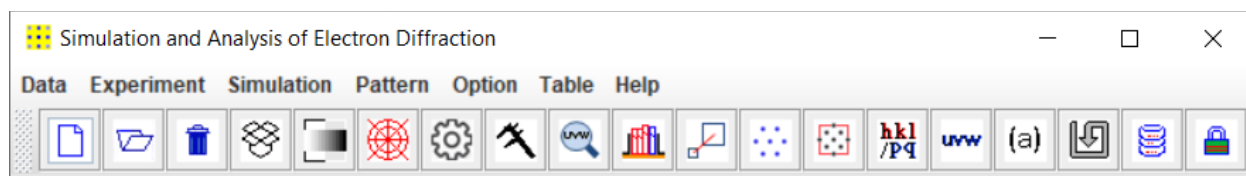


***LANDYNE***

# **User Manual**

Simulation and Analysis of Electron Diffraction Pattern

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## Highlights

1. A window frame with a panel is used to show the simulated pattern or match the preloaded experimental diffraction pattern.
2. Input parameters for the calculation can be initialized with an operational panel and several dialog windows.
3. Input structure data files can be easily prepared using a computer assistant.
4. Multiple phases can be loaded and calculated simultaneously to simulate the diffraction patterns for twins, coexisted phases with a fixed orientation, and for comparison of the similar patterns from a different phase.
5. An experimental pattern can be aligned, resized, and rotated.
6. Label tools are available to prepare figures for publication.

### 1. Introduction

Selected area electron diffraction analysis has been extensively used in materials science for phase identification, determination of structural intergrowth and growth directions, e.g. twin relation and fixed orientation of co-existing multiple phases.

Due to a much stronger interaction of electrons with matter compared to X-rays, electron diffraction has non-negligible advantages and disadvantage in comparison with X-ray diffraction. On one hand, nano-objects that are too small for conventional X-ray diffraction experiment and would have to be taken to a synchrotron can be studied in the laboratory by electron diffraction. Moreover, electron diffraction patterns can show reflections corresponding to a resolution beyond that available with X-rays for light atoms. On the other hand, the much stronger interaction of electrons with matter as well as very small diffraction angles also cause strong dynamical diffraction effects, such as multiple diffraction, which hinder structural interpretation of electron diffraction patterns.

Simulation of electron diffraction patterns plays a vital role in interpreting experimental results. 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 for advanced simulation and analysis of electron diffraction patterns. PCED4 is for selected-area electron diffraction patterns of polycrystalline samples. SAED is for selected-area electron diffraction patterns of single-crystal samples.

Software current available for simulation of electron diffraction is primarily designed for a single-phase only. For advanced simulation and analysis of electron diffraction patterns, the functionalities in such software are not enough, for example, in the analyses of twinning, coexisted multiple phases with a fixed orientation, and the comparison of two similar diffraction patterns from different phases. A practical task in electron diffraction analysis is to find the zone axis of the diffraction pattern and indexing; such an analysis can be used for phase identification, the orientation of a crystal grain, *et cetera*. A projected atomic potential (difference) map can be

used to interpret the HREM structural image and improve a structural model; the tasks are treated as an extension in PAPM. Thus, we have developed SAED; the current version is 6.

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]

SAED was written and compiled in Java 8. 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 the textbooks (e.g., Peng *et al.*, 2004, other books on electron diffraction theory) and literature references (e.g., Metherell, 1975).

The electron atom scattering 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  $\mathbf{g}(hkl)$  as

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

where  $L$  is the camera length,  $d=1/|\mathbf{g}(hkl)|$  and  $\lambda$  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:

$$I_g \propto |F_g|^2 \quad (2)$$

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***

Based on their diffraction patterns, twinned crystals may be grouped into three general categories. *Non-merohedral* twins have two or more crystalline domains with reciprocal lattices that either do not overlap or only partially overlapped. In contrast, *Merohedral* twins have domains with diffraction patterns that are completely overlapped. For merohedral twins, the symmetry operations relating the twinned domains are part of the sample's Laue group but are not a part of the space group. *Pseudo-merohedral* also has domains with completely overlapped diffraction patterns, but the symmetry operation relating to the domains is not part of the sample's Laue group.

Two phases or more may coexist with a fixed orientation relationship in a complex alloy system. Electron diffraction analysis can be used to determine the orientation relationship. Precipitates may have a fixed orientation with the matrix. To study the precipitates, it usually tilts the matrix to get a particular orientation of the precipitates since the precipitates are small particles.

For twins and multiple coexisting phases, the electron diffraction pattern simulation requires to be calculated based on multiple structures in one frame. SAED is designed to calculate the patterns from multiple structures one by one and easily adjusted any patterns to simulate the patterns from twins and multiple structures coexisted with a fixed orientation.

