LANDYNE

User Manual

Simulation and Analysis of Electron Diffraction Pattern

Simulation and Analysis of Electron Diffraction

Data Experiment Simulation Pattern Option Table Help

Contents

Highlights

1. A window frame with a panel displays the simulated pattern or matches a preloaded experimental diffraction pattern.
2. Input parameters for calculations can be initialized using an operational panel and several dialog windows.
3. Structure data files can be easily prepared using a computer assistant.
4. Multiple phases can be loaded and calculated simultaneously to simulate diffraction patterns for twins, coexisting phases with fixed orientations, and for comparing similar patterns from different phases.
5. Experimental patterns can be aligned, resized, and rotated.
6. Label tools are available to prepare figures for publication.

1. Introduction

Selected area electron diffraction analysis is widely employed in materials science for tasks such as phase identification, determining structural intergrowths, and establishing growth directions like twin relations and fixed orientations of co-existing phases.

Electron diffraction offers distinct advantages and disadvantages compared to X-ray diffraction due to its stronger interaction with matter. On one hand, nano-objects too small for conventional X-ray experiments can be studied in the lab with electron diffraction. Additionally, electron diffraction patterns can reveal reflections with higher resolution for light atoms than X-rays. On the other hand, electron diffraction's strong interaction with matter and small diffraction angles can lead to complex dynamical effects like multiple diffraction, complicating structural interpretation.

Simulation of electron diffraction patterns is crucial for interpreting experimental data. Patterns from single crystal grains and polycrystalline samples differ significantly, necessitating separate treatment for advanced simulation and analysis. PCED6 simulates electron diffraction from polycrystalline samples, while SAED focuses on single-crystal samples.

Current electron diffraction simulation software primarily supports single-phase simulations. However, for advanced analysis involving twinning, multiple phases with fixed orientations, and comparing diffraction patterns from different phases, existing functionalities may be insufficient. Key tasks in electron diffraction analysis include determining the zone axis, indexing diffraction patterns for phase identification, and orienting crystal grains.

To enhance structural interpretation and modeling, a projected atomic potential (difference) map can aid in interpreting high-resolution electron microscopy (HREM) images. This capability is integrated as an extension in ESPOT. Therefore, we have developed SAED, currently in its 6th version, to address these needs comprehensively.

JECP/ED: Journal of Applied Crystallography, 36 (2003) 956
SAED2: Proceedings of Microscopy & Microanalysis, 18 S2 (2012) 1262.
SAED3: Microscopy and Analysis, 2019 (May issue 16-19).

SAED4: Save diffraction data for ESPOT. formats, jpg, png, tif. Add functions for index label, zone axis label, mark label.
SAED5: Enhanced new (structural data) on non-standard space group. and add function of check for update.
SAED6: Enhanced new (structural data) on rhombohedral system, and enhanced function of find [uvw]. The executive code was compiled in openJDK21.

SAED was written in Java. Further code optimization (including obfuscation) was carried out for the compiled class files. A license file is needed to unlock the program (SAED.jar) for loading input data files. Please contact the LANDYNE (computer software) for licenses.

2. Theory background

2.1 Electron diffraction geometry and intensity

The kinematical and dynamical theories of high-energy electron diffraction have been well documented in textbooks (e.g., Peng *et al.,* 2004, other books on electron diffraction theory) and literature references (e.g., Metherell, 1975).

The electron atom scatting factor can be derived from the X-ray atom scatter factor using the Mott-Bethe relationship or directly obtained from a parameterized table of electron atom scatter factors (Peng *et al.* 1996). Here we use the second method.

Following the electron diffraction geometry, the reciprocal length (R) of a reflection in a diffraction pattern can be related to the length of the reciprocal vector *g(hkl)* as

$$R = \frac{L\lambda}{d} \frac{\sqrt{1-\left(\frac{\lambda}{2d}\right)^2}}{1-2\left(\frac{\lambda}{2d}\right)^2} \tag{1}$$

where L is the camera length, $d=1/|g(hkl)|$ and λ is the wavelength of an incident electron beam.

For high-energy electron diffraction, the Ewald sphere's radius is relatively large; thus, the electron diffraction pattern of the thin sample reveals the two-dimensional distribution of reciprocal lattice points.

Electron diffraction intensity in kinematical theory is given by:

$$I_g \propto \left|F_g\right|^2 \tag{2}$$

Here F_g is the so-called structure factor.

In SAED, dynamical electron diffraction intensities are calculated using the Bloch wave method (Metherell 1975). Readers should check the formulas in the original research papers.

2.2 Electron diffraction of twins and coexisted multiple phases

Crystals exhibiting twinning can be categorized based on their diffraction patterns into three main types. Non-merohedral twins consist of two or more crystalline domains whose reciprocal lattices either do not overlap or only partially overlap. In contrast, merohedral twins feature domains with completely overlapped diffraction patterns. The symmetry operations linking the twinned domains belong to the sample's Laue group but not its space group. Pseudo-merohedral twins also have completely overlapped diffraction patterns, but the symmetry operations relating to the domains are not part of the sample's Laue group.

In complex alloy systems, two or more phases may coexist with a fixed orientation relationship. Electron diffraction analysis plays a crucial role in determining these relationships. For instance, precipitates within a matrix often exhibit a fixed orientation. Researchers typically tilt the matrix to study these precipitates, as they are small particles requiring specific orientation for analysis.

Simulating electron diffraction patterns for twins and multiple coexisting phases involves calculating patterns from multiple structures within a single frame. SAED is designed to sequentially calculate patterns from multiple structures, making it easy to adjust and simulate patterns from twins and multiple coexisting structures with fixed orientations.

2.3 Determination of a zone axis and indexing

In electron diffraction analysis, a fundamental task is identifying the zone axis of the diffraction pattern and indexing, which are crucial for tasks such as phase identification and determining crystal grain orientation.

