enif/xzli/computer-programs and http://landyne.scienceontheweb.net. Decompress SIMPA.zip in a user-defined directory, e.g., c:\landyne_plus\, and execute landyne_plus.exe.

5.3 Licenses and feedback

The software works in two modes, demo mode, and license mode. The software is fully operational at demo mode but limited to the demo input file, SIMPA_demo.tif.

Both short-term and perpetual licenses are available at LANDYNE (jlandyne@gmail.com). Suggestions and comments are welcome.

6. References