## ***2.3 Determination of a zone axis and indexing***

A practical task in electron diffraction analysis is to find the zone axis of the diffraction pattern and indexing; such an analysis can be used for phase identification, the orientation of a crystal grain, *et cetera*.

SAED provides tools to measure the scale bar and to measure two basic reciprocal vectors' lengths and the angles between them on a diffraction pattern in jpeg or tiff format.

The two basic reciprocal vectors' lengths are matched to all possible (hkl) with a given tolerance. Then the angle between the two basic reciprocal vectors is checked, one of the zone axes with the least mismatch values is listed out, and possible zone axes can be saved to a file.

Since only the tolerance of reciprocal lengths is defined in the Find Zone Axis dialog, the angle is checked by the reciprocal length of the third edge in the triangle formed by the two basic reciprocal vectors.

### 3. The graphic user interface of SAED

#### 3.1 Main interface

The main interface of SAED is shown in Fig. 1. The usage of SAED for simulation needs to load structure data and to set up input parameters, then click the **Calculate** button in the **Calculation** control panel. The usage of SAED for zone axis search or phase identification needs to load experimental diffraction pattern first and then find zone axis and then match the calculated patterns by chosen structure data and input parameters. Multiple structure data can load simultaneously for comparison or simulation of various twins and coexisted structures with a fixed orientation.