SAED provides tools specifically designed for these purposes. Users can measure the scale bar and determine the lengths of two basic reciprocal vectors, as well as the angles between them, on diffraction patterns saved in jpeg, png, or tiff formats.

The lengths of the two basic reciprocal vectors are compared to all possible (hkl) indices within a specified tolerance. Subsequently, the angles between these vectors are evaluated using the reciprocal length of the third edge in the triangle formed by the vectors. The zone axis with the least mismatch in length values is identified and listed, and possible zone axes can be saved to a file.

In the "Find Zone Axis" dialog of SAED, users define the tolerance for reciprocal lengths, while the angle assessment is based on the reciprocal length of the third vector edge in the triangle.

3. The graphic user interface of SAED

3.1 Main interface

The main interface of SAED is depicted in Figure 1. SAED serves multiple purposes depending on its usage scenario:

1. Simulation:
   - o Load structure data and configure input parameters.
   - o Click the "Calculate" button in the Calculation control panel to simulate diffraction patterns.
2. Zone Axis Search or Phase Identification:
   - o Start by loading an experimental diffraction pattern.
   - o Identify the zone axis and match calculated patterns with chosen structure data and input parameters.

SAED supports loading multiple structure data simultaneously for comparison or simulation of twins and coexisting structures with fixed orientations.

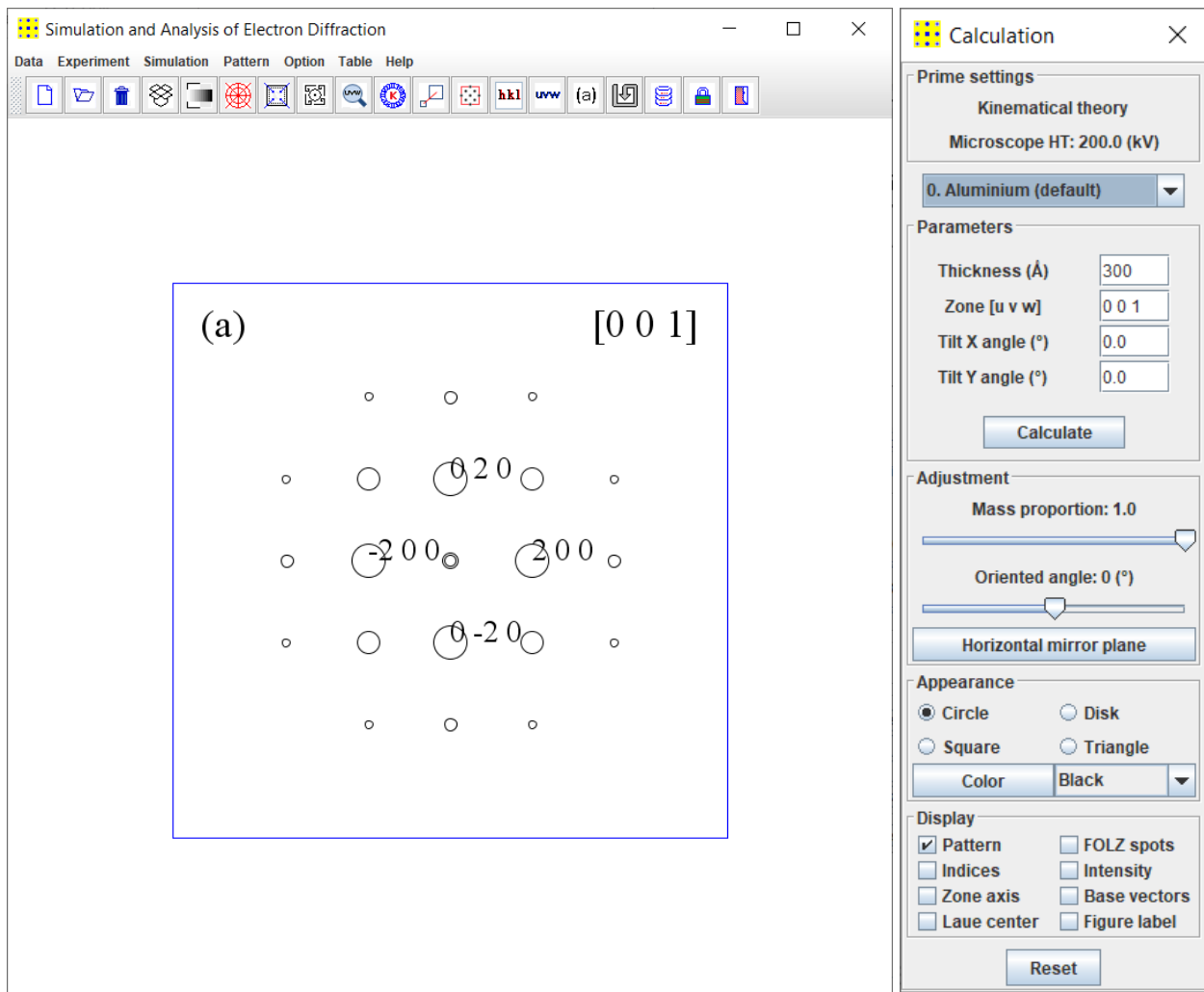Users can customize the software frame size, including the display panel, through the Auxiliary menu.

Figure 1. Snapshot of the main panels in SAED, a simulation of an electron diffraction pattern of Aluminum along [001] zone axis.

3.2 Menu and toolbar

The menu and toolbar in SAED provide essential functionalities through dialog pop-ups for data loading and parameter adjustment. Here's an overview of their capabilities:

Crystal Menu: Facilitates creating new structure data, loading input structures (which can be reloaded for twins), and clearing all loaded structures except the default (Al) structure.