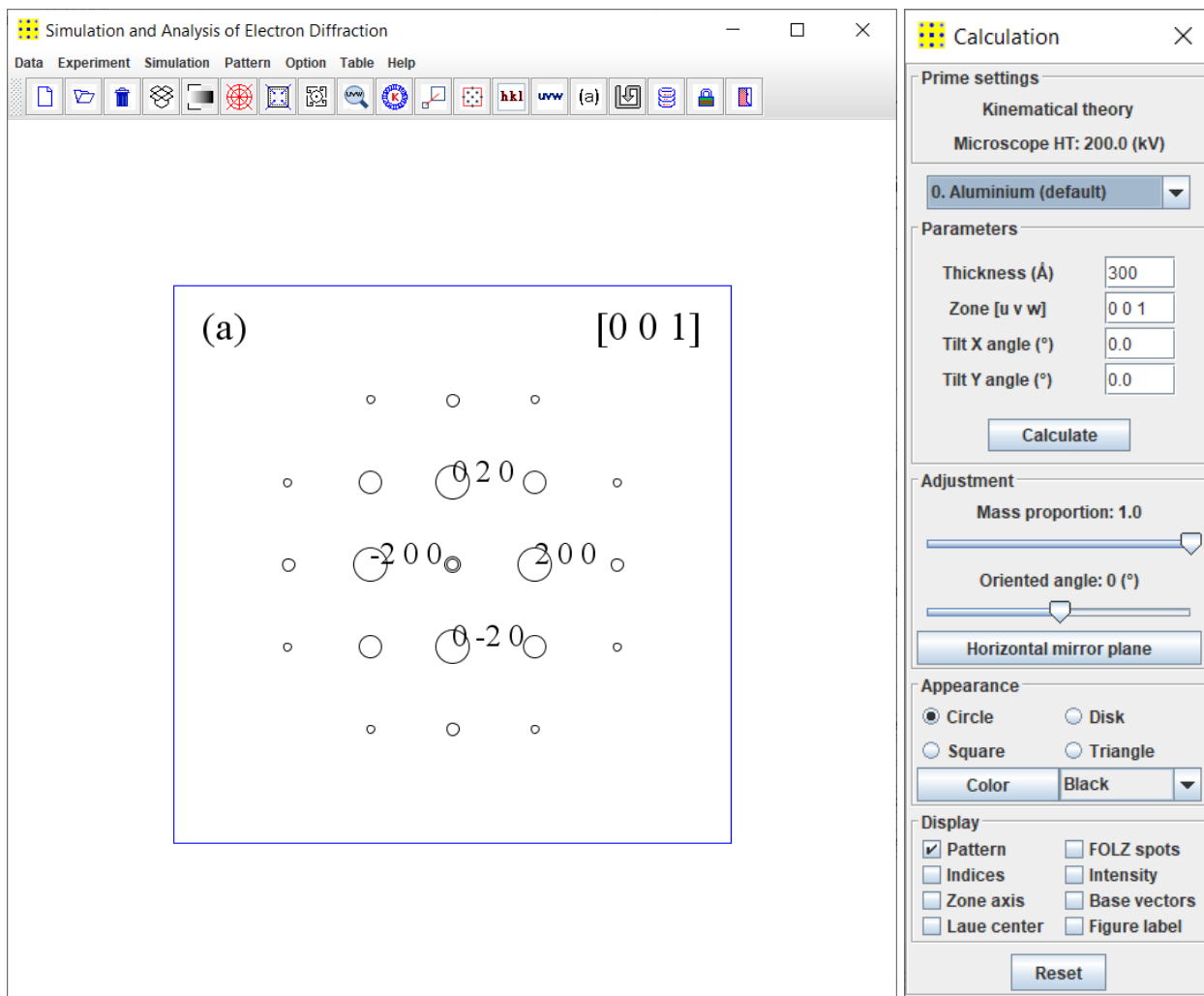


Figure 1. Snapshot of the main panels in SAED, a simulation of an electron diffraction pattern of Aluminum along [001] zone axis.

#### 3.2 Menu and toolbar

Menu and toolbar can be used to pop up dialogs for loading data or changing parameters. The menu gives more text descriptions and organizes in groups, while the toolbar shows in graphics and easy access.

**Crystal menu** provides an interface for creating the new structure data, loading the input structure (the same structure can reload for twins), and clearing all the loaded structures except the default (Al) structure.

**Experiment menu** provides an interface for loading experimental electron diffraction pattern (EDP) in JPEG and TIFF format. The loaded SAED pattern (image) can be set in inversed contrast or cleanup. The image can be resized and rotated and shifted/centered by drag-and-drop action, referring to a set of concentric circles and lines. Loading image by drag-and-drop: selecting an image file by the mouse pointer, press down the left button of the mouse, drop to the drop-box icon on the menu bar, and release the left button of the mouse. The position of the image can be set up in the **Image Operation** dialog, as shown in Fig. 2. A caliper is to adjust the reciprocal spacing using the scale bar in the experimental SAED pattern, as shown in Fig. 3. **Find [uvw]** provides a dialog for finding the basic reciprocal vectors of the EDP, and then the [uvw]. A zone axis with the least mismatching residue is shown, and detailed info on a list of all possible zone axes can be saved to a text file.

**Simulation menu** provides a submenu for the choice of theories between kinematical and dynamical diffraction theories. The default choice is the kinematical diffraction theory. The dynamical calculation may not be suitable for a crystal with a large unit cell since it will take a very long time in the Bloch wave method. The high voltage of the microscope and the maximum of the index number for the calculation can be set up. A dialog window for adjusting the pattern zoom and intensity scale simulates the camera length and exposure time and a dialog window for selecting the label of diffraction spots (reflections). The label on reflections can be used to select the scheme for index and intensity. Weak diffraction spots can be rescaled to a constant, or it can also be chosen to show reciprocal lattice only.

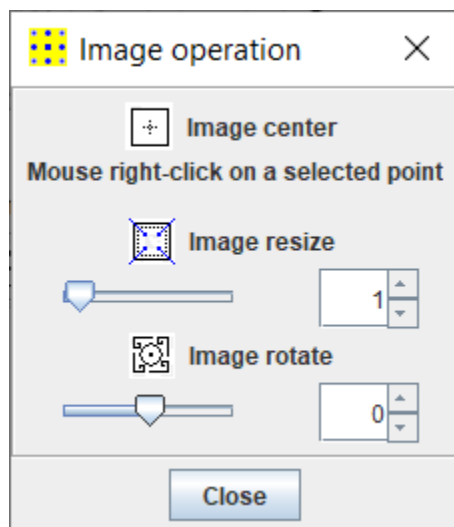


Figure 2. Snapshot of the supporting panels in SAED for analysis of experimental SAED patterns.



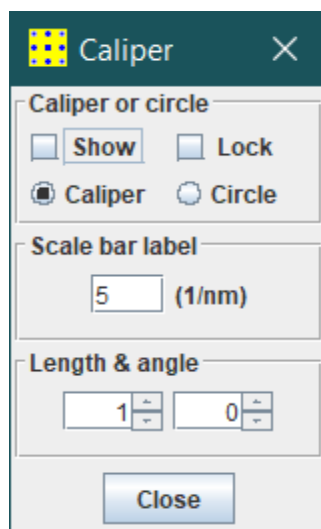


Figure 3. Snapshot of Caliper panel for adjusting the reciprocal spacing to the scale bar on the experimental SAED pattern.

**Pattern menu** provides a dialog for ROI and PPI; the simulated patterns can be saved as output files in JPEG 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 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 trial model. Contact Landyne for purchasing the license file.

#### 4. Usage of SAED

To run SAED, a user may use (1) Landyne launcher or (2) double click the icon of SAED.jar or (3) 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, similar to 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

A structure data file can be prepared using the **New Crystal Structure File** dialogue window in Figure 4. The dialogue window provides an automatic assistant for the user and makes sure to meet the requirement of the file format. The template is embedded with the 230 space groups in the Hermann-Mauguin notation, which list in the international table for crystallography. However, only b unique axis will be used in a monoclinic system. Two origin choices can be accepted as input parameters, but choice-2 will be converted to choose-1. To save the data structure, click the **Save** button; or make a new one click the **New** button.

The crystal file can be also converted from a previous data for modification or from a crystallographic information file (CIF). If a data file in an alternative setting of space group for triclinic, monoclinic and orthorhombic systems is used, please click on the alternative settings (1~74). A tool for the transformation of files in the nonconventional notations to the standard notations is provided.

**New Crystal Structure File**

Description  
New crystal structure

Space group  
☒ The standard settings (1~230) ☐ The alternative settings (1~74)  
Number 1~230 Symbol ? Origin [dropdown]

Lattice parameters  
a = [ ] (Å) b = [ ] (Å) c = [ ] (Å) α = [ ] (°) β = [ ] (°) γ = [ ] (°)

Coordinates of Atoms

atom	elem #	x	y	z	occ.
		0.0	0.0	0.0	1.0

Add Remove Clear View

Number of atom in the list: 0 Global isotropic temperature factor 0.0

Notes  
References etc.

New Load Save Close

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

#### 4.2 Simulation

Kinematical diffraction theory (default selection) and dynamical diffraction of Bloch wave theory are used in the simulation. Basic parameters for calculation, e.g., high voltage, pattern zoom, and intensity scale, can be adjusted in the **Simulation** menu.

The calculation in Bloch wave theory may take time for a crystal structure with relative large lattice parameters. In order to save the time, (i) the software provides an option for user to terminate the calculation process when the result is good enough or continue the calculation, as shown in Figure 5; (ii) the software will use previous calculated parameters to simulate a diffraction pattern when only the thickness is changed.

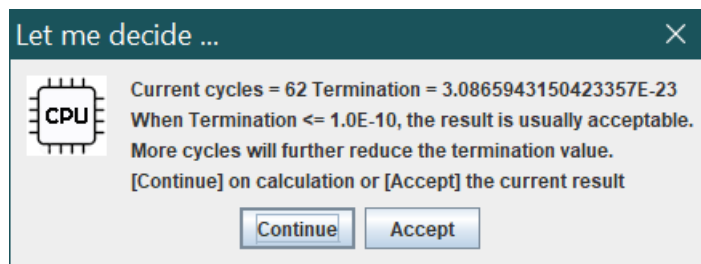


Figure 5. Snapshot of an option for user to terminate or continue the calculation.

A structure data for calculation should be selected in a list of loaded structure data. After choosing the thickness, zone axis, tilt angles to generate a new diffraction pattern, needs to click the **Calculate** button. The pattern can be adjusted by changing other parameters.

**Mass proportion** defines the same unit weight for all loaded structures as the default value. Mass proportion is meaningful only when two or more structural data are calculated at a composite diffraction pattern.

**Orientation and mirror operation** is used to orient the simulated pattern to match the experimental pattern and generate various twins.

**Diffraction Patterns** can be viewed with four predefined shapes and in various colors. Pattern (ZOLZ and FOLZ) can be displayed or hidden. Index and intensity can be labeled for basic reciprocal vectors and for diffraction spots selected by the intensity level. Basic vectors and Laue center can be displayed and hidden.

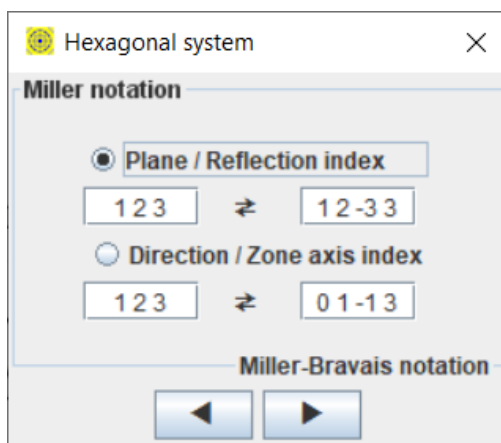


Figure 6. Miller-Bravais converter for hexagonal system.