Experiment Menu: Offers options for loading experimental electron diffraction patterns (EDP) in JPEG, PNG, and TIFF formats. Loaded SAED patterns can be adjusted by inverting contrast or cleaning up. The image can be resized, rotated, and shifted/centered using drag-and-drop actions relative to concentric circles and lines. Images can be loaded via drag-and-drop by selecting the file with the mouse pointer, pressing down the left button, dropping it onto the drop-box icon on the menu bar, and releasing the left button. The image position can be further adjusted in the Image Operation dialog (see Fig. 2). A caliper tool is available for adjusting reciprocal spacing using the scale bar in the experimental SAED pattern (Fig. 3). The "Find [uvw]" option opens a dialog to determine the basic reciprocal vectors of the EDP and identify the zone axis with the least mismatch residue. Detailed information on all possible zone axes can be saved to a text file.

Simulation Menu: Includes a submenu for selecting between kinematical and dynamical diffraction theories. Kinematical diffraction theory is the default choice due to its suitability for most crystals. Dynamical calculations, using the Bloch wave method, are cautioned for crystals with large unit cells due to extended computation times. This menu allows setting parameters such as microscope high voltage and maximum index number for calculations. Dialog windows enable adjustment of pattern zoom, intensity scale to simulate camera length and exposure time, and selection of diffraction spot labels (reflections). Labels can be configured for indexing and intensity schemes. Weak diffraction spots can be normalized to a constant scale, or the display can focus solely on reciprocal lattice points.
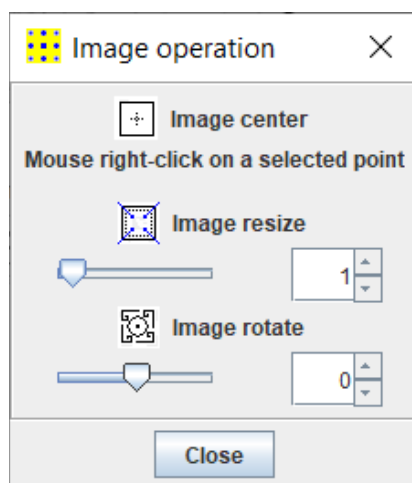

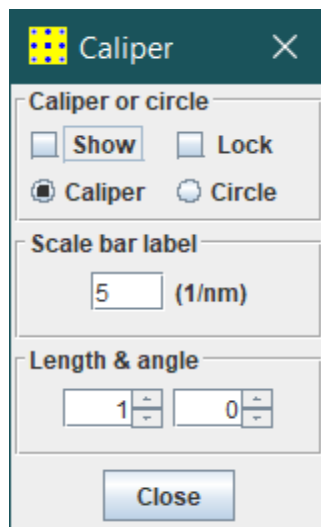Figure 2. Snapshot of the supporting panels in SAED for analysis of experimental SAED patterns.

Figure 3. Snapshot of Caliper panel for adjusting the reciprocal spacing to the scale bar on the experimental SAED pattern.

Pattern menu provides a dialog for ROI and PPI; the simulated patterns can be saved as output files in JPEG, PNG or TIFF format.

Table menu provides a periodic table of elements and a table of the space group.

Option menu provides freedom of customizing the appearance of SAED (look and feel skin), a switch to show or hide the graphic menu bar and set up the default position and the size of the panels.

Help menu can be used to find the current drive and the serial number (SN), which is required for license files, a version, and license information.

The toolbar provides a quick way to conveniently access the functions described above. The toolbar can be switched on/off. The functions of the toolbar are shown by both the icon image and tooltip text. Most frequently used menus and submenus are listed in the Toolbar. Drag-and-drop box only appears in the toolbar, allowing the drag and drop action to load an image in JPEG, PNG or TIFF format quickly. A lock icon is unlocked when a valid license file is the same fold. Without a license file, SAED can be evaluated in a demo model. Contact Landyne for purchasing the license file.

4. Usage of SAED

To run SAED, a user may use (1) Landyne launcher or (2) type: java -jar (-Xmx512m) SAED.jar in the command line. -Xmx512m is an option to locate the memory of a Java virtual machine up to 512 MB. The main window frame and the control interface of the program in Fig. 1 will show up.

In the following, we show step by step from preparing structure data file, common routine usage for simulation, and to the last steps of saving and printing the results. More details on specific topics are left to the next section.

4. 1 Prepare new crystal structure file

To prepare a structure data file in SAED, use the New Crystal Structure File dialogue window (Figure 4). This dialogue window features an automatic assistant to ensure compliance with file format requirements. The template includes the 230 space groups in Hermann-Mauguin notation, as listed in the international table for crystallography. Note that only the unique b axis is utilized in monoclinic systems. Two origin choices are available as input parameters, with choice-2 automatically converted to choice-1 for consistency. To save a data structure, click the "Save" button, or create a new structure by clicking "New."

Existing crystal files can also be modified or converted from a Crystallographic Information File (CIF). For systems with alternative space group settings in triclinic, monoclinic, and orthorhombic systems (settings 1 to 74), click on the appropriate alternative setting. SAED provides a tool for transforming files from nonconventional notations to standard notations.

Figure 4. Snapshot of the preparation of the new crystal structure file.

4.2 Simulation

SAED simulation offers two theories: the default kinematical diffraction theory and the dynamical diffraction theory using Bloch wave theory. Key parameters such as high voltage, pattern zoom, and intensity scale can be adjusted in the Simulation menu.