#### 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

$$U = u-t; u = (2U-V)/3$$

$$V = v-t; v = (2V-V)/3$$

$$W = w; t = -(U+V)$$

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

#### 4.4 Save 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.

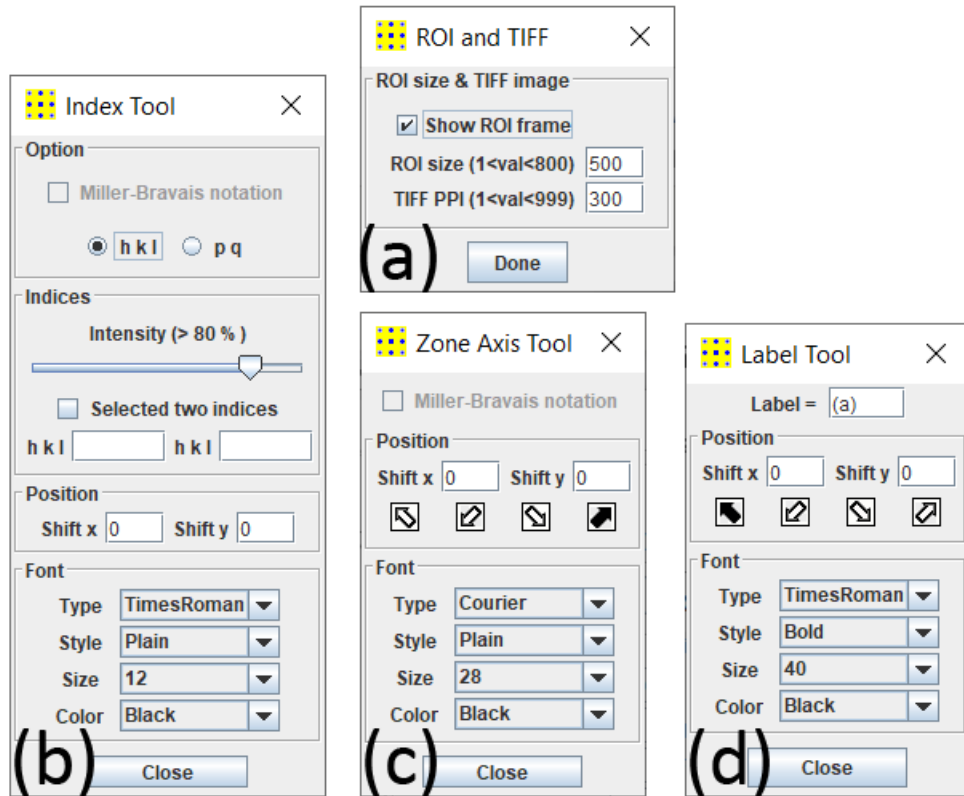


Figure 7. Snapshot of the tools for labeling a simulated pattern.

#### 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 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.

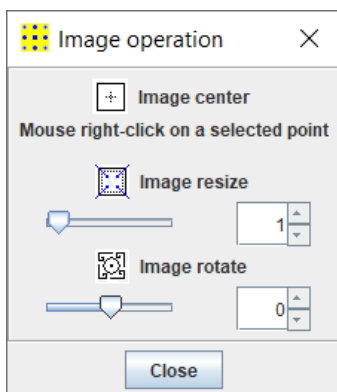


Figure 8. Experimental diffraction pattern (JPEG or TIFF format) can be loaded and centered by drag and drop operation.

**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 time as soon as the same experimental conditions were used.

**Step 2.** Find the basic reciprocal vectors  $g_1$  and  $g_2$ ; the length can be labeled in ( $1/\text{\AA}$ ).

**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,

$$\text{Percent error} = (V_e - V_k) / V_k \times 100\%.$$

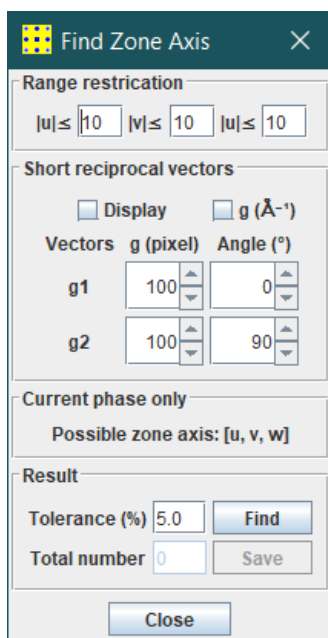


Figure 9. Snapshot of the [uvw] finder.

**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  $g_1$  and  $g_2$  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 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 center 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. In order to generate twinning 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 twinning 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 considerable interest in understanding various properties of Pt-Bi based compounds because of their high activity as fuel-cell anode catalysts for formic acid (HCOOH) or methanol (CH<sub>3</sub>OH) oxidation. Although Pt is regarded as one of the most efficient catalyst materials, the main problem with this conventional catalyst is that it is readily poisoned by carbon monoxide (CO) that is produced as a side product of the reaction. CO poisoning reduces the catalytic activity and cell efficiency because it remains firmly bound to the electrode surface. However, some recent reports show that the use of ordered intermetallic compound such as PtBi

as an electrode material exhibits an improved cell efficiency with a dramatic reduction in the CO adsorption.

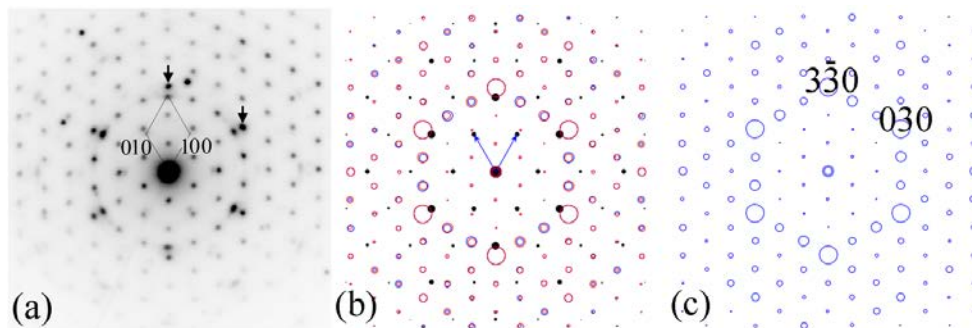


Figure 10. SAED pattern of Pt-Bi thin film, which consists of the twin of  $\gamma$ -PtBi<sub>2</sub> and coexisted hexagonal PtBi phase, (a) experimental electron diffraction pattern (EDP), (b) simulated EDP, and (c) simulated EDP with a single phase of  $\gamma$ -PtBi<sub>2</sub>.

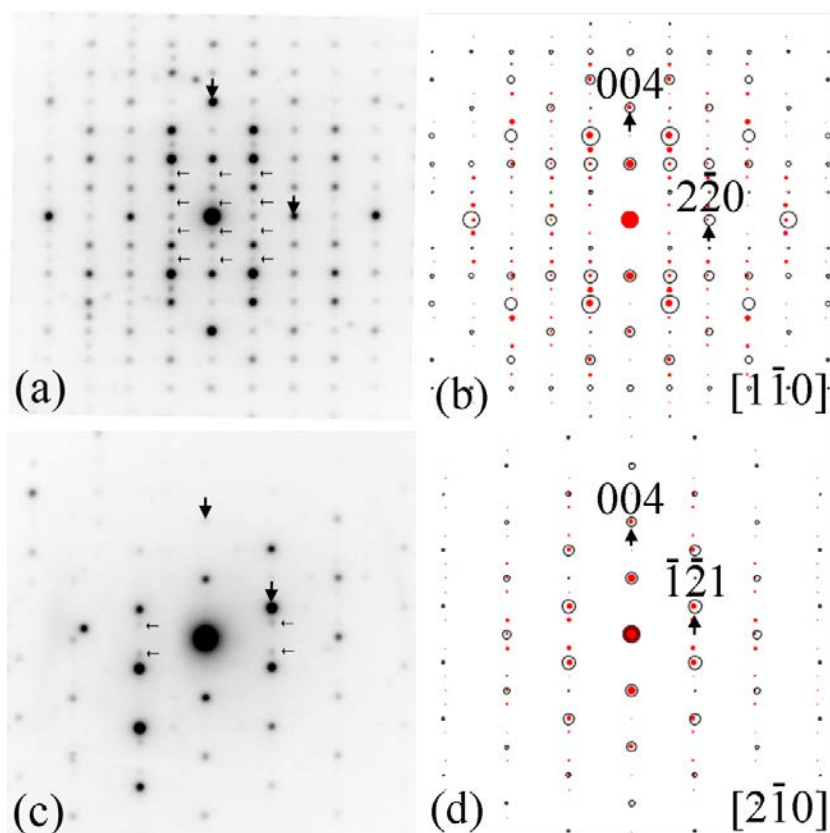


Figure 11. (a, c) experimental electron diffraction patterns of Pt-Bi thin film, which consists of  $\gamma$ -PtBi<sub>2</sub> and  $\beta$ -PtBi<sub>2</sub>, (b, d) the simulated EDP.

The three common intermetallic compounds based on Pt and Bi are PtBi, PtBi<sub>2</sub> and Pt<sub>2</sub>Bi<sub>3</sub>. Equiatomic PtBi phase is at the low temperature side of the phase diagram and may be off-stoichiometric towards Pt-rich side. PtBi<sub>2</sub> has four polymorphs namely  $\alpha$ -PtBi<sub>2</sub>(oP24),  $\beta$ -PtBi<sub>2</sub>(cP12),  $\gamma$ -PtBi<sub>2</sub>(hP9) and  $\delta$ -PtBi<sub>2</sub>(oP6) from low to high temperature in equilibrium phase