Calculation using the Bloch wave theory may require significant time for crystals with large lattice parameters. To optimize efficiency:

- The software includes an option for users to terminate the calculation process once an acceptable result is achieved or to continue calculation, as depicted in Figure 5.
- When only the thickness parameter changes, the software utilizes previously calculated parameters to simulate a diffraction pattern, saving computation time.
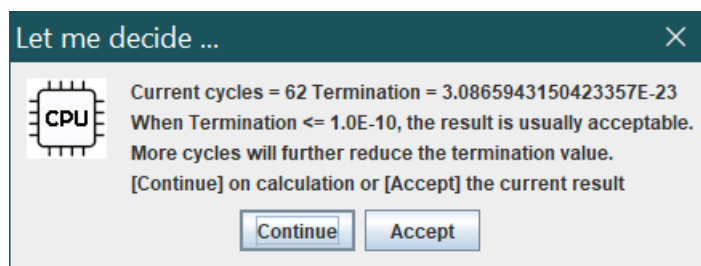

Figure 5. Snapshot of an option for user to terminate or continue the calculation.

In SAED, structure data for calculation should be selected from a list of loaded structure data. Once the thickness, zone axis, and tilt angles are chosen to generate a new diffraction pattern, click the Calculate button. Adjustments to the pattern can be made by modifying other parameters.

The mass proportion setting assigns equal weight to all loaded structures by default. This parameter becomes relevant when calculating a composite diffraction pattern from two or more structural data sets.

Orientation and mirror operations are utilized to align the simulated pattern with the experimental pattern and to generate various twin configurations.
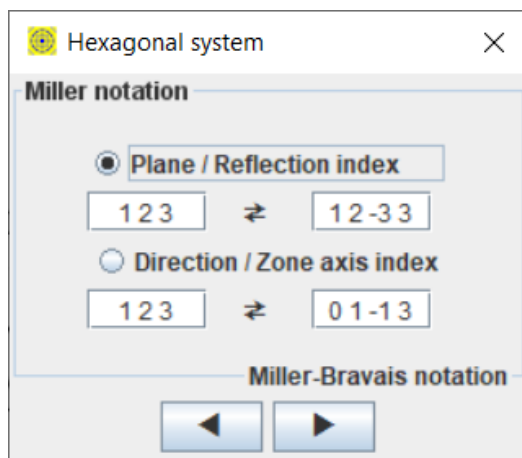

Figure 6. Miller-Bravais converter for hexagonal system.

Diffraction patterns in SAED can be viewed in four predefined shapes and various colors. Options include displaying or hiding patterns (ZOLZ and FOLZ), labeling index and intensity for basic reciprocal vectors, and labeling diffraction spots based on intensity levels. Basic vectors and Laue centers can also be toggled to display or hide.

4.3 Miller-Bravais convertor

The hexagonal system is more conveniently described by 4 basis vectors (Miller-Bravais index notation), 3 of which are co-planar and therefore, not linearly independent. Hence, the tendency to describe planes in hexagonal crystal using the Miller-Bravais system (hkil) where $i=-(h+k)$ and can be omitted in writing (hk.l); The zone axis is [uvtw] in Miller-Bravais system and [UVW] in Miller system, where

$$U = u\text{-}t; u = (2U\text{-}V)/3$$
$$V = v\text{-}t ; v = (2V\text{-}V)/3$$
$$W = w; t = -(U+V)$$

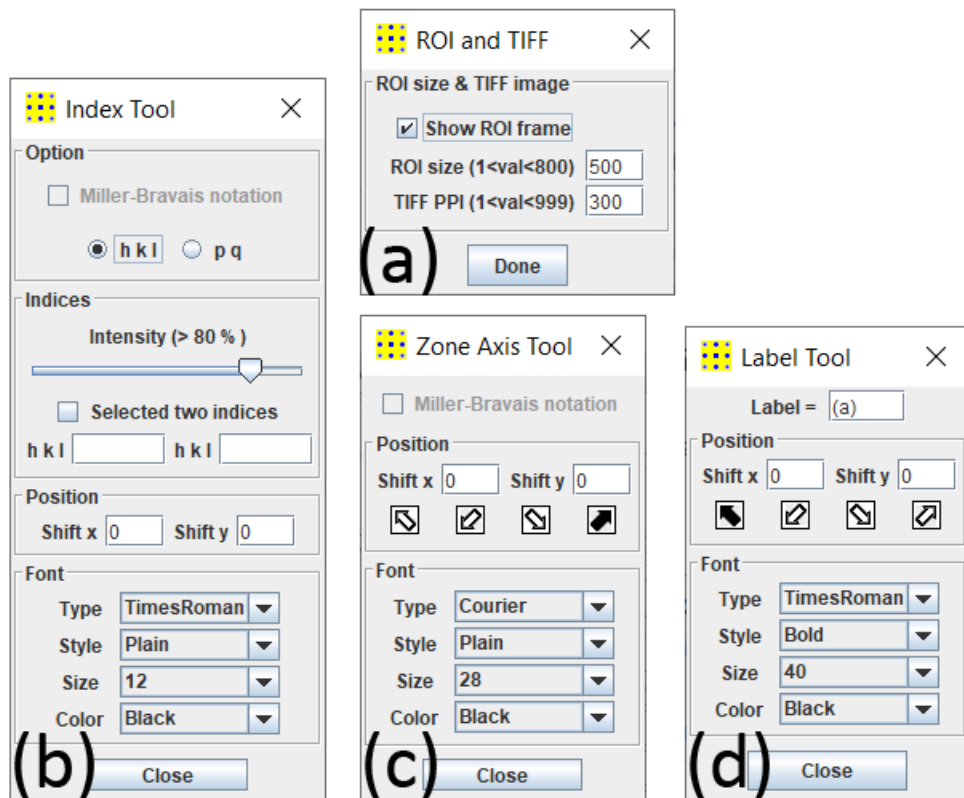This converter was built to convert between Miller and Miller-Bravais indices, as shown in Figure 6.

Figure 7. Snapshot of the tools for labeling a simulated pattern.