diagram. PtBi and Pt<sub>2</sub>Bi<sub>3</sub> adopt the hexagonal NiAs structure (PtBi:  $a = 4.3240$  and  $c = 5.501$  Å; Pt<sub>2</sub>Bi<sub>3</sub>:  $a = 4.13$  and  $c = 5.58$  Å) whereas the three polymorphs of PtBi<sub>2</sub> crystallize in the AuSn<sub>2</sub> type Orthorhombic ( $\alpha$ -PtBi<sub>2</sub>:  $a = 6.732$ ,  $b = 6.794$  and  $c = 13.346$  Å), FeS<sub>2</sub> cubic pyrite ( $\beta$ -PtBi<sub>2</sub>:  $a = 6.701$  Å), and trigonal ( $\gamma$ -PtBi<sub>2</sub>:  $a = 6.57$ , and  $c = 6.16$  Å) crystal structures, respectively.

PtBi and PtBi<sub>2</sub> 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<sub>2</sub> with a small trace of PtBi. Although TEM analysis shows a signature of  $\beta$ -phase PtBi<sub>2</sub>, the  $\gamma$ -phase is the dominant phase in these samples. The PtBi and PtBi<sub>2</sub> samples are textured, but the  $\gamma$ -PtBi<sub>2</sub> 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  $\gamma$ -PtBi<sub>2</sub> and coexisted hexagonal PtBi phase, (b) the simulated EDP in comparison with (c) simulated EDP with a single phase of  $\gamma$ -PtBi<sub>2</sub>. The orientation relationship between the  $\gamma$ -PtBi<sub>2</sub> and the PtBi phases is

$$\begin{aligned} &[001] \gamma\text{-PtBi}_2 // [001] \text{PtBi} \\ &(100) \gamma\text{-PtBi}_2 // (110) \text{PtBi} \end{aligned}$$

Figure 11. shows (a, c) experimental electron diffraction patterns of Pt-Bi thin film, which consists of  $\beta$ -PtBi<sub>2</sub> and  $\alpha$ -PtBi<sub>2</sub>, (b, d) the simulated EDP.

## 6.2 Cu<sub>2</sub>S nanofiber

Hierarchical nanostructures are increasingly attractive for application in optics, electronics, sensing, *et cetera*. Specifically, core-branch heterostructures (i.e., branches of nanowires or nanorod on a central nanowire or nanofiber core), having core and branches composed of different materials, allow targeted properties of the nanowires and the base, offer high surface-to-volume ratio and nanowire-to-base ratio, and bring the promise of novel functional membranes. A novel hierarchical architecture in our recent work, inorganic Cu<sub>2</sub>S nanowires standing on organic polyacrylonitrile (PAN) nanofiber, has been produced by combining the electrospinning technique and room-temperature gas-solid diffusion-assisted chemical growth.

The produced nanowires are 1.5~1.8  $\mu\text{m}$  long with a uniform diameter of about 80 nm (Figure 12a). The single nanowires' experimental EDPs match the monoclinic Cu<sub>2</sub>S crystal phase. They indicate that the nanowires' growth direction is perpendicular to the (2,0,-4) crystal plane, i.e., parallel to the monocrystal c axis (Figure 12b, 12c). The nanowires' growth seems to precede the formation of Cu<sub>2</sub>S sheath on the nanofibers' surface.

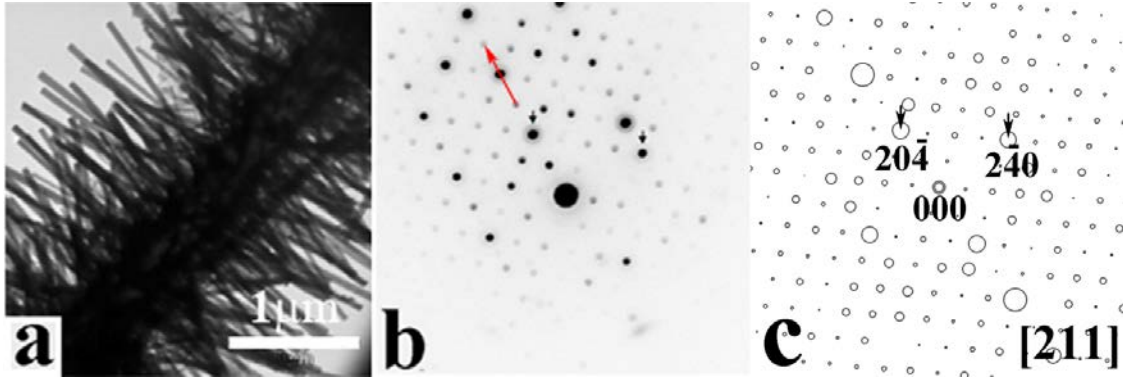


Figure. 12. TEM images of the hierarchical structure (a). Experimental EDPs of the  $\text{Cu}_2\text{S}$  nanowires (b), arrows show the nanowire growth direction and corresponding simulated patterns of monoclinic  $\text{Cu}_2\text{S}$  crystal structure (c).