4.4 Sava figures for publication

Together with experimental images, these simulated patterns can be saved to images, which are ready for publication. Figure 7 shows the tools of (a) region of interest, (b) index, (c) zone axis, and (d) figure label. The option of hkl is the indices based on the vectors of the reciprocal lattice and the option of the pq is the indices based on the vectors of this diffraction pattern (for ESPOT). An example in Figure 1 is to show a simulated image within a region ready for saving in .tif, .jpg, or .gif formats.

4.5 Determination of zone axis and indexing

SAED can be used to determine the zone axis of an experimental diffraction pattern if it belongs to one of the known structures which were loaded into the structure list.

Experimental diffraction pattern (in JPEG, PNG or TIFF format) can be loaded and centered by drag and drop operation in Figure 8. Gray contrast can be converted if needed. Figure 9 shows the [uvw] finder dialog window.
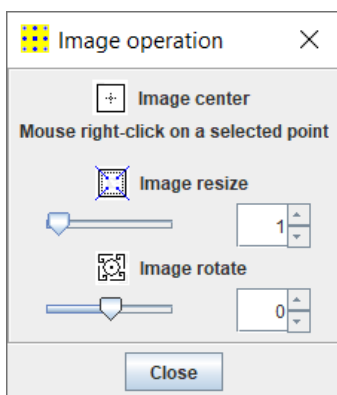

Figure 8. Experimental diffraction pattern (JPEG, PNG or TIFF format) can be loaded and centered by drag and drop operation.

Step 1. Update the match factor. Use a **Scale marker** to calibrate the simulated pattern to match with the experimental one (or a single diffraction spot/ring). The match factor can be saved, so it does not need to be calibrated all the time as soon as the same experimental conditions were used.

Step 2. Find the basic reciprocal vectors g1 and g2; the length can be labeled in (1/Å).

Step 3. Define the tolerance value (default as 5%) and find
the possible zone axis. The one with the least mismatching residue is shown, and the whole list can be saved to a text file.
The tolerance value is defined as the maximum of percent errors: V_e = experimental value and V_k = known value,
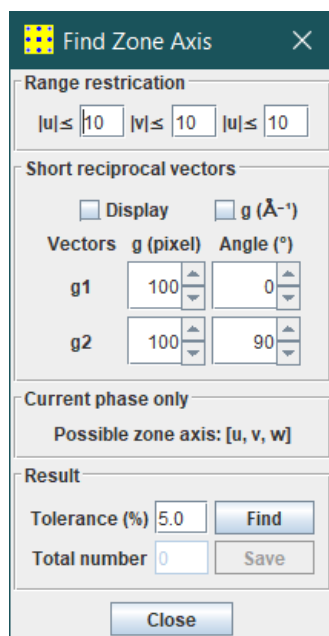
$$\text{Percent error} = (V_e - V_k)/ V_k \times 100\%.$$

Figure 9. Snapshot of the [uvw] finder.

Step 4. The zone axis is obtained by matching the reciprocal length and angle between them. The zone axis should be confirmed by comparing a simulated pattern to the experimental one.

Step 5. The list of all possible zone axes within the tolerance can be saved to an ASCII text file. The zone axes, the measured g1 and g2 and angle, and their percentage errors are listed in the file.

5. Special topics on SAED

5.1 Partial occupancy factor and isotropic temperature factor

Some atom coordinates maybe not be in full occupancy in a crystalline structure. In this case, the occupancy factor (default value 1.0) should be changed to the values according to the crystalline structure in preparation of the structure data file for electron diffraction simulation.

The partial occupancy factor can also be used to simulate a certain level of chemical order in structure. For example, the chemical ordered FePt $L1_0$ phase, see section 6. In this case, a different type of atoms may be assigned to the same atomic coordinates with a different occupancy according to the chemical ratio, but the sum of the occupancy factors of the two atoms is 1.0.

The Isotropic temperature factor is used here to simulate the effect of lattice vibration (Debye model). Although the isotropic temperature factor is a rough model, it can be used to simulate the decrease of the diffraction intensity with the variation of the |g| value. The higher the value of |g|, the more decrease of the diffraction intensity.

5.2 Load and align EDP

Experimental electron diffraction patterns can be loaded up and centered for analysis and compare with simulated patterns. The experimental pattern in jpeg (.jpg) and tiff (.tif) formats can be loaded using the window file system or the drag-and-drop box in the graphic menu bar. The experimental pattern can be processed, e.g., invert, resize and rotate, and then center by using **Center** in the **Experiment** menu. Once the **Center** is clicked, five concentric circles will appear in the main panel. The pattern can be adjusted into the center of the panel by selecting the center of the pattern while holding the left button of the mouse; Click the Center in the **Experiment** menu, the pattern is locked up in the position, and concentric circles disappear. More adjustments in small steps may be needed to find the accurate position. The number of concentric circles can be changed using the **Number of Reference Circle** in the **Option** menu.

5.3 Determination of weight ratio of a multiple-phase system

The SAED program provides a way to roughly estimate the weight ratio of a composite diffraction pattern of multiple phases. Adjust the mass proportion mp(i) of each phase to match the relative intensities of its diffraction pattern to experimental patterns, then the final mass ratio of phase i is,

$$\frac{mp(i)}{\sum_i mp(i)}$$

5.4 Simulation of twins，precipitation, and coexisted multiple phases

Electron diffraction patterns of twins can be simulated using SAED. To generate twining diffraction patterns, the same structure data needs to be loaded multiple times according to the number of twin components. In reciprocal space, the twin patterns may be generated by rotation, mirror, or inverse operations. For the rotation twin, the twinning component can be rotated in the calculation control panel. For reflection twin, the twining component can be reflected at the horizontal mirror and then rotated to the requested angle. For inversion twin, the twin component can be calculated using zone axes of [uvw] and [-u,-v,-w]. Similarly, we can load the data of the coexisted multiple phases or the data of the precipitation and matrix, then make the simulation of each phase and make the adjustment to match the experimental electron diffraction patterns.

6. Examples

6.1 Pt-Bi thin film

There has been significant interest in exploring the properties of Pt-Bi based compounds due to their exceptional performance as fuel-cell anode catalysts for the oxidation of formic acid (HCOOH) or methanol (CH3OH). While platinum (Pt) is highly effective as a catalyst, a major drawback is its susceptibility to poisoning by carbon monoxide (CO), a byproduct of the reaction. CO adsorption on the electrode surface diminishes catalytic activity and overall cell efficiency.

Recent studies indicate that using ordered intermetallic compounds like PtBi as electrode materials can significantly enhance cell efficiency while markedly reducing CO adsorption. This improvement is attributed to the unique properties of PtBi, which mitigate the adverse effects of CO poisoning, thereby enhancing the performance and longevity of fuel-cell systems.
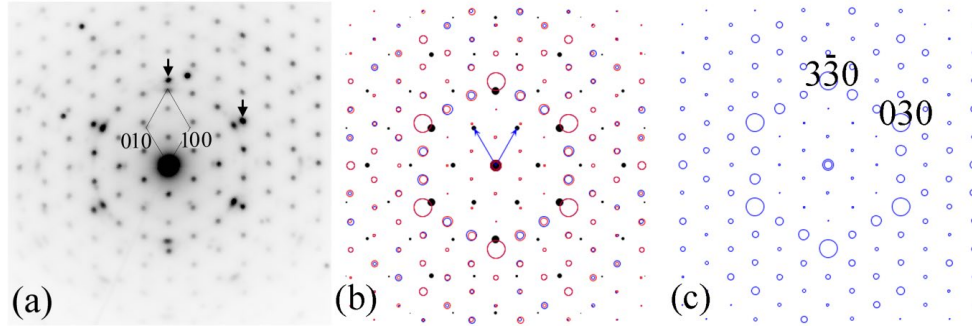

Figure 10. SAED pattern of Pt-Bi thin film, which consists of the twin of γ-PtBi$_2$ and coexisted hexagonal PtBi phase, (a) experimental electron diffraction pattern (EDP), (b) simulated EDP, and (c) simulated EDP with a single phase of γ-PtBi$_2$.
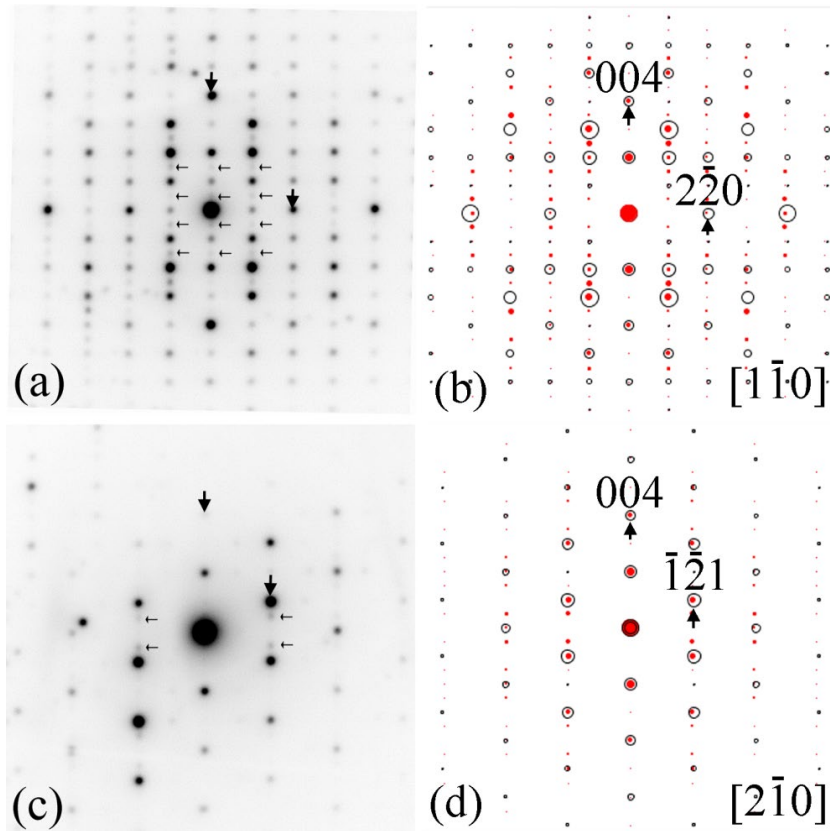

Figure 11. (a, c) experimental electron diffraction patterns of Pt-Bi thin film, which consists of γ-PtBi$_2$ and β-PtBi$_2$, (b, d) the simulated EDP.

The three common intermetallic compounds based on Pt and Bi are PtBi, PtBi$_2$ and Pt$_2$Bi$_3$. Equiatomic PtBi phase is at the low temperature side of the phase diagram and may be off-

stoichiometric towards Pt-rich side. $PtBi_2$ has four polymorphs namely α-$PtBi_2$(oP24), β-$PtBi_2$(cP12), γ-$PtBi_2$(hP9) and δ-$PtBi_2$ (oP6) from low to high temperature in equilibrium phase diagram. PtBi and Pt_2Bi_3 adopt the hexagonal NiAs structure (PtBi: a = 4.3240 and c = 5.501 Å; Pt_2Bi_3: a = 4.13 and c = 5.58 Å) whereas the three polymorphs of $PtBi_2$ crystallize in the $AuSn_2$ type Orthorhombic (α-$PtBi_2$: a = 6.732, b = 6.794 and c = 13.346 Å), FeS_2 cubic pyrite (β-$PtBi_2$: a = 6.701 Å), and trigonal (γ-$PtBi_2$: a = 6.57, and c = 6.16 Å) crystal structures, respectively.