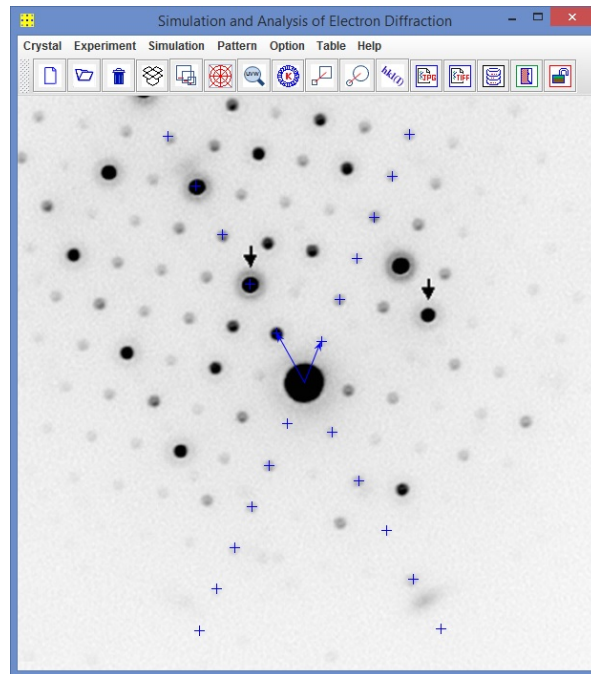


Figure. 13. Measurement of basic reciprocal vectors in the experimental EDP of  $\text{Cu}_2\text{S}$  nanofiber. The basic reciprocal vectors for the experimental EDP are measured, as shown in Figure 13. The calibrated matching factor and basic reciprocal vectors for the experimental EDP are listed 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.

**Find Zone Axis** ✕

---

Short reciprocal vectors

☒ Display ☐ g (Å<sup>-1</sup>)

Vectors	g (pixel)	Angle (°)
g1	43.8	67.5
g2	54	118.5

---

Current phase only

Possible zone axis: [2, 1, 1]

---

Tolerance (%) 5.0 Find

Total number 7 Save

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%.

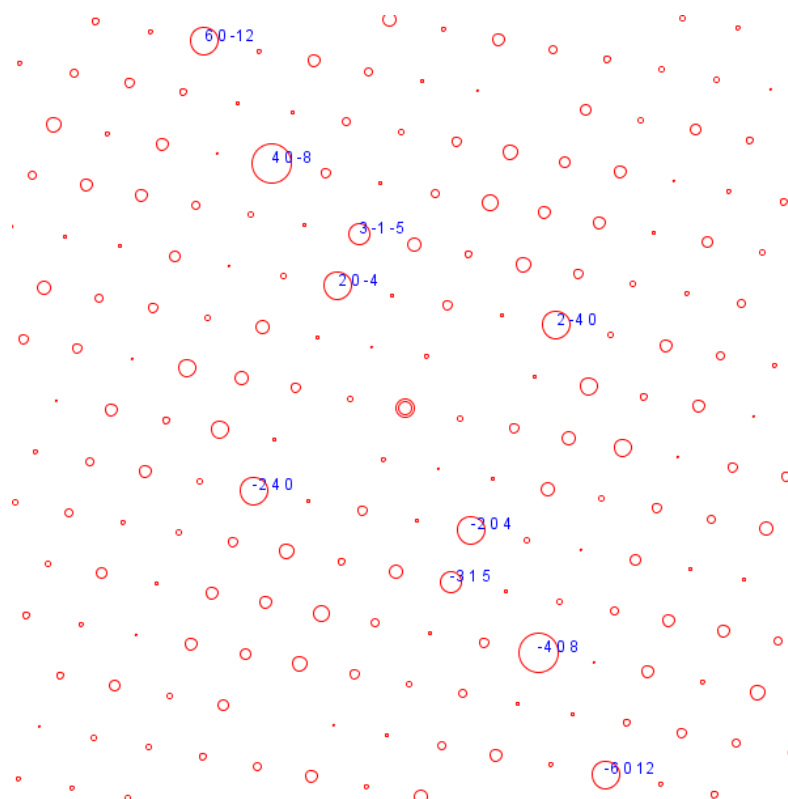


Figure. 15. Simulated EDP of Cu<sub>2</sub>S with zone axis [2 1 1].

## 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 Landy suite, becomes obvious with the growth of the programs and users.

### **7.2 SPICA**

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

### **7.3 PCED**

PCED4 is an upgraded version of the previous JEC/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; SAKI4 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.

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