PtBi and $PtBi_2$ films were synthesized on glass and thermally oxidized silicon substrates by e-beam evaporation and annealing. TEM analysis shows that the films prepared by post-deposition annealing of 300 °C and 400 °C are mostly polymorphic $PtBi_2$ with a small trace of PtBi. Although TEM analysis shows a signature of β-phase $PtBi_2$, the γ-phase is the dominant phase in these samples. The PtBi and $PtBi_2$ samples are textured, but the γ-$PtBi_2$ films are highly c-axis oriented, where the c-axis is perpendicular to the film plane. Figure 10. shows (a) experimental electron diffraction pattern of Pt-Bi thin film, which consists of the twin of γ-$PtBi_2$ and coexisted hexagonal PtBi phase, (b) the simulated EDP in comparison with (c) simulated EDP with a single phase of γ-$PtBi_2$. The orientation relationship between the γ-$PtBi_2$ and the PtBi phases is

[001] γ-$PtBi_2$ //[001] PtBi
(100) γ-$PtBi_2$ //(110) PtBi

Figure 11. shows (a, c) experimental electron diffraction patterns of Pt-Bi thin film, which consists of β-$PtBi_2$ and α-$PtBi_2$, (b, d) the simulated EDP.

6.2 Cu_2S nanofiber

Hierarchical nanostructures, particularly core-branch heterostructures where nanowires or nanorods extend from a central nanowire or nanofiber core, are gaining increasing attention for their applications in optics, electronics, sensing, and other fields. These structures, composed of different materials in the core and branches, offer tailored properties, high surface-to-volume ratios, and significant nanowire-to-base ratios, promising novel functional membranes.

In our recent work, we have developed a novel hierarchical architecture featuring inorganic Cu_2S nanowires grown on organic polyacrylonitrile (PAN) nanofibers. This architecture was achieved through a combination of electrospinning and room-temperature gas-solid diffusion-assisted chemical growth techniques.

The produced Cu_2S nanowires measure 1.5 to 1.8 μm in length with a uniform diameter of approximately 80 nm (Figure 12a). Experimental Electron Diffraction Patterns (EDPs) of single nanowires confirm their crystalline phase as monoclinic Cu_2S. The EDPs indicate that the growth direction of the nanowires is perpendicular to the (2,0,-4) crystal plane, parallel to the monocrystal c axis (Figure 12b, 12c). Interestingly, the growth of the nanowires appears to precede the formation of a Cu_2S sheath on the surface of the PAN nanofibers.

This innovative hierarchical architecture not only demonstrates controlled nanowire growth but also opens avenues for exploring advanced applications in nanotechnology and material sciences.
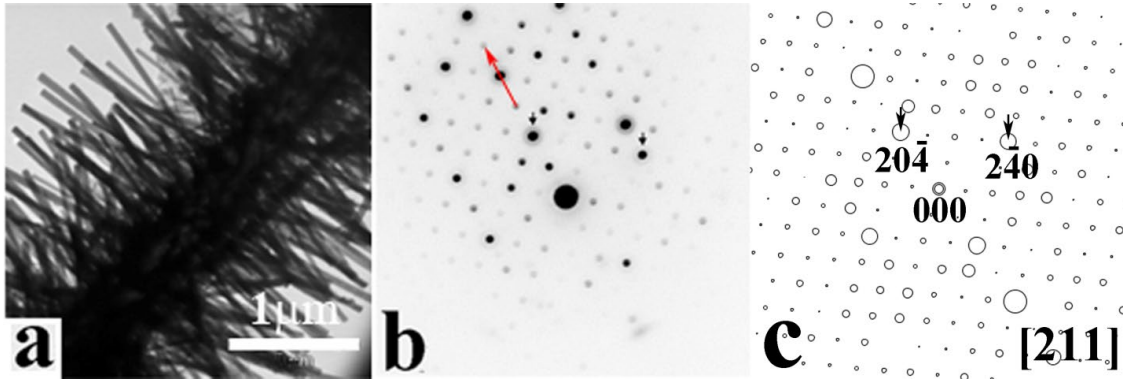
Figure. 12. TEM images of the hierarchical structure (a). Experimental EDPs of the Cu$_2$S nanowires (b), arrows show the nanowire growth direction and corresponding simulated patterns of monoclinic Cu$_2$S crystal structure (c).

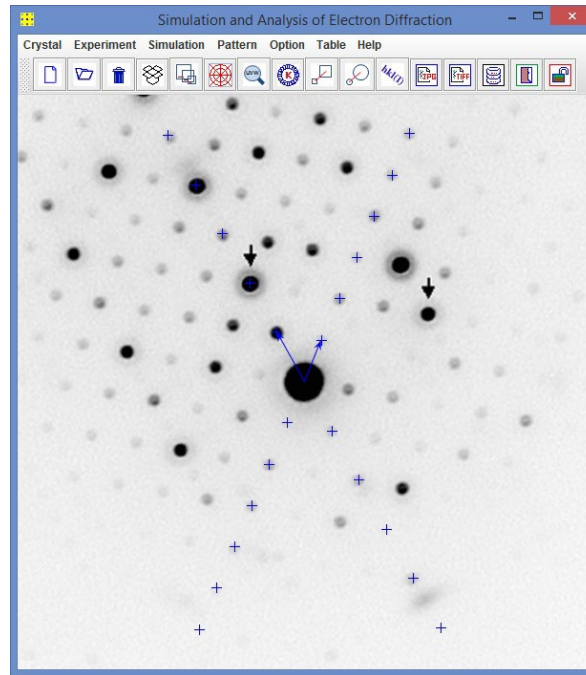

Figure. 13. Measurement of basic reciprocal vectors in the experimental EDP of Cu$_2$S nanofiber.

The basic reciprocal vectors for the experimental EDP are measured, as shown in Figure 13. The calibrated matching factor and basic reciprocal vectors for the experimental EDP are listed in Figure 14. The tolerance is chosen as 5%. The possible zone axis is found to be [2 1 1], and there are seven possible zone axes, which can be saved to a file. Figure 15 shows the simulated pattern of [2 1 1] zone axis matches well with the experimental EDP; thus, the zone axis and index of the EDP are determined.

Figure 14. Matching factor and g lengths and angles of the basic reciprocal vectors. The possible zone axis is found to be [2 1 1] with a tolerance of 5%.
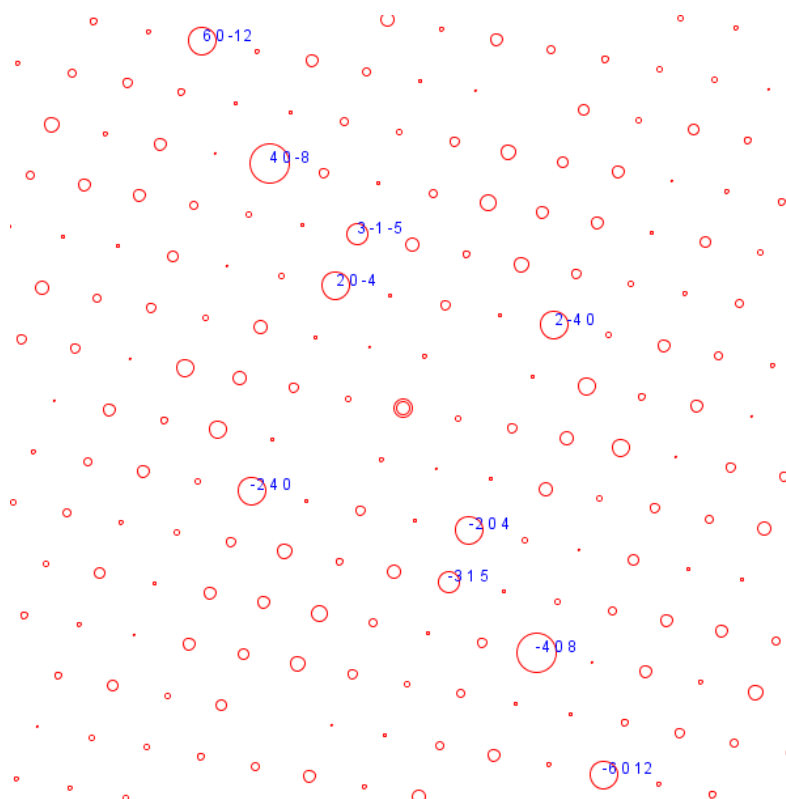

Figure. 15. Simulated EDP of Cu$_2$S with zone axis [2 1 1].

7. Related programs: SVAT, SPICA, PCED, SAKI, and ESPOT

All programs in the Landyne suite use the input structure data in the same format. A few of them are listed here, which can be used in combination with SAED. Users may check the program specification or user manual for each program in detail.

7.1 SVAT

The need for a structure visualization/an analytical tool, using the same input data format in the Landyne suite, becomes obvious with the growth of the programs and users.

7.2 SPICA

SPICA is the next version of early JECP/SP, which was designed for stereographic projection with an application for specimen orientation adjustment using TEM holders. SPICA3 inherits JECP/SP functions and extends to many new functions for crystallographic analysis with a more user-friendly GUI design.

7.3 PCED

PCED is an upgraded version of the previous JECP/PCED. New features include (i) Blackman's theory, an integral two-beam dynamical theory, for intensity calculation, (ii) Match model for out-of-plane and in-plane texture, (iii) pseudo-Voigt function for peak profile of diffraction ring, and (iv) improvement on diffraction pattern indexing and matching to an experimental pattern.

7.4 SAKI

SAKI can be viewed as an extension of the SAED. SAKI can be used to simulate the Kikuchi pattern and double diffraction effect; SAKI can also be used to determine the precise orientation of a crystal using three pairs of Kikuchi lines.

7.5 ESPOT

ESPOT is an extension of SAED for generating an electrostatic potential (difference) map of a crystal structure. SAED provides the calculated diffraction data for ESPOT. The experimental diffraction data for ESPOT can be generated using QSAED.

Reference:

Humphreys, C.J., The scattering of fast electrons by crystals, Rep. Prog. Phys., 42 (1970) 122.

Li, X.Z., PCED2.0 - A computer program for advanced simulation of polycrystalline electron diffraction pattern. Ultramicroscopy 110 (2010) 297-304.

Li, X.Z., SAED3: simulation and analysis of electron diffraction patterns. Microscopy and Analysis, May issue (2019) 16-19.

Li, X.Z. SVAT4: a computer program for visualization and analysis of crystal structures. Journal of Applied Crystallography 53 (2020) 848-853.

Metherell, A.J.F., Diffraction of electrons by perfect crystals, Microscopy in Materials Science II, ed. by Valdre, U. and Ruedl, E., CEC Brussels, 1975.

Peng, L.M., Dudarev, S.L., and Whelan, M.J., High Energy Electron Diffraction and Microscopy, Oxford University Press, 2004.

Peng, L.M., Ren, G., Dudarev, S.L., and Whelan, M.J., Robust Parameterization of Elastic and Absorptive Electron Atomic Scattering Factors, Acta Cryst. A52 (1996) 257.

Self, P.G., O'Keefe, M.A., Buseck P.R., Spargo, A.E.C. Practical computation of amplitudes and phases in electron diffraction, Ultramicroscopy 11 (1983) 35-52.